2021 SUMMER

UNDERGRADUATE RESEARCH SYMPOSIUM

WEDNESDAY, JULY 21

9:00 - 11:45 a.m.

Jordan Hall of Science

SUMMER UNDERGRADUATE RESEARCH SYMPOSIUM

July 21, 2021

SESSION 1: 9:00 to 10:00 a.m. (ET)

#	PRESENTER	PROJECT TITLE	ADVISOR	DEPARTMENT
1	Zoe Barnette	Optimizing CO2 Capture using a Poly(4-vinylpyridine)-Based Catalytic Membrane System	Dr. Casey O'Brien	Chemical and Biomolecular Engineering
2	Steven Broussard	Comparing Machine Learning Techniques for Social Science Event Classification	Dr. Paul Brenner	Center for Research Computing (CRC), Computer Science and Engineering
3	Andrew Christy	Energy Transfer in Lead-Halide Perovskites with Various A-Site Cations	Dr. Prashant Kamat	Chemistry and Biochemistry
4	Brenda Cruz González	Gold-Silica Janus Nanoparticles	Dr. Prakash D. Nallathamby	Aerospace and Mechanical Engineering
5	Nicholas DeLuca	Generating Continuous Spark Discharges Through High-Frequency Mechanical Actuation of Piezoelectric Crystals	Dr. David B. Go	Aerospace and Mechanical Engineering
6	James Ernst	Phased Arrays and Lenses for Low-Power 5G MMW Communications	Dr. Jonathan Chisum	Electrical Engineering
7	Christopher Ferguson	N-Distance – Mapping Interpersonal Interactions to limit the spread of COVID-19	Dr. Aaron Striegel	Computer Science and Engineering
8	Ria Goyal	Regulation of Endocrine Therapy Resistance in Breast Cancer by ZNF217	Dr. Laurie Littlepage	Chemistry and Biochemistry
9	Argerie Guevara	Optimizing PLGA derived Gel for Steady Release of Phage-Mimicking Antimicrobial Nanoparticles	Dr. Prakash Nallathamby	Aerospace and Mechanical Engineering
10	Peter Halloran	Catalytic Hydrocracking of Low-Density Polyethylene	Dr. Hicks	Chemical and Biomolecular Engineering
11	Ian Havenaar	Event Classification on Coups with Greater Machine Learning Specificity and Accuracy	Dr. Paul Brenner	Center for Research Computing (CRC)
12	Charlotte Hirsch	Predicting Middle School Students' Self-Efficacy in Computer Programming Using Linear Mixed Models	Dr. Ying (Alison) Cheng	Psychology
13	Colton Kammes	Neural Network Optimzed Wireless Side Channel Attacks	Dr. Siddharth Joshi	Computer Science and Engineering, Electrical Engineering
14	Cellina (Inhye) Kim	Even More Disadvantaged: The Disproportionate Effect of Macroeconomic Conditions on Black Unemployment	Dr. Taryn Dinkelman	Economics
15	Schuyler Louie	Female Representation on Appointed Boards Forecasts Closer Gender Parity in Elected Positions	Dr. Lakshmi Iyer	Economics
16	Marion Madanguit	Supporting College Admissions with Information Visualization	Dr. Ronald Metoyer	Computer Science and Engineering
17	Andrew Marquardt	Exploring Advanced Sampling Applied to Model Host-Guest systems	Dr. Jonathan Whitmer	Chemical and Biomolecular Engineering
18	Hailey Meyer	Controlling Gold Nanostructure Dimensions Using an Etching Solution	Dr. Svetlana Neretina	Aerospace and Mechanical Engineering
19	Nathaniel Moller	Development of Polymeric Piezo-Electrolytes for Self-Charging Batteries	Dr. Jennifer Schaefer	Chemical and Biomolecular Engineering
20	Vongaishe Mutatu	Utilizing Photonic Sintering to Develop High-Performing Silver-selenide Thermoelectric Films for Wearable Electronic Applications	Dr. Yanliang Zhang	Aerospace and Mechanical Engineering
21	Amala Ozumba	Exploring Maternal Mistreatment: A Comparative Study of Factors that Effect Care in Public and Private Kenyan Maternal Health Facilities	Dr. Vania Smith-Oka	Anthropology
22	Elena Parial	Using Total Internal Reflection Absorption Spectroscopy to Measure Plasma-Injected Solvated Electrons in Non-Aqueous Solvents	Dr. David B. Go	Aerospace and Mechanical Engineering
23	Alexander Perez	Data-Enabled Optimization of Printing Chemical Patterns on Nanostructured Membranes	Dr. Alexander Dowling	Chemical and Biomolecular Engineering
24	David Tzu-chien Lin	The Effect of Informal STEM Experience on Interest and Career Aspiration in Computer Programming Among Middle Schoolers: A Mediation Analysis	Dr. Ying (Alison) Cheng	Psychology
25	Jackson Vyletel	Binding of Per- & Polyfluoralkyl Substances (PFAS) to Cucurbit[7]-uril	Dr. Matthew J. Webber	Chemical and Bimolecular Engineering
26	Austin Wyman	What You Won't Do For Pleasure: Illuminating the Relationship Between Anhedonia and Risk Taking	Dr. David Watson	Psychology

SESSION 2: 10:00 to 10:35 a.m. (ET)

	PRESENTER	PROJECT TITLE	ADVISOR	DEPARTMENT
	Scott Manning	Using Molecular Simulations to Understand Behavior and Structure of Ionic Liquid Crystals	Dr. Jonathan Whitmer	Chemical and Biomolecular Engineering
	Salmady Ramos	Computational Generation and Characterization of Crystalline Soft Porous Coordination Polymers for Gas Storage	Dr. Yamil Colón	Chemical and Biomolecular Engineering

SESSION 3: 10:45 to 11:45 a.m. (ET)

#	PRESENTER	PROJECT TITLE	ADVISOR	DEPARTMENT
27	Brian Beas	Maximizing the Piezoelectric Response from Inorganic-Organic Composite Electrospun Nanofibers	Dr. Nosang V. Myung	Chemical and Biomolecular Engineering
28	Hannah Collins	Structure-property relationships in ionic liquid crystal electrolytes	Dr. Jennifer Schaefer	Chemical and Biomolecular Engineering
29	Anuj Gajjar	Smart Breast Clips for Breast Cancer Treatment	Dr. Thomas O'Sullivan	Electrical Engineering
30	Eric Gallagher	Combining Ultrasound and Diffuse Optical Imaging for Compact and Noninvasive Diagnosis of Breast Lesions	Dr. Thomas O'Sullivan	Electrical Engineering
31	Kathleen Hart	Characterization of triple junction enhanced thermally-driven plasma on the surface of pyroelectric crystals	Dr. David B. Go	Aerospace and Mechanical Engineering
32	Nathaniel Hiott	An Exploration of Electron Transfer Processes in Two-Dimensional Lead-Halide Perovskites	Dr. Prashant Kamat	Chemistry and Biochemistry
33	Nathan Jensen	A Novel Curriculum for Wireless Communication in Congested and Contested Environments	Dr. Nicholas Laneman	Electrical Engineering
34	Brian Kang	Incorporation of Ternary Semiconductors in Bipolar Membranes for Photocatalysis	Dr. Prashant Kamat	Chemistry and Biochemistry
35	Tipton Lichtenstein	Binary data and thermodynamic modeling are sufficiently accurate to inform early process design and IL screening for the Separation of Ternary Azeotropic Hydrofluorocarbon Mixture R-410A	Dr. Alexander Dowling	Chemical and Biomolecular Engineering
36	Nicholas Lowe	Water Remediation via Electrospun MIL-101@ZIF-8-Embedded Nanofibers as Copper Filters	Dr. Nosang V. Myung	Chemical and Biomolecular Engineering
37	Nate McGhie	Local prohibition's effect on contemporaneous alcohol-related mortality, 1908-1920	Dr. Kasey Buckles	Economics
38	Stephanie Mueller	Synthesis of a Zn(II) carbene	Dr. Vlad Iluc	Chemistry and Biochemistry
39	Erin Neu	Engineering Biomimetic Materials to Promote Lymphangiogenesis	Dr. Donny Hanjaya-Putra	Aerospace and Mechanical Engineering, Bioengineering
40	Stephanie Nonamaker	Exploratory Factor Analysis of the Computer Programming Attitudes Scale: Evidence of Proximal and Distal Outcome Expectations	Dr. Ying (Alison) Cheng	Psychology
41	Sofia Rodriguez	Accuracy of Human Coding and Machine Learning for Political Science Event Classification	Dr. Paul Brenner	Center for Research Computing
42	Hakim Sanfo	Testing Efficient Techniques to Absorb Copper (II) Chloride using Nanostructured Membranes	Dr. William Phillip	Chemical and Bimolecular Engineering
43	Junji Shen	Bringing 5G Smarts to Network Measurement	Dr. Aaron Striegel	Computer Science and Engineering
44	Nicholas Slusher	The Effect of Solution Dipping Temperature on the Properties of Anodized-Aluminum Pressure-Sensitive Paint	Dr. Hirotaka Sakaue	Aerospace Mechanical Engineering
45	Lauren Stark	HF Characterization and Modeling of GaN Transistors	Dr. Patrick Fay	Electrical Engineering
46	Katelyn Wendt	Task Specific, Thermo-responsive Ionic Liquids for Directional Solvent Extraction Water Desalinations	Dr. Brandon L. Ashfeld	Chemistry and Biochemistry
47	Tia Williams	Here I Am: The Stories of University Women Learning and Growing during COVID-19	Dr. Maria McKenna	Institute for Educational Initiatives; Africana Studies
48	Qinxiao Wu	Magnetic Nanocarrier based, Precision Combinatorial Chemotherapeutics Treatment Against Metastatic Cancer Cells	Dr. Prakash Nallathamby	Aerospace and Mechanical Engineering
49	Alejandra Zaleta Lastra	Adversity During Multiple Periods of Development Does Not Influence Adult Parasite Loads in Wild Baboons	Dr. Elizabeth Archie	Biological Sciences

SESSION 1

9:00 to 10:00 a.m.

Jordan Hall of Science

Galleria

Optimizing CO2 Capture using a Poly(4-vinylpyridine)-Based Catalytic Membrane System

By:
Zoe Barnette
ND Energy (Slatt Fellowship)

Faculty Advisor:
Dr. Casey O'Brien
Department of Chemical and Biomolecular Engineering
College of Engineering

Other Contributors:
Renxi Jin

Abstract:

Current industrial scale CO2 capture and CO2 conversion technologies rely on inefficient steps, such as energy-intensive regeneration and limited mass transfer due to dilute atmospheric CO2 concentrations. The development of a catalytic polymeric membrane technology could improve upon current practices by acting as both the capture and conversion medium of CO2, eliminating the regeneration step and producing value-added chemicals. Quaternized poly(4-vinylpyridine)-based membranes are particularly promising polymeric membranes because of their high CO2 permeance and high selectivity of CO2 over N2, derived from their unique facilitated CO2 transport mechanism and their high catalytic activity for cyclic carbonate synthesis. The current research involves analyzing the exact permeance and selectivity of solutions of various PVP polymers, pH levels, and concentrations to determine the optimum conditions for effective CO2 capture and conversion at mild and high temperatures. Our recent data shows that a bromoethane quaternized PVP-based polymer (C2-PVP) performs the best overall to achieve a high CO2 permeance and a decent CO2 to N2 selectivity ratio when tested at room temperature. Adjusting the pH level of the solution to about 8 allowed for best mixing with a basic fixed-carrier polymer — polyvinylamine (PVAm) — which aids CO2 transport, increasing both CO2 permeance and selectivity. The concentrations of PVP and PVAm were also varied to improve solution mixing as well as to adjust for any imbalance between permeance and selectivity due to polymer-type or pH changes. The best mixed solution so far is 20% C2-PVP with a pH 8 mixed with 0.6 % PVAm. Further experimentation is needed to find the optimal solution to produce both high permeance and selectivity, which would aid future work on CO2 conversion via epoxides into cyclic carbonates.

Comparing Machine Learning Techniques for Social Science Event Classification

By:
Steven Broussard
Center for Research Computing (CRC)

Faculty Advisor:
Dr. Paul Brenner
Center for Research Computing (CRC)
Notre Dame Research

Abstract:

The Triggers of Mass Killings (ToMK) project uses machine learning and data science techniques to identify triggering events that may lead to state-led mass killings. Between 1989 and 2017, 59 countries experienced 74 mass killing events, defined as an event where the number of civilian killings exceeded the yearly average by two standard deviations. This project focuses on Change in Political Control (CPC), one of the nine potential triggers. Three different machine learning algorithms, SVM, BERT, and Longformer, were used to classify potential articles to identify whether they contained a CPC event. To obtain our data, we downloaded articles from the Lexis-Nexis database that contained keywords corresponding to the CPC trigger. To classify these articles, I used training data provided by the political science team, consisting of article text and a label stating whether the trigger was described in the text. The three machine learning algorithms were trained on this dataset and made predictions on the unlabeled data we downloaded.

This project investigated why these three machine learning tools produced different results, even though they were trained on the same labeled data and predicted on the same articles. While the SVM classified roughly 13,000 of 146,000 articles as yes at a 75.11% accuracy rate, the two neural networks, BERT and Longformer, classified at a lower accuracy rate (65-70%) and classified far more articles (45-65k) as yes. I analyzed the overlap of these articles to investigate why the neural networks were classifying more articles as yes. I also looked into whether to include "alternative positive" articles and studied the importance of balanced datasets for machine learning. Alternative positive articles were articles containing a CPC event, but outside of the two-year window before a mass killing event. Excluding these articles resulted in a more precise dataset but resulted in far more no articles than yes articles, which led to a deceptively high accuracy score and harmed the machine's ability to identify articles containing a trigger.

We aim to improve our accuracy scores by implementing knowledge graphs. The coup trigger had accuracy scores of 90-95%, and our goal is to achieve similar results for the CPC trigger, which would be a significant step towards our goal of performing Event Coincidence Analysis (ECA) to determine which triggers cause mass killings. Knowledge graphs, which analyze word relationships in articles, may be helpful for complex triggers such as CPC, in contrast to triggers like coups and protests that are more straightforward to classify.

Energy Transfer in Lead-Halide Perovskites with Various A-Site Cations

By:
Andrew Christy
ND Energy (Slatt Fellowship)

Faculty Advisor:
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Department of Chemistry and Biochemistry
College of Science

Other Contributors:
Jeff Dubose

Abstract:

Harvesting light to drive chemical reactions (photocatalysis) requires careful control of the flow of energy. Recently, two-dimensional (2D) lead halide perovskites have been demonstrated to have a wide range of beneficial properties for photocatalysis: strong light absorption, tunable optoelectronic properties, and ease of synthesis. One way to harvest the energy from perovskite nanomaterials is to store that energy in long-lived molecular states called triplets. These triplet states can be used to increase visible light absorption for solar cell applications through photon upconversion or can be used to drive selective photocatalytic reactions. Molecules such as pyrene, benzophenone, and naphthylethylene have been well-studied for their triplet-forming properties and are good model systems. However, attempts to combine the beneficial properties of perovskites and triplet-forming molecules are lacking. Herein, we attempted to synthesize lead halide perovskites which incorporate these molecules into their structure. Although aminopyrene and aminobenzophenone-based 2D perovskites could not be formed, we were successful in forming perovskites with naphthylethylamine (NEA). The syntheses of (NEA)2PbI4 and (NEA)2PbBr4 2D perovskites were confirmed through their UV-visible absorption and photoluminescence spectra. Films of (NEA)2PbI4 and (NEA)2PbBr4 were made by spin-coating the substrates onto FTO glass. Solution-stable colloidal particles of both were also made by diluting in toluene. The colloids of (NEA)2PbBr4 showed phosphorescence at higher concentrations, which signifies migration of energy from the lead halide (PbBr4) unit to the NEA through triplet energy transfer (TET). Future studies will investigate the TET process through transient absorption measurements and measurements of the phosphorescence signal at liquid nitrogen temperatures (77 K). Beyond TET as an energy harvesting mechanism, we also explored electron transfer from (NEA)2PbBr4 to C60 molecules. At room temperature, addition of small amounts of C60 quenched the fluorescence signal of the (NEA)2PbBr4 colloids, which implies electron transfer is occurring. Future studies will characterize the energy- and electron-transfer capabilities of this NEA system to better understand how to control the flow of energy in these photocatalysts.

Gold-Silica Janus Nanoparticles

By:
Brenda Cruz González
NDnano (NURF)

Faculty Advisor:
Dr. Prakash Nallathamby
Department of Aerospace and Mechanical Engineering
College of Engineering

Abstract:

Nanotechnology has become one of the most important sciences for innovation in material sciences nowadays and mostly in the medicine field. In this research is reported a Gold Nanoparticles with Janus behavior (Janus AuNPs) as a novel method to do drug delivery to cancer cells. The novelty in this Janus nanoparticle is the immiscible nature of two thiol-derived polymers on the gold surface, Polyethylene glycol (PEG) and Polystyrene (PS), which can self-assemble on the gold in a tunable fashion by varying the size, polymer ratio and temperature, among other experimental parameters [1] but at the same time, one of the two polymers used (PEG) acts as a primer and therefore a partial SiO_2 coating is added to the gold nanoparticle to create a Janus structure [2]. This means that we could improve the biocompatibility and stability in biological environments, such as the human body. Therefore, Janus AuNPs in the future seems to be a promising noble nanoparticle that improve the drug delivery in cancer cells while incorporating multiple modalities.

References

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2. Fang, L., Wang, W., Liu, Y., Xie, Z., & Chen, L. (2017). Janus nanostructures formed by mesoporous silica coating Au nanorods for near-infrared chemo–photothermal therapy. Journal Of Materials Chemistry B, 5(44), 8833-8838. doi: 10.1039/c7tb02144e

Generating Continuous Spark Discharges Through High-Frequency Mechanical Actuation of Piezoelectric Crystals

By:
Nicholas DeLuca
NDnano (NURF)

Faculty Advisor:
Dr. David B. Go
Department of Aerospace and Mechanical Engineering
College of Engineering

Other Contributors:
Jinyu Yang

Abstract:

Conventional methods of producing plasmas requires the use of high voltage power supplies, which primarily constrain plasma generation to laboratory settings. Piezoelectric crystals have been recently explored as an alternative source for high breakdown voltages as they are relatively inexpensive and generate electric potential purely from mechanical deformation. Previous work has shown that certain piezoelectric crystals exhibit relaxation times on the nanosecond scale, suggesting high frequency actuation as a feasible method for continuously generating spark discharges, which are atmospheric pressure, non-equilibrium plasmas. These plasmas have been shown to produce promising results in pollutant removal, specifically with regards to agriculture and water purification. A mechanical system consisting of a motor, belt, and pulleys was designed and constructed to actuate a piezoelectric crystal at frequencies from 1-10 kHz. The design involves teeth on a rotating piece that strike a steel electrode pressed against a lead zirconate titanate (PZT) crystal, compressing the structure. A tungsten needle wired to the electrode routes the discharge towards a grounded copper plate. Testing consisted of spinning this piece up to speed before slowly raising the electrode into its path for impact. Various tooth designs were 3D printed from PLA to best optimize impact angle and frequency. High-speed footage was taken of each design to compare these parameters. Future work includes manufacturing the impact piece from steel. High voltage probes will be used in conjunction with an oscilloscope to measure both voltage and current of the discharge to assess the efficiency of the system as well as its potential for further improvement.

Phased Arrays and Lenses for Low-Power 5G MMW Communications

By:
James Ernst
Wireless Institute (AWaRE)

Faculty Advisor:
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Department of Electrical Engineering
College of Engineering

Other Contributors:
Nicholas Estes, Nicolas Garcia, Wei Wang

Abstract:

5G and satellite-based internet systems both types of systems rely upon beam-scanning antennas while in the millimeter-wave bands to allow target tracking and to close links in real-time. The traditional solution for antennas with beam scanning capabilities is a phased array that combines potentially 1000's of antenna elements, each element has its own active electronics, so synthesizing beams is very costly and consumes large amounts of power. In our research, we are exploring hybrid solutions of widely spaced antenna arrays combined with low-cost lens antennas to achieve similar performance as a traditional phased array, but at a fraction of the active elements. In addition, in our design, less than 10% of the elements are active at a time which dramatically reduces dynamic power consumption. Our main objective is to characterize a hybrid lens/array system to find the maximum performance for the number of elements used at different spacing. We have measured the radiative electric far-field for each antenna feed in a virtual array using a planar near-field scanner for our hybrid system and 27 GHz and analyzed the possible beams for such a system. The work demonstrates that this method reduces the number of feeds by more than a factor of two while still being able to produce acceptable beam scanning capabilities. Leaving us with a promising method for commercial applications which require millimeter-wave beam scanning.

N-Distance – Mapping Interpersonal Interactions to limit the spread of COVID-19

By:
Christopher Ferguson
Wireless Institute (AWaRE)

Faculty Advisor:
Dr. Aaron Striegel
Department of Computer Science and Engineering
College of Engineering

Other Contributors:
Stephen Mattingly

Abstract:

One way of limiting the spread of the ongoing COVID-19 pandemic is reducing contact between infected and uninfected individuals. “Contact tracing”, in which people provide a summary of interpersonal interactions via clinician interview, allows authorities to monitor the spread of the disease. Using this information, authorities can inform individuals of their possible exposure, allowing them to restrict their interactions and avoid further spread.

The N-Distance project aims to create a system using passive and privacy sensitive sensors to achieve a similar effect for a localized area, such as a college campus. This information is utilized in a visual format to allow easy identification of areas that have a high risk of spreading disease based on proximity between individuals, and to identify these patterns historically and in real time, allowing for timely intervention by college officials. In addition, this tool provides individuals the ability to assess risk and modify behavior accordingly, e.g. seeking out a less crowded area to study in.

This system is based on phone location and Bluetooth sighting data gathered from participants who install an app and carry a beacon. By collecting this data, the N-Distance system is able to generate a heatmap of roughly when and where interactions occur on campus. Because data is collected passively and with an emphasis on privacy, the system may reduce the need for self-reporting that may interfere with privacy.

Regulation of Endocrine Therapy Resistance in Breast Cancer by ZNF217

By:
Ria Goyal
Independent Summer Undergraduate Research

Faculty Advisor:
Dr. Laurie Littlepage
Department of Chemistry and Biochemistry
College of Science

Other Contributors:
Parinda Tennakoon

Abstract:

Around 70% of breast cancer tumors are estrogen receptor positive (ER+). Although endocrine therapy has been the mainstay for ER+ breast cancer patient treatment, about 33% of patients have tumors that eventually relapse and develop as recurrent metastatic tumors that are resistant to endocrine therapy. The molecular mechanisms that result in endocrine therapy resistance are poorly understood. The overexpression of ZNF217, an oncogene and transcription factor, has been shown to promote resistance to the endocrine drug tamoxifen in mammary epithelial cells in culture. However, no studies have detailed the mechanisms behind the molecular events that cause tamoxifen resistance after ZNF217 overexpression.

To investigate the role of ZNF217 in promoting endocrine therapy resistance, Zfp217 (mouse analogue) overexpression was examined in vivo by treating Zfp217-overexpressing breast tumors with tamoxifen. The control tumors responded to tamoxifen, whereas Zfp217-overexpressing tumors did not respond. The use of RNA sequencing led to the finding that key pathways are altered in a ZNF217 dependent manner after growth factor induction. These current results suggest that Zfp217 overexpression causes resistance to endocrine therapy in vivo and that growth factor induction promotes a differential ZNF217 dependent gene expression signature in ER+ breast cancer cells. A Cut&Tag assay revealed several target genes that contain estrogen receptor binding sites dependent on both ZNF217 and NRG1 signaling. We are currently working to functionally annotate estrogen receptor binding sites that are upstream of the PCK1 gene, in order to assess their regulatory capability on gene expression through our utilization of a luciferase reporter assay in MCF-7 human breast cancer cells. The eventual identification and understanding of the mechanisms by which ZNF217 causes endocrine therapy resistance will be critical to the development of novel drug targets to overcome endocrine therapy resistance.

Optimizing PLGA derived Gel for Steady Release of Phage-Mimicking Antimicrobial Nanoparticles

By:
Argerie Guevara
NDnano (NURF)

Faculty Advisor:
Dr. Prakash Nallathamby
Department of Aerospace and Mechanical Engineering
College of Engineering

Abstract:

There is a huge unmet need for a novel class of anti-infective, unlike the antibiotics currently available in the market, to counter drug resistant bacterial infections. One answer is to mimic antimicrobial viruses (Phages) that have successfully exploited the evolutionarily constant shape and membrane composition of bacteria for millions of years. But phages' biological origin makes them susceptible to immune reactions from the patient. Interestingly, the Nallathamby lab has been synthesizing phage-mimicking nanoparticles (PhANPs) made from non-immunogenic components. The antibiotic-free, phage-mimicking nanoparticles demonstrated a > 99.9% bacterial kill rate against four clinically relevant multi-drug resistant infectious bacterial cultures (Staphylococcus aureus USA300, Pseudomonas aeruginosa FRD1, Enterococcus faecalis, and Corynebacterium striatum) in suspension and on implants 1. Our new class of phage-mimicking core-shell nanoparticles are modularly assembled with a silica core (65 nm or 130 nm) and a discontinuous shell composed of controllably spaced, 1.8-3.5 nm, gold-silver nanoalloys1.

The current version of the PhANPs are geared towards topological applications. This project aims to design a PhANPs formulation that will release the PhANPs from a resorbable gel at a steady rate for prolonged antimicrobial action. We aim to incorporate the PhANPs into a PLGA derived gel 2. As part of optimization we are determining the kinetics of release of gel encapsulated phage-mimicking antibacterial nanoparticles for a better way to stop the growth of harmful bacteria. By referencing published literature, poly(lactic-co-glycolic acid) (PLGA) nanoparticles (NPs) will be synthesized and later incorporated with fluorescein for release study purposes. This will help determine the dissolution rate of PLGA and maximize the efficiency of payload incorporation into PLGA NPs. We have also synthesized AlexaFluor 750 incorporated PhANPs for in vivo tracking of the fluorescent PhANPs release from PLGA gel.

References
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Catalytic Hydrocracking of Low-Density Polyethylene

By:
Peter Halloran
ND Energy (Slatt Fellowship)

Faculty Advisor:
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Department of Chemical and Biomolecular Engineering
College of Engineering

Other Contributors:
Aubrey Jeffries

Abstract:

Mid-range hydrocarbon fuel, derived from waste plastic degradation, is a promising source of modern-day alternative fuel. However, selective catalysts and more efficient processes are needed to recycle waste plastics into fuels. In this study, we used low density (0.91-0.94 g/cm3) polyethylene (LDPE) as a well-defined polymer to represent a waste plastic. We subjected the LDPE to distinct environments in which the solvent and catalyst was varied. All trials were run in a Parr 4848 250ml batch reactor with an initial H2 pressure of ~3450 kPa. The temperature was raised to 598K and held for two hours. Qualitative analysis of gas products using a GC with TCD and FID suggested the formation of low carbon number gases in all conditions (C1-C8). Without n-hexanes as a solvent, no liquid product was formed, while with a solvent, the liquid phase was analyzed in a GC-MS. Results suggested the lack of formation of mid-range hydrocarbons present in the liquid phase using Pt/Al2O3. Taken cumulatively, the outcome suggests the conditions tested favor chain-end scission, a useful approach to maximize gas production. Due to the limited research investigating the solvent relationship with catalytic hydrocracking of polymers, future research in this area will investigate the effects of the solvent on the liquid and gas yields.

Keywords: alternative fuel, LDPE, hydrocracking

Event Classification on Coups with Greater Machine Learning Specificity and Accuracy

By:
Ian Havenaar
Center for Research Computing (CRC)

Faculty Advisor:
Dr. Paul Brenner
Center for Research Computing (CRC)
Notre Dame Research

Abstract:

The Triggers of Mass Killings project uses machine learning algorithms to classify news articles about triggers of mass killings. It is part of a larger project investigating nine types of triggers of mass killings (coups, assassinations, etc.) for purposes of atrocity prevention. I focus on the trigger of coups. This project seeks to classify large numbers of articles according to whether they contain information on a coup or attempted coup (positive classification) or not (negative) using three machine learning algorithms (SVM, BERT, Longformer). For each of the nine potential triggers, the first step is to pull down articles from the Lexis-Nexis database. We search for given keywords for each trigger, and if the article contains this keyword(s), it is pulled down from the database. The articles for the coup trigger have previously been pulled down, so I focused on improving the machine learning classification for these events. Our team has previously discovered that the SVM often performs with the highest accuracy score, which is likely because of the smaller training set for each trigger. However, for the coups trigger, the SVM still is not highly specific when classifying positive articles with the result being 28,552 positively classified articles (of 660,967 total articles). Even though the number of articles has decreased, there are still numerous articles that do not contain a coup or attempted coup event. Our primary objective in resolving this issue was a greater specificity for positively labeled coup articles, preferring a Type II error or a “false negative” over a “false positive.” One possible solution is to deal only with articles that have been classified as positives by all three machine learning algorithms (SVM, BERT, and Longformer), which decreases the number of positive articles from 28,552 articles to 20,984 articles. This solution accounts for greater specificity in positively labeled articles, but this number of articles is still extensive. Following feedback from the political science team, I identified more false-positive coup or attempted coup events. One such case was labeled a Russian coup in January 1997, but this event was instead a Russian-backed coup in Afghanistan. This false positive is an example of the machine learning algorithms failing because all three algorithms perceived several mentions of “Russia” and “coup” and therefore mislabeled the article as a positive coup article in Russia. Another issue arose in false positives coming from the use of the keyword “overthrow” in pulling down the articles because the word refers to the overthrow of something other than a government. A potential solution for this is to use another synonym in pulling down the articles initially. In the future, we wish to implement knowledge graphs, a helpful tool in analyzing word associations, with the keyword “overthrow.” We also intend to utilize this same greater specificity classification on the other eight triggers of mass killings as those articles are pulled down from Lexis-Nexis.

Predicting Middle School Students' Self-Efficacy in Computer Programming Using Linear Mixed Models

By:
Charlotte Hirsch
Center for Research Computing (CRC)

Faculty Advisor:
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Department of Psychology
College of Arts and Letters

Other Contributors:
Teresa Ober

Abstract:

Self-efficacy refers to an individual's beliefs regarding their performance and capacity in a particular domain (Lent et al. 2002). According to Lent and other Social Cognitive Career Theorists, low self-efficacy due to sociocultural expectations or stereotypes can constrain career development (2002). In an effort to boost self-efficacy in STEM and computing (STEM+C) among female and underrepresented minority students (URM; see Hamrick, 2021), the web-based app Curated Pathways to Innovation (CPI) provides an assortment of engaging STEM+C activities for middle schoolers. Students complete STEM+C modules on the app to earn badges; after each badge they are prompted to respond to a short survey measuring self-efficacy. Self-efficacy is operationalized through two Likert questions in the post-badge survey: "I am good at the kinds of activities that were in this badge" (corresponding to task-specific self-efficacy) and "I am good at computer programming" (corresponding to global self-efficacy). This study examines the following questions: 1) Taking into account the nested structure of the data, does task-specific self-efficacy predict global self-efficacy?; 2) Are there differences in students' task-specific and global self-efficacy on the basis of gender, URM-status, or the interaction of these two demographic variables after accounting for the nested data structure?; and 3) Does gender, URM-status, or the interaction of these two variables predict global self-efficacy after accounting for variation explained by task-specific self-efficacy? The sample consists of 869 participants (mean age = 11.2, 42.8% female, 55.9% URM), 122 badges, and 6082 survey responses (only including responses in which both self-efficacy items were answered). The data was fitted to linear mixed-effect models using the lme4 package in R with unique student-ID and badge included as random effects. To address RQ1, global self-efficacy was modelled with task-specific self-efficacy as the fixed effect. For RQ2, task-specific, then global self-efficacy were modelled with gender, URM-status, and the gender-URM interaction as predictors. For RQ3, global self-efficacy was modelled with task-specific self-efficacy, gender, URM-status, and the gender-URM interaction as predictors. Task-specific self-efficacy was significantly and positively predictive of global self-efficacy ($\beta=0.49$, $p<0.001$) (RQ1). Gender significantly predicted task-specific but not global self-efficacy; female students tended to have lower task-specific self-efficacy ($\beta=-0.20$, $p=0.048$) (RQ 2). Neither URM-status nor the interaction of gender and URM-status significantly predicted task-specific nor global self-efficacy (RQ2). After accounting for variation explained by task-specific self-efficacy, neither gender, URM-status, nor the interaction of the two were significantly associated with global self-efficacy; task-specific self-efficacy was the only significant predictor ($\beta=0.49$, $p<0.001$) (RQ3). The dichotomous coding of gender and the homogenous label of "underrepresented minority" to categorize a heterogeneous group present limitations to this analysis. Nonetheless, this study provides a valuable contribution to our understanding of middle schoolers' self-efficacy in STEM+C. The robust relationship between task-specific and global self-efficacy demonstrates that boosting confidence through specific activities may correspond to higher self-efficacy across the board in STEM+C areas. These findings reinforce the importance of resources such as CPI to encourage all students that they are capable of pursuing STEM+C, regardless of gendered and racialized stereotypes surrounding this field.

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Hamrick, K. (2021, April 29). Executive Summary. Women, Minorities, and Persons with Disabilities in Science and Engineering. https://ncses.nsf.gov/pubs/nsf21321/report/executive-summary.
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Neural Network Optimzed Wireless Side Channel Attacks

By:
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Wireless Institute (AWaRE)

Faculty Advisor:
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College of Engineering

Other Contributors:
Mark Horeni, Tanner Waltz

Abstract:

System-on-Chips (SoCs) are integrated circuits that integrate multiple components of a computer. These devices are typically used in IoT and Smartphone applications and typically have radios in close proximity to the other components such as the processor and memory. Due to the proximity, CPU and Memory activity can propogate through the radio and leak data wirelessly through RF communications. When encryption (such as AES-128) is occurring on the chip, leakage is transmitted which can be used to determine the encryption key through template attack algorithms like canonical correlation analysis. Such algorithms require many traces to attack a single key, but a Multi-Layer Perceptron (MLP) can attack multiple keys with fewer traces. To train the MLP, a large, clean, and consistent dataset must be collected. After training, a MLP can collect a single trace from a target and recover information such as an encryption key. Single trace MLP attacks are a vast improvement to classic algorithms as they are faster and require significantly less data at the time of attack.

Even More Disadvantaged: The Disproportionate Effect of Macroeconomic Conditions on Black Unemployment

By:
Cellina (Inhye) Kim
Center for Research Computing (CRC)

Faculty Advisor:
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College of Arts and Letters

Abstract:

In the United States, the Black unemployment rate is twice as large as White's. Many studies in the past related this consistent Black-White gap to the changes in business cycle. In other words, Blacks are disproportionately affected by the changes in macroeconomic conditions compared to Whites.

To test this hypothesis, we analyzed the monthly Current Population Survey from 2011 to 2021 using a linear probability model. The variation in unemployment rate in a given state, year, and month was used as an indicator of economic conditions. The results showed a significant difference in the effect of worsening economic conditions on the two racial groups. This implies that the Black-White gap in unemployment is wider when the US economic conditions are poor, meaning that Blacks become more disadvantaged as the economy takes a downturn. We also found that socioeconomic status, such as education level and occupation, only partially explains the Black-White unemployment gap.

Our findings suggest that Blacks are losing jobs at a higher rate and/or getting hired at a lower rate than Whites as the economy weakens. It has also been observed that Blacks' transition into and out of the labor force is different from that of Whites'. Hence, further studies are needed to better understand the variation in the Black-White response to cyclical changes in the economy.

Female Representation on Appointed Boards Forecasts Closer Gender Parity in Elected Positions

By:
Schuyler Louie
Center for Research Computing (CRC)

Faculty Advisor:
Dr. Lakshmi Iyer
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College of Arts and Letters

Abstract:

The historic underrepresentation of women in government has been well documented over time. Recent efforts in the last couple of decades have been made at the local and federal level to have more female representation on legislative bodies. These endeavors have an end goal of putting women in elected positions, which are more prestigious and consequential to society. Some believe that encouraging women to get appointed positions in government will lead to them having a larger share of the elected positions later on. Previous qualitative research concludes that having more women on appointed boards leads to an increase of women in elected positions through political networking. Although this qualitative study has been done with respect to this matter, there have been no empirical studies that prove having women fill appointed positions leads to a higher share of women in elected positions later on. We use unique data scraped from the Office of the City Clerk of the City of Los Angeles Database and computational gender-assigning tools to determine whether having higher female representation on appointed boards leads to better representation in elected office. We regress the percentage of women who are in elected office on the percentage of women on appointed boards in the previous election cycle. We also control for economic and political variables, as well as municipal government expansion. Consistent with previous qualitative studies, we have found that greater women's representation on appointed boards leads to an increase in representation of elected officials for the following election cycle. Our findings may be used to predict future policy impact regarding gender diversity, such as the recent gender quota legislation passed by Los Angeles Mayor, Eric Garcetti.

Supporting College Admissions with Information Visualization

By:
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Wireless Institute (AWaRE)

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College of Engineering

Abstract:

The role of a college admissions officer is one of sensemaking and storytelling, yet few tools have been created to actually support them in these tasks. In this paper, we operationalize our prior research on the needs of admissions officers to re-imagine one of their key devices: the decision sheet. The decision sheet lays at the center of all discussions of an applicant and is the way that admissions officers capture the relevant information for making a decision about a student. We present artifacts and evidence from our co-design sessions that validate our prior findings, and highlight a number of other challenges and opportunities in designing for holistic review processes. We develop a prototype in support of storytelling, bias mitigation, and overall support/efficiency and plan to perform a comparative study to understand how our design impacts the process itself.

Exploring Advanced Sampling Applied to Model Host-Guest systems

By:
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Chemical and Biomolecular Engineering (CBE)

Faculty Advisor:
Dr. Jonathan Whitmer
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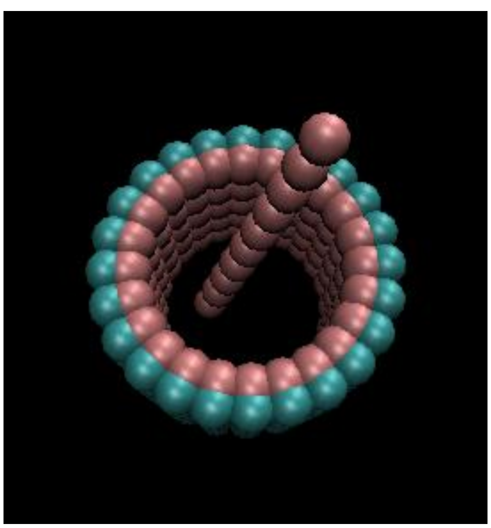
College of Engineering

Abstract:

A host-guest molecular binding system consists of a host molecule containing a binding site, often in the form of a cavitand or pocket, and a guest with a significant binding affinity for that site. Binding affinity is often codified in terms of a dissociation constant or binding free energy which may be computed using molecular simulations. This is typically done via alchemical methods such as thermodynamic integration, which utilize an unphysical but computationally and thermodynamically valid pathway between bound and unbound states involving the gradual removal of interactive forces between the host and guest, reapplication of those forces to a novel configuration, and determination of the changes in system free energy due to these steps. While standard, it can be computationally expensive to obtain high accuracy. Recently, unrestrained advanced sampling methods have shown promise in precisely and efficiently calculating binding free energy within a small collection of simulations. In this study, we apply one such method, unrestrained Adaptive Biasing Force (ABF), to a coarse-grained cavitand host-guest system in order to explore the phenomena that arise in the time-dependent estimate of the system's free energy of binding. Our observations of the system behavior, especially surrounding geometries in which the guest length is similar to the host inner diameter, characterize the free energy landscape of such a binding event as well as the physical bottlenecks resulting from an unrestrained calculation method, and allow us to conjecture whether alternative methods are required to better characterize the system.



Controlling Gold Nanostructure Dimensions Using an Etching Solution

By:
Hailey Meyer
NDnano (NURF)

Faculty Advisor:
Dr. Svetlana Neretina
Department of Aerospace and Mechanical Engineering
College of Engineering

Abstract:

Gold nanostructures are readily synthesized via colloidal chemistry, yet these particles can be produced on a substrate from a seed, ideal for specific applications. The thickness of these nanostructures relies heavily on the initial seed size, a dimension that is not easily reduced. However, by utilizing solution-based methods, the thickness and diameter of the gold structures can be decreased to exhibit greater control over the final dimensions. Here, a solution of hydrochloric acid and hydrogen peroxide is utilized to etch these gold nanostructures. This etching solution preserves the hexagonal corners of gold nanostructures and can be utilized to reduce the thickness of the seeds. When these etched seeds are grown into hexagonal nanoplates, the structures appear more rounded but show the desired geometric growth tendency. To reduce the diameter of gold nanostructures, a modification to the etch allows the reaction to preferentially etch the sides, parallel to the substrate. When applied to gold hexagonal nanoplates, this etch rounds the corners, producing disk-like structures. However, the reaction must be slowed to ensure an isotropic etch on the hexagonal corners. This etching solution allows the dimensions of substrate bound gold nanoparticles to be controlled, and with modifications to the etch, various gold structure geometries are achieved.

Development of Polymeric Piezo-Electrolytes for Self-Charging Batteries

By:
Nathaniel Moller
NDnano (NURF)

Faculty Advisor:
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Department of Chemical and Biomolecular Engineering
College of Engineering

Abstract:

Typically, energy generation and storage are two distinct processes that occur in different entities. In this project, the two processes are coupled together where mechanical energy is converted into electrical energy and then stored as chemical energy to create a self-charging battery. More specifically, a charge will be generated across the piezoelectric separator when a stress is applied, and the polymer electrolyte will enable ion transport, converting the electrical charge generated from the piezoelectric into electrochemically stored energy. Polymeric piezoelectric material such as polyvinylidene fluoride (PVDF) and polyacrylonitrile (PAN) can facilitate this process because of the charged poles that are created when a stress is applied to the material.

Here, we surround these piezoelectric mats, made of ZnO in both PAN and PVDF, with a polymer of crosslinked polyethylene glycol diacrylate (PEGDA), a common polymer battery electrolyte precursor, onto electrospun piezoelectric mats. This is achieved by a simple process of soaking the mats in the pre-polymer solution followed by thermally initiated polymerization. The condensed polymer piezoelectric mat can then be swelled in an electrolyte to produce a piezo-electrolyte and used in a self-charging battery. To test the piezoelectric properties of the polymerized piezoelectric mat, a cantilever is used, which is a device that applies different stresses to the material and measures the voltage across the sample. It has been found that the piezoelectricity of the mats increases when the polymer is applied, suggesting that these polymerized piezoelectric mats have the potential to be very effective in a self-charging battery. If this project succeeds, this self-charging battery could be useful in sports watches or other materials where mechanical energy is constantly supplied. Further research needs to be done to test the effectiveness of the electrolyte on the polymerized piezoelectric mat.

Utilizing Photonic Sintering to Develop High-Performing Silver-selenide Thermoelectric Films for Wearable Electronic Applications

By:
Vongaishe Mutatu
Independent Summer Undergraduate Research

Faculty Advisor:
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Department of Aerospace and Mechanical Engineering
College of Engineering

Other Contributors:
Mortaza Saeidi-Javash

Abstract:

Flexible thermoelectric generators (TEG) are desirable devices due to their ability to convert waste thermal energy to electrical energy and provide perpetual power for flexible electronics such as self-powered sensors and wearable health monitors. TE generators have advantages such as no battery requirement, scalable to nanoscale size, long life span, reliability, no mechanical motion or moving fluids, no noise generation, and low maintenance. In addition, TE generators have the potential to play a role in the worldwide battle against climate change by utilizing waste thermal energy. Currently, there are conventional rigid and bulk TEG, but it is proven difficult to develop flexible TEG with comparable power generation. This research tackles this problem and focuses on developing high-performing silver selenide TE films which can be integrated with flexible substrates such as plastics and clothing fabric, while maintaining their TE properties under various strains such as bending. An important factor in developing high performance TE films is sintering which improves the TE properties. Conventional thermal sintering requires long periods of time and is not effective for low melting temperature substrates (e.g., plastics, polyimide, and fabric clothing). Instead, this research utilizes Intense Pulsed Light (IPL) sintering (i.e., photonic) to sinter the films in milliseconds allowing for the sintering of the TE films on flexible substrates with low melting temperatures. Photonic sintering involves a Xenon lamp emitting a pulse of high energy on the TE film with four sintering variables including the applied voltage to the lamp, pulse duration, number of pulses, and pulse delay time. In this research, silver selenide TE films were fabricated using the vacuum-assisted filtration method. To assess the performance of the silver selenide films and the impact of photonic sintering, the Seebeck coefficient and electrical conductivity of both unsintered and sintered films were measured using a home built apparatus. The results showed a more than 11 fold increase in the power factor in just 1 millisecond compared to the unsintered films. Future work involves determining the optimum photonic sintering conditions which leads to the maximum power factor of the silver selenide TE films.

Exploring Maternal Mistreatment: A Comparative Study of Factors that Effect Care in Public and Private Kenyan Maternal Health Facilities

By:
Amala Ozumba
The Graduate School (SROP)

Faculty Advisor:
Dr. Vania Smith-Oka
Department of Anthropology
College of Arts and Letters

Abstract:

Maternal mortality rates remain a pressing global health issue across many regions of the world. Studies suggest that two important factors are essential to reducing the number of preventable deaths during childbirth and labor: skillful service provided by healthcare staff during labor and delivery and access to facility-based obstetric care in the event of complications. While the Kenyan government has since made efforts to reduce maternal mortality rates through the implementation of free maternity care, many women are still hesitant to receive care during childbirth at health facilities due to the multiple forms of mistreatment they endure. Previous studies done on maternal mistreatment in Kenya suggests that women have been subject to physical abuse, verbal abuse, discrimination, neglect, and other forms of abuse. This study utilized qualitative research methods to explore the forms of mistreatment affecting women who visited different public and private healthcare facilities in an urban slum in Kenya in 2016. The study discovered that mistreatment during facility-based childbirth was widespread. The trend of mistreatment occurring within public and private care facilities was a consequence of a broken healthcare system that was suffering from many transitions due to changing maternal health policies that affected relationships between healthcare providers and patients and other governmental changes. In order to combat mistreatment in Kenya, it is imperative that further policies be enforced to provide healthcare facilities with adequate resources for maternity wards, such as increasing the number of staff members and providing more equipment to accommodate a large influx of patients.

Using Total Internal Reflection Absorption Spectroscopy to Measure Plasma-Injected Solvated Electrons in Non-Aqueous Solvents

By:
Elena Parial
NDnano (NURF)

Faculty Advisor:
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College of Engineering

Other Contributors:
Daniel C. Martin

Abstract:

Solvated electrons are of interest in chemistry because they are strong reducing agents and can be used to drive chemical reactions. One way to produce them is by an electrolytic cell. This method utilizes a plasma electrolytic cell to create solvated electrons at the plasma-liquid interface. The goal of this project is to study plasma-injected solvated electrons in alcohol solutions, such as glycerol, using total internal reflection absorption spectroscopy, also known as TIRAS. TIRAS detects the solvated electrons, which absorb light, by reflecting a laser off the plasma-liquid interface and into a photodetector. Absorbance can be found by comparing the laser intensity before and after passing through the interface so the concentration of solvated electrons can be calculated. Measurements show that TIRAS absorbance decreases with increasing glycerol concentration in the electrolytic cell, which is hypothesized to be caused both by the change in reaction from second order recombination (solvated electrons reacting with water molecules) to a slower reaction between injected electrons and glycerol in addition to a shift in the absorbance spectrum. This shift is observed because the spectrum of solvated electrons changes in different solutions thus changing the wavelength of maximum absorbance as the solution changes. Future work will explore other types of alcohols and vary the laser wavelength in order to further understand the interaction between plasma injected electrons and alcohols.

Data-Enabled Optimization of Printing Chemical Patterns on Nanostructured Membranes

By:
Alexander Perez
NDnano (NURF)

Faculty Advisor:
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College of Engineering

Other Contributors:
Xinhong Liu

Abstract:

This project focuses on developing a data-enabled optimization framework for modeling reactive inks to improve printing chemical patterns on nanostructured membranes. Through data-enabled optimization, we seek to accelerate the design of chemically patterned membranes, which have shown unique ion transport properties when designed using the copper-catalyzed azide-alkyne cycloaddition (CuAAC) reaction, when a reactive ink is deposited on the membrane surface. Time and cost are reduced significantly with the implementation of computational design and optimization, enabling models that can produce reliable data for designing the reactive inks that produce the desired chemical patterning. In this context, my ND Nano summer research experience focused on modeling the CuAAC reaction, specifically the alkyne reactions. The components of the studied solutions are copper(II) sulfate pentahydrate, ascorbic acid (AA), and dimethylaminopropyne (DMA). Modeling of the kinetics of reaction mechanisms for the CuAAC reactions was done using a python framework enabling parameter estimation for the reaction rate constants of the kinetic model using non-linear optimization with the least-squares method. Fully dynamic models, as well as models with pseudo-steady-state assumptions, are derived. We found the predictions agree well with experimental data and performed an uncertainty analysis to inform the user of the reliability of the model and the fit. Experimental data for the CuAAC reactions were available in the form of time-series pH measurements to a steady-state point, additional experiments were conducted over the summer period to gather useful data to fit the second step of the CuAAC reactions kinetic model. UV spectroscopy experiments were conducted to measure the Cu2+ conversion. Specifically, measuring the peaks at 800nm informed the percentage reduction of Cu2+ in the solution as a function of time. Additional time-series pH measurements were taken from the Cu-AA-DMA reactions to inform the production of H+ as a function of time. It was observed that for excess concentrations of DMA in a 2:1 ratio to Cu2+ a significant conversion of Cu2+ is observed. With lower ratios of DMA to Cu2+, pH Measurements showed a higher generation of H+ with low ratios of DMA to Cu2+. These data will enable the derivation of a more sophisticated model to recapitulate high conversions at a wide range of initial concentrations. As ongoing work, we are using these data to make predictions to test the models and subsequently fit the data to the aforementioned experimental measurements to test the validity of the model and verify uncertainty and reliability. Efforts are being made to make our Python code highly automated and general; this will facilitate future extensions to model any alkyne group.

The Effect of Informal STEM Experience on Interest and Career Aspiration in Computer Programming Among Middle Schoolers: A Mediation Analysis

By:
David Tzu-chien Lin
ND International (iSURE)

Faculty Advisor:
Dr. Ying (Alison) Cheng
Department of Psychology
College of Arts and Letters

Other Contributors:
Teresa Ober

Abstract:

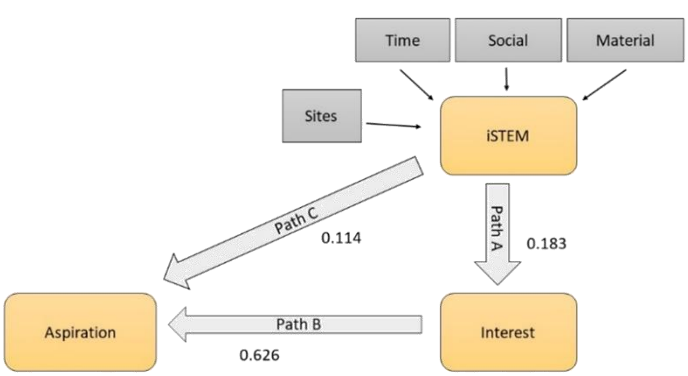
As early as middle school, many programs have been implemented by schools and organizations to encourage female and underrepresented minority (URM) students to pursue a career in STEM+C (Dou et al., 2019; Shahali et al., 2019). However, students' interest in STEM, a strong predictor of their career aspiration, generally decreases during middle school if no intervention is taking place (George, 2006; Osborne, Simon, & Collins, 2003). Studies have suggested that such decreases may be due to lack of exposure to STEM subjects outside of school and their low Science Achievement Value (SAV) and Perception of Family SAV (Shahali, 2019; Jones et al., 2021). SAV refers to the person's science self-efficacy and academic self-concept, while Perception of Family SAV "includes an individual's perceptions about the interest and expectations their family holds relative to science"; both are influenced by the person's resources in science capital, opportunities for exposure to science practitioners, and time for extracurricular engagement (Jones et al., 2021).

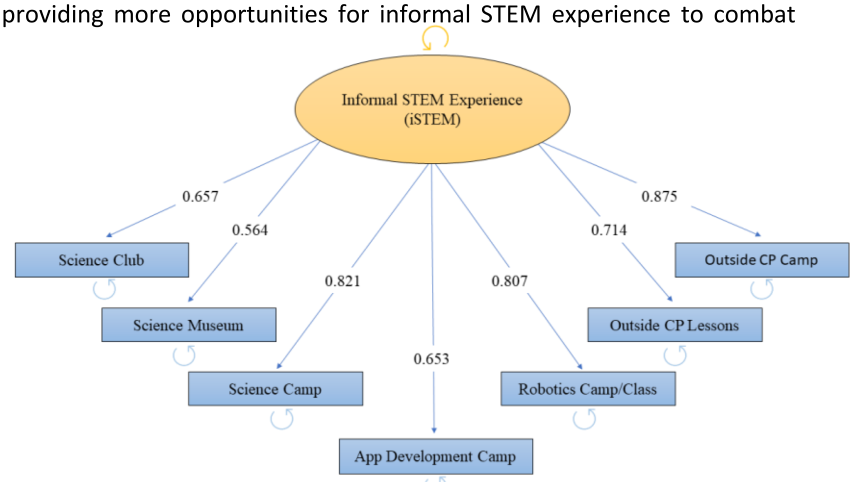
This study explored the relationship between middle schoolers' informal STEM experience (iSTEM), SAV, and Interest and Aspiration in computer programming (CP). The research questions were 1) Can the seven-item scale for "informal STEM experience" be modeled as a single latent factor model? 2) How do students' informal STEM experiences vary based on their SAV? 3) After controlling for students' differences in resources (i.e., material, social, time), does interest mediate the association between informal STEM experience and CP Aspiration?

Data were pulled from the survey responses administered by the Curated Pathway to Innovation (CPI) project, a web app designed for middle schoolers to learn about and foster interest in computer programming. Participants (N = 636, mean age = 13.5 years, 43.4% female, 45.4% URM) are from 15 sites in the US. Scores for iSTEM, and interest and aspirations in CP were computed as an average scale score, and the three resources variables were operationally defined and dichotomized. R Studio was used to perform confirmatory factor analysis (CFA), two-sample t-tests, and mediation analysis, respectively addressing each research question.

The result of the CFA suggested the iSTEM scale is a well-fitted model. The t-tests revealed significant differences in iSTEM score based on all resources variables, including parental educational attainment. The mediation analysis between iSTEM, resources variables, and interest and aspirations in CP indicated a partial mediation, with a significant indirect effect of iSTEM on career aspirations by way of interest, as well as a significant direct effect of iSTEM on career aspirations.

Being correlated with interests ($r = 0.19$, $p < 0.001$) and aspirations in CP ($r = 0.23$, $p < 0.001$), iSTEM showed signs of effects on promoting interest and aspiration in STEM among young students, which is in accordance with the finding of differences in interest pre and post iSTEM intervention (Young, Ortiz, & Young, 2017). Therefore, schools and organizations that wish to encourage adolescents to pursue a career in STEM+C may consider providing more opportunities for informal STEM experience to combat declining interest in STEM among middle schoolers.





Binding of Per- & Polyfluoralkyl Substances (PFAS) to Cucurbit[7]-uril

By:
Jackson Vyletel
NDnano (NURF)

Faculty Advisor:
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Department of Chemical and Biomolecular Engineering
College of Engineering

Other Contributors:
Brant Gates

Abstract:

The broad consumer, industrial, and military uses of per- and polyfluoroalkyl substances (PFAS) have become increasingly problematic for health and the environment since the original classification of the toxins in the 1930s [1]. PFAS and other related molecules have been used for coatings for various surfaces and have a range of applications in the aerospace, photographic imaging, semiconductor, automotive, construction, electronics, and aviation industries [2]. While PFAS have proven useful for a number of applications, their limited natural degradation leads to bioaccumulation and ultimately harmful effects in animals and humans such as liver damage, damage to the immune system, and increased risk of kidney or testicular cancer [3]. In this work, we demonstrate a new route to capture and detect various PFAS molecules. We test multiple PFAS and model their respective association constants (Ka) in order to show technologies that capture PFAS with sufficient binding affinity. Furthermore, the pH dependence of these binding groups can be leveraged to modulate the affinity of capture. These studies ultimately show promise for the applications of non-covalent binding of PFAS, with future sights set on large-scale industrial capture technologies for remediation of contaminated waters and waste streams.

What You Won't Do For Pleasure: Illuminating the Relationship Between Anhedonia and Risk Taking

By:
Austin Wyman
The Graduate School (SROP)

Faculty Advisor:
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Department of Psychology
College of Arts and Letters

Other Contributors:
Claire Scott-Bacon

Abstract:

Background: Anhedonia is a symptom of multiple mental illnesses that causes individuals to feel less pleasure from ordinarily pleasurable activities. Literature shows that anhedonia is responsible for deficits in the reward system and that the reward system is responsible for risk-taking behavior; however, there is a lack of research on the direct relationship between anhedonia and risk-taking behavior. If pleasure motivates risky behavior and individuals with anhedonia experience diminished pleasure, are individuals with anhedonia more likely to be risk averse? This question guided the present study to examine the direct relationship between anhedonia and risk taking, both independently and within the context of other important variables like personality and age. Methods: Using the Personality Inventory for DSM-5 (PID-5), Comprehensive Assessment of Traits relevant to Personality Disorder (CAT-PD), and Faceted Inventory of the Five-Factor Model (FI-FFM) measures within the Relations Among Personality and Symptoms (RAPS) dataset (N = 439), the present study conducted four hierarchical regressions to predict the effect of anhedonia, extraversion, and age on risk-taking behavior. Results: Findings were inconclusive about the direct relationship between anhedonia and risk taking in stage one; however, the higher stages of the hierarchical regressions generally indicated that anhedonia predicted a weak increase in risk taking, extraversion predicted a moderate increase, and age predicted a very weak decrease. Discussion: The present data help identify anhedonia, extraversion, and age as significant components to a comprehensive model for predicting risk-taking behavior. Future research should continue exploring the direct relationship between anhedonia and risk taking, and should work to identify additional factors that predict risk-taking behavior in order to establish a more complete model of risk taking.

SESSION 2

10:00 to 10:35 a.m.

Virtual Presentations

Jordan Hall of Science

Room 105

Using Molecular Simulations to Understand Behavior and Structure of Ionic Liquid Crystals

By:
Scott Manning
ND Energy (Slatt Fellowship)

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College of Engineering

Other Contributors:
Michael Quevillon

Abstract:

Clean energy is a promising technology, but widespread adoption requires the development of more effective battery storage technologies. The need for better batteries has led researchers to consider next-generation material technologies that incorporate new chemical compounds into battery composition to improve energy storage density and battery safety. Ionic liquid crystals (ILCs) are a promising class of conducting polymer electrolytes which exhibit ordered bulk mesostructures. These properties may improve ion transport and conductivity when integrated into battery design. Unfortunately, ILCs also exhibit a range of complex phase behaviors depending on operating conditions, thereby making analysis of these electrolytes difficult with conventional tools in the laboratory. Given this challenge, computer-based molecular simulations are one strategy to better understand the structure and phase behaviors of these conducting electrolytes. This research project focused on modeling a set of ILCs [Li+][CnTFSI-] recently synthesized by the Schaefer group at Notre Dame. Focusing on alkyl tail lengths from 8 to 18, we have built models capable of examining the phase behavior and conductive properties of these novel materials, and we have begun to explore their novel properties.

Computational Generation and Characterization of Crystalline Soft Porous Coordination Polymers for Gas Storage

By:
Salmady Ramos
ND Energy (Slatt Fellowship)

Faculty Advisor:
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Department of Chemical and Biomolecular Engineering
College of Engineering

Other Contributors:
Christian Villa Santos

Abstract:

In the need to find efficient adsorbents, porous materials have been studied for their great potential, especially in gas storage. Soft porous coordination polymers (SPCPs) are a new class of materials composed of metal-organic polyhedra (MOP) and organic linkers, with the promising properties of permanent porosity, high surface area and pore volume, low weight, flexibility, processability, among others. There are many challenges regarding hydrogen and methane storage, some of these are finding more efficient, lower-cost hydrogen storage systems, higher storage capacity, with reduced weight and volume. To advance technologies for SPCPs applications, studies on structural properties and performance are needed. We use computational molecular modeling and simulations to generate idealized crystalline structures, and calculate adsorption of these gases. Characterization simulations were performed on structures composed by MOP with different nodes (Rh, Co, Cu, Zn) and Rh-MOP with different linkers by calculating their surface area and pore volume. We then perform adsorption simulations at different temperatures and pressures. It is noted that since the values for uptake are based on ideal crystalline structures, adsorption in real systems would be lower. These adsorption simulations findings provide better understanding of the potential of these materials and how their structural characteristics and temperature play a role in their adsorption capacity.

SESSION 3

10:45 to 11:45 a.m.

Jordan Hall of Science

Galleria

Maximizing the Piezoelectric Response from Inorganic-Organic Composite Electrospun Nanofibers

By:
Brian Beas
NDnano (NURF)

Faculty Advisor:
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Department of Chemical and Biomolecular Engineering
College of Engineering

Other Contributors:
Dr. JoAnna Milam-Guerrero

Abstract:

To reach environmental sustainability and address climate changes, it is critical to develop new renewable energy sources. Piezoelectric materials have been effective at improving energy harvesting and storage in nanogenerators as they are capable of coupling mechanical stress and electrical polarization processes. Inorganic Zinc Oxide (ZnO) nanoparticles have commonly been utilized in piezoelectric generators. Energy generation might be further enhanced by adding the flexibility to the generator by fabricated inorganic ZnO nanoparticles embedded in an organic polymer matrix.

In this work, ZnO nanoparticles were embedded onto piezoelectric organic polyacrylonitrile (PAN) and polyvinylidene fluoride (PVDF) nanofibers where we hypothesize that power generation can be maximized by enhancing synergistic effects such as leveraging the strong piezoelectric response of ZnO with the flexibility of piezoelectric organic nanofibers. Various composite nanofibers were systematically synthesized by altering the ratio of ZnO to polymer, solution feed rate, and voltage supplied while electrospinning. Additionally, ZnO with different morphologies were examined and correlated to their piezoelectric response to maximize the piezoelectric response. Our work demonstrates the feasibility of fabricating a scalable source of piezoelectric generators that, when combined with a gel electrolyte to form a piezo-electrolyte, can be incorporated into existing battery technology to produce Self-Charging Power Cells (SCPC). SCPCs can be used to harvest 'waste energy' from everyday activities such as walking for use in wearable technology.

Structure-property relationships in ionic liquid crystal electrolytes

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Abstract:

Advancements in battery technology are becoming increasingly important for the future of transportation and energy storage, especially for the grid-scale implementation of intermittent renewables. Improvements to today's lithium-ion batteries must overcome problems such as flammability and have sufficiently high conductivity to be viable. The study of ionic liquid crystals or other solid-state materials for use as electrolytes in energy storage devices is an investment in safety and capacity for use with a lithium metal anode. Liquid crystalline materials have potential in this area because of the range of possible phases and degrees of molecular order. In addition, percolation of ionic aggregates in ordered structures within these materials is hypothesized to enhance the metal ion transport properties of the electrolyte. Lithium bis(trifluoromethane)sulfonimide octadecane (C18LiTFSI) is the ionic liquid crystal base molecule for the materials studied, and high dielectric moment additive molecules with varying effects on free volume in the material structure were hoped to enhance the properties when mixed with C18LiTFSI.

Four sulfonyl derivatives, with 18-carbon alkyl chains and polar head groups of varying sizes, were synthesized as additives to the C18LiTFSI molecule. Mixtures of these molecules with C18LiTFSI in multiple ratios were analyzed to ascertain the effects on the thermal properties and liquid crystal phases of the materials using differential scanning calorimetry (DSC) and small and wide-angle X-ray scattering (SAXS/WAXS). DSC and SAXS measurements were in agreement that there is no significant difference in crystallization temperature across all ratios, while there is wide variation in the temperature of the isotropic to smectic transition, which decreases with increasing additive content.

Dielectric impedance spectrometry was also used to establish DC conductivity of these materials across a wide temperature range. Preliminary results indicate high ratios of additive molecules to C18LiTFSI decrease the ionic conductivity of the material. However, with the current parallel plate electrodes setup, the ordering and orientation of the molecules and ionic aggregation within the material is uncertain. Future work will be focused on temperature dependent conductivity measurements using interdigitated electrodes. The much smaller scale than a parallel plate electrode, and hydrophobically modified surfaces should allow for increased alignment, and a better assessment of the effects of molecular ordering and ionic aggregation.

Smart Breast Clips for Breast Cancer Treatment

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Abstract:

Breast tissue markers are tiny radiologically-visible grain-sized implants which are routinely implanted into suspicious breast lesions during biopsy procedures. These “breast clips” enable clinicians to radiologically locate breast lesions and group diseased areas for more precise monitoring. We are developing similarly-sized “smart” breast clips that can provide real-time information of a tumor to optimize treatment and extend survival. These smart clips consist of hyperspectral optical sources, photodetectors, and wireless power receiver and communication circuitry. These hyperspectral sources detect changes in concentrations and chemical states of three biomarkers: hemoglobin (oxygenated and deoxygenated), water (protein-bound or free), and lipids (saturated or unsaturated), which are directly related to tumor composition, metabolism, and vascularity. Such biomarkers can also predict a pathologic complete response (pCR) to chemotherapy.

The smart breast clip performs this molecular sensing of tumor composition and hemodynamics via two microchip vertical-cavity surface-emitting lasers (VCSELs) covering the optical bandwidth (visible and near-infrared light) used to measure the above biomarkers. The implant also includes an analog front end to control the VCSELs and photodetectors, a receiver coil and impedance matching and rectification circuitry for wireless power transfer, as well as load-modulation of the RF power field for wireless communication. All sensor components and circuitry are integrated into a single printed circuit board sized to standard syringe needle sizes for in vivo implantation.

To enable the final development aim of preclinical evaluation of the device, the accuracy, precision, dynamic range, stability, and tissue depth range must be well characterized. This characterization involves simulating the optical performance of the sensor, profiling the power performance of the VCSELs, profiling the response of the sensor’s photodetectors, and testing performance in an optical and electromagnetic phantom. In this poster, we describe our work to enable repeatable characterization of smart breast clips.

The first goal was to perform Monte-Carlo-based tissue optical simulations of the device to obtain metrics about the overall expected optical performance of the breast clip. The second goal of this work was to automate a characterization procedure for the breast clip, which involved reading measurements from various external detectors that characterize laser and photodetector performance, as well as controlling the analog front end within the sensor. Using a combination of Python and C++ programming, a modular software system was built to achieve both goals, and thus provide progress toward preclinical evaluation of the breast clip.

Combining Ultrasound and Diffuse Optical Imaging for Compact and Noninvasive Diagnosis of Breast Lesions

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Abstract:

Ultrasound (US) is a commonly used imaging modality for the diagnosis of breast cancer. Although its high-resolution and deep tissue imaging provides a good visualization of breast masses where lesion characteristics such as size and architecture can be determined, its low contrast makes determination between benign and malignant tumors difficult. Therefore, surgical or needle biopsies are required to make a final diagnosis. While effective, all biopsies require taking tissue samples, which not only causes pain and scarring but can take several days or longer to get results which increases anxiety. Alternatively, US paired with Diffuse Optical Imaging (DOI), another imaging modality which measures functional information— such as concentrations of oxyhemoglobin, deoxyhemoglobin, water, and lipid— can be used to differentiate between benign and malignant tumors. This noninvasive method of breast cancer diagnosis would reduce the number of biopsies needed. We hypothesize that a combined DOI/US imaging system, which is handheld and easy-to-use, can provide more accurate characterization of breast lesions and lead to improved noninvasive breast cancer diagnosis.

Our specific aims are to design and fabricate an optical imaging attachment for the handheld Butterfly US system, characterize the accuracy and precision (e.g., lesion size, optical property recovery) of the combined US/DOI imaging system in vitro using tissue phantoms, and perform a proof-of-concept measurement of a human breast lesion using the combined system. The current system shows promise in its ability to obtain optical data with the aid of US imaging while remaining relatively compact. We chose to incorporate a silicon photomultiplier (SiPM) detector with a higher sensitivity to light rather than a conventional avalanche photodiode (APD) to allow for larger source-detector separations dictated by the dimensions of the ultrasound probe. Testing of breast lesion detection is being conducted on custom fabricated optoacoustic phantoms which simulate the optical absorption and scattering, acoustic scattering, and acoustic impedance of lesion tissue surrounded by “healthy” tissue. Considerations for future work include a redesign of the current optical attachment that places the SiPM detector directly in contact with the tissue being measured; this would remove the need for fiber coupling and sensitivity losses associated with it.

Characterization of triple junction enhanced thermally-driven plasma on the surface of pyroelectric crystals

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Abstract:

Low temperature non-equilibrium plasmas are a form of ionized gas with many applications, such as sterilization of medical equipment or pollution mitigation. However, they typically require high voltages to operate; hence, developing ways to convert other forms of energy, such as thermal energy, could make them better suited for application. Pyroelectric crystals can drive the production of low temperature non-equilibrium plasmas when exposed to a significant temperature gradient, what is termed an energy-conversion plasma source. The addition of a triple junction, a feature where a metal, dielectric and air meet, on the surface of the crystal enhances the electric field that produces these plasmas. Recently, preliminary research indicated that creating an angle in the metal layer produces a 3D effect at the triple junction that enhances plasma production, however the physics of this effect has not been extensively studied. In this work, we used lithium tantalate crystals with a layer of silver to create various angles. The crystal was placed on a heater, and a silicon wafer was mounted just above the crystal to act as a counter-electrode. The wafer allows us to simultaneously measure the current induced by the plasma in the wafer using a picoammeter and the temperature of the crystal. The results indicate that the amount of charge density induced on the wafer decreases with increasing distance between itself and the crystal. There is also an angle dependence, where the charge density decreases with increasing angle. With these results, we can determine the relationship between triple junction angle and charge density, which would add to our understanding of the behavior of the electric field and plasma production around a 3D triple junction.

An Exploration of Electron Transfer Processes in Two-Dimensional Lead-Halide Perovskites

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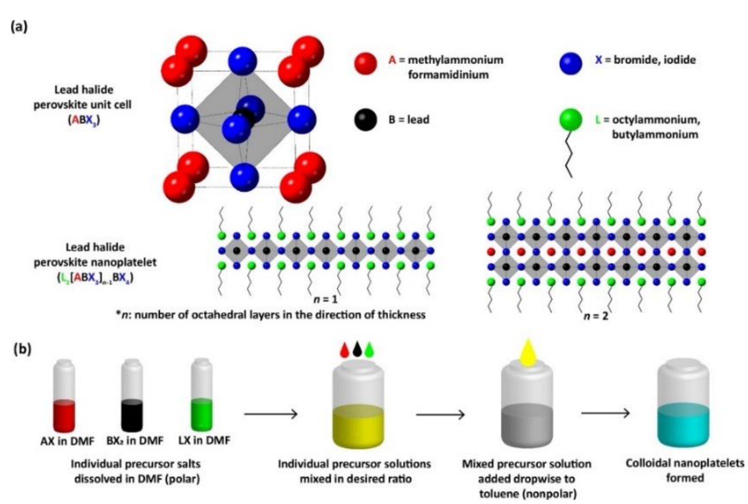
Abstract:

Lead-halide perovskites have recently emerged as a frontrunner for future semiconductor research and applications. The bulk of this research has focused on three-dimensional perovskites, which now have power conversion efficiencies similar to the best silicon solar cells. However, the limited composition possibilities and moisture instability of the 3D structure hinder its further utilization. Two-dimensional perovskites solve these problems by using organic cations as spacers between layers of variable thickness. The tuning of the layer thickness adjusts the band gap and exciton binding energy of the material, while the organic spacers allow it to be more stable in polar solvents. The superior photophysical properties of 2D perovskites make them suitable candidates for photocatalysis applications in light-emitting diodes (LEDs) and solar cells.

This research focuses on investigating the interactions between colloidal two-dimensional perovskites and the electron acceptor fullerene. The synthesis of colloidally stable 2D perovskites remains a major challenge, but this method allows for fine-tuning of the layer thickness of the 2D perovskites. Single, double, and triple-layered perovskites (n = 1, 2, and 3) were synthesized by varying the ratios of the organic cation methylammonium to the concentrations of the lead source and the butylammonium and octylammonium spacers. This allowed us to explore the photoinduced electron transfer processes from colloidal 2D perovskites to electron acceptors like fullerene. The experiment was designed such that a solution of fullerene dissolved in toluene was added to solutions of single, double, or triple thickness perovskites also in toluene. By observing the absorbance and photoluminescence of each sample as the electron acceptor was added, the recombination pathway of the excited electrons could be determined. The fullerene addition quenched the photoluminescence of the samples without significantly degrading the 2D perovskite, indicating that the excited electrons get transferred to fullerene. We confirmed this conclusion by characterizing the negatively charged fullerene since the reduced fullerene has characteristic absorption peaks.

The next step is to focus on quantifying the rate of electron transfer and to elucidate the mechanism. Femtosecond transient absorption spectroscopy will be utilized to determine the rate constant of electron transfer. In addition to the rate constant of electron transfer, the mechanism of electron transfer can be determined using the Stern-Volmer method and the charge carrier separation from the photocurrent response of the sample. Investigating this further will open new opportunities in exploring 2D perovskites in photocatalytic applications which has not yet been explored in the scientific community.



A Novel Curriculum for Wireless Communication in Congested and Contested Environments

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Abstract:

Modern communication networks rely heavily on wireless technology which demands a reliable link be established between the sender and receiver of a transmission. A tremendous deal of largely successful research has been performed to increase the data rates achievable via wireless communication. However, very little research exists addressing the issues of maintaining link quality in the presence of antagonistic signal sources. Congested and contested networks are becoming increasingly prevalent issues. We are creating an upper level university course which will expose these to students, thus enabling them to engineer communication networks capable of maintaining link quality in these adverse conditions. The lab for this class involves exposing the students to the various components and signal processing techniques required for building a solid radio transmitter and receiver system. Most recently, we upgraded the radio hardware to include tunable phase locked-loops serving as the local oscillators, active mixers for the modulators and demodulators, and fully differential amplifier drivers supporting dual channel operation. The use of these various integrated circuits- some of which operate at radio frequencies- involves careful circuit design to maintain system integrity and flexibility. Furthermore, combining the various hardware components to build a functional radio is far from trivial, and therefore extensive unit and system testing was performed to determine system performance. Finally, various signal processing techniques were utilized to ensure a robust and high performing communication network. The second version of the course hardware kit has been finalized, allowing continuous streaming over a wireless link to be realized utilizing the homodyne radio architecture.

Incorporation of Ternary Semiconductors in Bipolar Membranes for Photocatalysis

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Abstract:

Photocatalysis - the use of light to drive chemical reactions - is a viable route toward forming sustainable chemical fuel sources. In traditional photocatalysis, an absorber material promotes oxidation and reduction processes of interest. One way to enhance photocatalysis is to separate the different photocatalytic steps. This can be done using a bipolar membrane (BPM) - a polymer membrane with cation-selective and anion selective layers. This affords fine tuned control over the parameters that influence reduction and oxidation (e.g. pH, concentration, etc.) for optimizing the overall process. To date, it has been shown that light-absorbing semiconductors such as CdS and electron-acceptors such as gold particles can be loaded into BPMs and used for photocatalysis. However, this provides only a limited set of photo-active materials for BPM-based photocatalysis. Finding new semiconductor light absorbs that are compatible with the BPM is thus of interest. In this work, we investigated methods to load two ternary semiconductors - $AgInS_2$ and $CsPbBr_3$ - into BPM films. $AgInS_2$ provides a non-toxic alternative to traditional semiconductors, and $CsPbBr_3$, while it contains lead (Pb), has several beneficial properties for photocatalysis. The general method for formation of ternary semiconductors in the BPM was to first soak the films in a solution to load the cations (e.g. Ag^+ or Cs^+), then react that film to form an intermediate compound (Ag_2S or CsBr). Next, cation exchange reactions were employed to form the final material - either reaction with indium to form $AgInS_2$ or reaction with lead to form $CsPbBr_3$. Although successful formation of Ag_2S was confirmed via UV-visible spectroscopy, the conversion to $AgInS_2$ so far has remained elusive. Similarly, formation of CsBr within the BPM was successful (confirmed via UV-vis), but the cation exchange to $CsPbBr_3$ has proved difficult. Future directions will focus on adding chemical catalysts to promote cation exchange. Once successful, photocatalytic reduction of a model dye compound such as methyl viologen will be done to demonstrate the viability of loading ternary semiconductors within the BPM.

Binary data and thermodynamic modeling are sufficiently accurate to inform early process design and IL screening for the Separation of Ternary Azeotropic Hydrofluorocarbon Mixture R-410A

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Abstract:

In recent years, an increasing amount of attention has been placed on CFC and HFC refrigerants due to their ozone depletion potentials (ODP) and global warming potentials (GWP). Due to the risks posed by their continued use, there have been international attempts to curtail the usage of specific CFCs with high ODPs, such as the phase-out of R-22 (Freon) as laid out within the Montreal Protocol [1]. Additionally, the EPA has plans to reduce the overall HFC production and imports by 85% within the next 15 years [2]. This presents an issue as there are thousands of tons of HFC compounds in use that are set to be phased out in the foreseeable future. Furthermore, although HFCs do not have high ODPs like their CFC counterparts, many have high GWPs. For example, R-410A, a commonly used ternary near-azeotropic HFC mixture of R-32 and R-125 with a GWP of 2088 [3], is scheduled for phase-out under current environmental regulations. Thus, the need for separating azeotropic HFC mixtures into their components is apparent as these separations would reduce the emissions and waste from HFCs. In the case of R-410A, the components could be recycled.

However, there are currently no methods to feasibly achieve azeotropic separation of HFCs due to either unrealistically high energy requirements or lack of adequate separating agents. Through experimental trials, it has been demonstrated that ionic liquid (IL) entrainers have the potential to selectively separate certain azeotropic mixtures into their components [4,5]. Furthermore, Shifflett and coworkers collected experimental data for the solubility of HFC compounds within ILs and have created an ASPEN simulation demonstrating an IL-enabled extractive distillation process that selectively separates an HFC mixture [5, 6]. However, the study primarily focused on a single IL and HFC. To make these results applicable to a wider range of HFC mixtures, the next step is to evaluate the ability of custom IL entrainers to break azeotropic HFC mixtures.

To address this gap, we seek to create a framework to optimize HFC separation processes and develop a method for screening ILs for HFC separations. This framework would help avoid the trial-and-error process that might otherwise be required to determine which IL entrainer is best suited to each HFC mixture. In this context, my NDnano summer research project has focused on establishing tests for the heat integration network to ensure the process is operating with the lowest possible heat input and number of exchangers. This has enabled us to verify the process is accurately reporting the cost for utilities and to evaluate the economic impact of these separations.

As ongoing work, we utilize experimental data and molecular simulations [8] to model and optimize a process system for the separation of R-410A at scale while remaining economically viable. Through this work, we model the VLE of R-410A with IL entrainers and then predict the ternary phase behavior of R-32 and R-125 from binary solubility data to within 10% error of the compositions. By using binary data, we avoid expensive experiments with ternary mixtures in favor of relatively inexpensive solubility experiments. Then, we are comparing the volatilities of four custom ILs based on binary/ternary phase data, which was another focal point of my NDnano research. This volatility study will serve as one of many methods for screening ILs for HFC separations in the future.

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Water Remediation via Electrospun MIL-101@ZIF-8- Embedded Nanofibers as Copper Filters

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Abstract:

Heavy metals are toxic contaminants found in drinking water that present adverse health effects in humans including organ failure, severe illnesses, or death1. Historically, lead has been a prevalent contaminant due to lead piping for houses contaminating the water2. These have often been replaced by copper, which has been shown to corrode into drinking water recently and thus has become a more prevalent contaminant3. Development of efficient, high-capacity point-of-use heavy metal filters is critical, as carbon filters typically used by popular water filter brands like Brita cannot remove heavy metals. This research addressed this challenge using electrospun nanofiber filters as a support scaffold for a composite of metal organic frameworks (MOFs), MIL@ZIF, which has a high surface area capable of collecting contaminants. MOF-embedded electrospun nanofibers have emerged as a superior filter design for their high porosity, flexibility, MOF immobilization, scalability, and ease of use.

This work showed that the Zeolitic Imidazolate Framework 8 (ZIF-8), a subset of MOFs, is an efficient adsorbent for aqueous copper in both powder and nanofiber forms. There are two potential mechanisms of copper adsorption onto ZIF-84. In one mechanism, the metal in ZIF-8 (zinc) is replaced by copper ions and then released into the water. The other mechanism is a coordination reaction in which copper ions form a covalent bond with nitrogen in the ligand of ZIF-8 (imidazole). While zinc is a nutrient, its presence in drinking water is EPA regulated5, making the second mechanism desirable. Additionally, zinc retainment in the second mechanism creates the potential for filter reuse, as the structure of the MOF is preserved.

In order to constrain the copper adsorption to the second mechanism, this work presented a core-shell MOF@MOF design, in which ZIF-8 (shell) was synthesized on NH2-MIL-101(Al) (core). Compared to freestanding ZIF-8, the MOF@MOF composite increased the removal of copper and other heavy metals while restraining adsorption to the desired mechanism6. Using a MOF-based core forced ZIF-8 to grow in nanosheets rather than its typical rhombic dodecahedral and cubic morphology, making zinc sites inaccessible to copper cations. This work utilized this interaction by electrospinning MIL@ZIF within a polymer scaffold for domestic heavy metal water filters that limit zinc leaching. This design sets the stage for future work in making these filters reusable, as well as potential detection methods of aqueous copper via the reported fluorescence properties of MIL@ZIF6.

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Local prohibition's effect on contemporaneous alcohol-related mortality, 1908-1920

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Abstract:

This project examines the magnitude of the effect of alcohol prohibition on contemporaneous alcohol-related mortality, specifically deaths caused by alcohol poisoning and cirrhosis of the liver. Although national prohibition is generally considered a failed policy, I investigate whether the state and county prohibition movement that preceded it had any effect on mortality and attempt to estimate the size of that effect. Economic theory posits that making a substance illegal raises its cost and disincentivizes its purchase, thereby decreasing consumption of the substance. To test this theory, I create a novel dataset that checks Law and Marks' (2019) state-level data and Sechrist's (2012) county-level data against historical Anti-Saloon League yearbooks, the result being the most thoroughly corroborated panel dataset of county prohibition laws that is currently available. I use the 1910 US Census to construct a "percent dry" statistic for 46 states in each year from 1908-1920, reflecting the percentage of a state's population that is "dry", or under prohibition. With CDC mortality reports for death data, I then use a fixed-effects linear regression to analyze the effect of dry policy on alcohol-related mortality, finding that increasing a state's dry population by 10 percentage points leads to a 6% decrease in alcohol-related deaths (or 1.8 fewer alcohol-related deaths per 100,000). Additionally, I observe spikes in alcohol-related deaths after statewide prohibition becomes effective, despite the general trend of county-level prohibition decreasing alcohol-related mortality. This apparent anomaly suggests a quirk of prohibition policy: some people's preferences for alcohol are such that in the absence of legal options, they will substitute for stronger, uncontrolled, and more dangerous substances (such as moonshine or bootlegged whisky), which contributes to the spikes in alcohol-related death upon an entire state going dry.

Synthesis of a Zn(II) carbene

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Abstract:

Transition metal carbenes have been studied due to their ability to activate inert molecules in catalytic cycles.1 Such activation provides an energy efficient method to utilize inexpensive and readily available feedstocks in synthesis. Zinc is of interest due to its low cost and unique reactivity, as its chemistry is not typical of transition metals. Zinc's reactivity comes from the fact that its valence shell consists of completely filled 3d orbitals, giving it only one attainable oxidation state.2 In order to synthesize a zinc carbene, the pincer ligand Li[PCHP] was first added to ZnCl2 to generate [PC(sp3) HP]ZnCl. In three attempts to deprotonate the backbone carbon to produce [PC(sp2) P]ZnL (where L is a neutral ligand), KN(TMS)2, CH3Li, or tBuLi were added to a solution of [PC(sp3)H P]ZnCl. Deprotonation was unsuccessful, leading to the following products [PC(sp3) HP]ZnN(TMS)2, [PC(sp3)H P]ZnCH3, and [PC(sp3)H P]ZntBu. These precursor molecules were characterized by 1H, 31P, and 13C NMR and small crystal X-ray diffraction, which showed a tetrahedral geometry around the metal center. This geometry prevents resonance from stabilizing a carbene. To induce a bipyramidal geometry, which could allow for resonance stabilization and subsequent deprotonation, phenanthroline, a bidentate-chelating agent was added. An intensely dark purple compound was formed. While attempts to grow a single crystal have been unsuccessful, NMR analysis suggests that the compound is a radical: Evan's method was used to show the presence of 2 unpaired electrons. Future steps include fully characterizing this paramagnetic complex and testing its reactivity in the presence of inert substrates.

Engineering Biomimetic Materials to Promote Lymphangiogenesis

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Abstract:

The lymphatic system is a secondary circulatory system, composed of vessels and nodes, that has essential roles in fluid homeostasis and multiple disease processes through multifarious actions, including immunosurveillance and lymph transport from tissues and organs. Lymphangiogenesis is the process of forming new lymphatic vessels from pre-existing vessels. Hyaluronic-acid based (HA)-hydrogels provide a platform for the development of a promising, new model to recapitulate lymphangiogenesis and to study its mechanisms by mimicking the body's natural ECM, which will aid in understanding lymphangiogenesis in tumor microenvironments.

Results from lymphatic endothelial cells (LECs) encapsulated in HA gels portray the importance of vascular endothelial growth factor-C (VEGF-C), which binds to vascular endothelial growth factor receptor-3 (VEGFR-3) on the surface of LECs, and matrix stiffness in controlling lymphangiogenesis. Within the breast cancer microenvironment, increased lymphatic vessel density is observed, suggesting that somehow the tumor microenvironment promotes lymphangiogenesis. Increased matrix stiffness and increased VEGF-C, secreted by cancer cells, are found within the tumor microenvironment and further highlight how these factors can influence lymphangiogenesis. The preliminary results from our HA-hydrogel platform serve as benchmarks for future experiments to characterize mechanical and biochemical factors found within the tumor microenvironment and their effect on lymphangiogenesis. By controlling lymphangiogenesis within these synthetic matrices, a novel therapeutic treatment would be presented where these hydrogels could be transplanted into the patient to restore their lymphatic circulation. Up to 40% of breast cancer patients and survivors suffer from secondary lymphedema caused by cancer treatments. These synthetic matrices would expand current therapeutic options which are currently limited to only manual drainage and compression garments. The results of these experiments catalyze future experimental directions which include co-culturing LECs with breast cancer condition media and breast cancer cells, and investigating cancer cell intravasation into lymphatic vessels using a microfluidic chip model.

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Exploratory Factor Analysis of the Computer Programming Attitudes Scale: Evidence of Proximal and Distal Outcome Expectations

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Abstract:

Curated Pathways to Innovation (CPI) is a web application designed to steer students towards careers in computer science fields. As students complete learning activities through the application, surveys are periodically administered to measure how students' attitudes towards computer programming change over time. Student answers to survey questions have been used to develop a "computer programming" attitudes scale with four domains: interest, awareness, career aspirations, and self-efficacy in computing. This research seeks to answer the question: What is the best fitting factor solution for the full 20-item "computer programming" attitudes scale when fitted to data from the 2019-2020 school year? To answer this question, an exploratory factor analysis (EFA) was conducted with varimax rotation, with a secondary goal of condensing the attitudes scale. Factor analysis investigates the underlying structure and internal reliability of the scale. Student answers to twenty survey questions meant to measure their attitudes towards computer programming were used for this analysis, with 472 observations. In phase 1, parallel analysis predicted that a 6-factor solution would best fit the data from the 20-items, so EFA was conducted from 2 up to 6 factors. Three survey questions did not load well onto any of the factor solutions, and were eliminated from the scale. In phase 2, EFA was conducted again, without these three items, from 2 to 6 factors, as parallel analysis suggested. The 2-factor solution and 3-factor solution were both identified as promising, and were evaluated based on content, as well as having a minimum number of complex loadings. Two more items were not loading well onto both the 2 and 3 factor solutions, so these items were removed. In phase 3, a final factor analysis was conducted with the remaining 15 items. The 2-factor solution was the best fitting factor solution for the 2019-2020 CPI data, where two latent factors were identified: One factor measured proximal attitudes towards computer programming, while the other measured long-term, distal attitudes towards computer programming (Perez et al., 2019). It is important that this scale accurately measures changes in attitudes towards computer programming, because according to expectancy-value theory, students' expectations for success in computer programming can influence their academic and career outcomes in computer science (Perez et al., 2019). Now informed about the underlying structure of the scale, the next step is to run a confirmatory factor analysis with a test dataset, with CPI data from the 2020-2021 school year.

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Accuracy of Human Coding and Machine Learning for Political Science Event Classification

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Abstract:

Social scientists continue to be interested in developing ways to leverage the massive amounts of available digital textual data to study important social issues. Political Science and International Relations researchers have used machine coding methods for political event data since the 1990's and continue to shift their attention from the classic method of content analysis coding by hand. In an effort to continue improving the techniques for political event extraction from news article sources scientists have turned to Machine Learning and Natural Language Processing (NLP) for their ability to handle large amounts of textual data. The Triggers of State-led Mass Killings project is a new attempt at developing computational tools to create an event dataset mapping the occurrence of trigger-type events from news articles between 1989-2017. The project is a collaboration between Computer Scientists and Political Scientists, allowing for the development of computational tools while remaining wedded to the larger goal of understanding mass killings for prevention efforts. The process includes coding by human readers to create the training datasets that develop the inference engines that identify trigger events. Human readers also perform various validity checks on the ML predictions to improve their accuracy. My project explores the benefits and drawbacks between text classification using Machine Learning tools and content analysis by human coding. I hypothesize that the computer will struggle to code events that are processes like change in political control and will have better accuracy for discrete events like coups or assassinations. By analyzing accuracy scores across triggers for human coders and the ML models, we find that both struggle to accurately code the assassination trigger and overreport positive cases across triggers. For event data in this case, we conclude that Machine Learning and NLP techniques are a promising tool for projects using large amounts of textual data. Though neither method is perfect, ML tools can analyze more data than is possible by humans alone and allow flexibility to adjust the codes of interest without losing any past work. Moving forward, researchers should continue to sharpen computational tools to address social science questions while prioritizing transparency and clarity in communicating what we gain and what we potentially lose out on with these methods.

Testing Efficient Techniques to Absorb Copper (II) Chloride using Nanostructured Membranes

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Abstract:

The objective of the proposed research is to develop and evaluate a novel nanostructured membrane sorbent for the recovery of phosphorus resources from municipal wastewaters. In this research, we will be using reactive polymers to produce the nanostructured membrane sorbent. The pore wall chemistry can be tailored to allow for targeted capture profiles through the functionalization of the allyl functional groups that line the pore walls. Therefore, using coupling chemistry, we propose to load our membrane adsorbents with functional groups that target PO43- and enabling the use of the membrane as a filter for PO43-. As an initial proof of concept and to learn the tools and techniques needed, the start of the project has been executed with Cu2+. Cu2+ is easier to use due to the fact that it is easily detected using UV-Vis spectroscopy and is visible on the membrane itself (i.e., it turns the membrane blue upon adsorption). The techniques during the process of Cu2+ will be applied to the PO43- which will allow that characterization process to be as accurate as possible. The results of the uptake isotherm experiments show that as the concentration of the feed becomes larger, there is a direct correlation with the growth of the mmol G^{-1} that the membrane absorbs. However, at a certain concentration the graphs start to level off and becomes almost like a linear line instead of a logarithmic. This is when the Cu^{2+} concentration of the feed is 10. The dynamic uptake experiment has a similar curve to the isotherm experiment and grows logarithmically and levels off to create a linear line.

Bringing 5G Smarts to Network Measurement

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Abstract:

The current free analysis of Internet access performance like Speedtest.net measures the data throughput and latency by sending larger and larger data flows until the network fails to handle additional traffic with the process generally taking on the order of 10-20 seconds. The advantage of this approach is that it is easy to implement and can accurately measure the achievable throughput of the network. However, during the Speedtest.net measuring process, tens of megabytes of data can be sent between devices and the network can be congested for quite some time, resulting in a large cost in terms of both mobile device energy and link utilization. For instance, for a single tests on a link of 10 Mb/s, the resulting test will use approximately 20 MB of data making it difficult to justify running tests longitudinally to measure network performance. Moreover, the majority of the users do not necessarily need to know the exact bandwidth of the network, rather all the users care about is if the network can handle their normal online activities. Therefore, a method that can reduce the data being transmitted with reduced bandwidth and shorter times could be a significant improvement. The focus of this work is to explore the extent that QUIC and the Go language, a new variant for network transfers and a newly emergent language for concurrency, could help advance existing works in a more scalable and effective manner towards measuring network performance.

The Effect of Solution Dipping Temperature on the Properties of Anodized-Aluminum Pressure-Sensitive Paint

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Abstract:

Anodized aluminum pressure-sensitive paint (AA-PSP) is widely used to correlate luminescent output to pressure in unsteady flow measurements. During the production of AA-PSP, anodized aluminum is submerged into a solution containing the luminophore. It is necessary to understand the effect of temperature during the dipping process has on the characteristics of the AA-PSP. The temperature of the solution was regulated, and various samples were created at different temperatures ranging from 0°C to 35°C. The pressure and temperature sensitivity of the AA-PSP samples were determined by exciting the luminophore with a spectrometer. The results demonstrated that a change in solution temperature affects pressure sensitivity, temperature sensitivity, and intensity. The amount of variability and possible error throughout the collected data was high. Therefore no clear trend could be established. The findings demonstrate that this area of study is promising though more refinement to testing methodology is required.

HF Characterization and Modeling of GaN Transistors

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Abstract:

Transistors are the workhorse device that underpins all modern electronics. While silicon-based transistors have come to dominate in digital applications due to their scalability and high degree of integration, for wireless communications and RF applications, silicon devices have limitations in terms of their output power, frequency range, and noise performance. One attractive solution to this problem that is being explored is the use of Gallium Nitride (GaN) based transistors. Because of the material properties of GaN (larger band gap, higher electron mobility) GaN transistors have the ability to function at a higher power levels, higher frequencies, and at higher temperatures than silicon. However, an open question is what are the ultimate limits of GaN transistors, and how can they best be used in circuits? To address this question, a nonlinear model (suitable for circuit design) is being extracted based on measured electrical characteristics of devices. Example research-grade GaN transistors, with gate lengths of approximately 50 nm and gate periphery of 37.5 microns, were placed under a microscope on a probe station. Two microwave-style probes were used (one on each side) that allowed different voltages to be applied the device, and the resulting currents to be measured. The outcome of this test created multiple data sets that quantify the device's response to these applied measurements.

Task Specific, Thermo-responsive Ionic Liquids for Directional Solvent Extraction Water Desalinations

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Abstract:

The ability to desalinate high salinity water is critical to addressing the ongoing global water shortage.(1) Undertaking this problem by minimizing energy consumption on a production level scale is necessary for rendering current polluted water to potable levels of saline content while also limiting waste. Our project focuses on the design and synthesis of new N-heterocycle-based ionic liquids (ILs) as environmentally benign, non-toxic fluids in an energy efficient directional solvent extraction (DSE) process for the desalination of industrial and residential water resources.(2) Thermo-responsive ILs exhibit Lower Critical Solution Temperature (LCST) and Upper Critical Solution Temperature (UCST) behaviors, allowing them to undergo phase separation above (LCST) and below (UCST) specific temperatures. While UCST behavior is commonly observed in liquids and is well accepted, LCST behavior is poorly understood. My project focuses on the analysis of LCST behavior of select ILs that exhibit phase separation behavior through temperature-dependent NMR with the goal of investigating the chemical physics behind LCST behavior in comparison to what is known about UCST behavior. Our lab has reported an IL suitable for DSE processes that enables a tenfold increase in freshwater yield over current techniques. We will improve and expand upon these results by synthesizing derivatives of this specific IL and performing TD NMR. Current methods for saltwater purification (e.g., reverse osmosis, etc.) are effective at treating hypersaline in small quantities, but these techniques are inefficient on large scale due to the need for large membranes and higher temperatures. The utilization of ILs exhibiting LCST behavior has the potential to substantially improve the energy efficiency of DSE processes and would enable DSE systems for water treatment on a global scale.

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Here I Am: The Stories of University Women Learning and Growing during COVID-19

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Abstract:

This qualitative study captures the stories of university women attending school in the United States during COVID-19 in their own words. As these women returned home for extended periods of time and resumed university classes for the academic year during the pandemic, this research examines how those experiences have impacted their relationships, identity development, lifestyles, and education. Women in the United States experience life differently than their male peers, especially in home and academic environments. Through this, the study aimed to amplify the women’s voices and further develop the body of work currently available relating to identity development in emerging adulthood, the emotional and relational impacts of COVID-19, and university women's perceptions of family life and lifestyles.

Magnetic Nanocarrier based, Precision Combinatorial Chemotherapeutics Treatment Against Metastatic Cancer Cells

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Abstract:

The leading cause of fatalities in breast cancer is metastasis. To increase the success rate of metastasis-free survival, there is a need to tackle therapy-resistant metastatic forms of the disease with novel, patient-friendly, combinatorial treatment regimens. At present, doxorubicin (Dox) regimens are standard of care for tumor debulking but do not stop metastatic recurrence and present cardiotoxicity. Vacuolar ATPase (V-ATPase) H + pump inhibitors (e.g., diphyllins) prevent metastasis, but the ubiquitous occurrence of this target raises concerns of off-target toxicity. A solution is targeted delivery to reduce off-target effects while also minimizing drug dose side-effects. So, here we present the successful demonstration of targeted combinatorial-delivery of V-ATPase inhibitors (Diph) and standard chemotherapeutics (Dox) to two metastatic cancer cell lines (A2780 and PC3) with positive cell clearance and affirmative inhibition of cancer cell invasion.

Recently developed magneto-silica nanoparticles (Mag-Si-Ns of ~5-8 nm) in our lab have been tuned to selectively permeabilize cancer cells in an external magnetic field, followed by a triggered release of a drug cocktail through an external oscillating, AC electromagnetic field. The MagSiNs possess a cobalt ferrite core and a piezoelectric fused silica shell. Anticancer drugs (Dox and Diph) which are encapsulated on MagSiNs, are co-administered, to specifically inhibit cancer growth and metastasis in the cell lines tested, while avoiding toxic side-effects on healthy control endothelial cells (HUVEC). The dosages of Dox and Diph tested were 20 nM and 500 nM. Dose-dependent cancer cell viability, cancer cell invasion capacity, MagSiNs uptake, and intracellular MagSiNs distribution were all assessed to ascertain cell clearing and anti-metastatic capabilities of our combinatorial chemotherapeutic regimen.

In conclusion, the drugs@MagSiNs formulations were magnetically permeabilized into the cancer cells, the active form of the drugs were released through a magnetic trigger, the drugs were selectively compartmentalized into the cancer cells, and the V-ATPase inhibitor worked synergistically with the doxorubicin to reduce cancer cell numbers and inhibit cancer metastasis. We are confirming these results in mouse animal model. We are also extending these results to test carboplatin and paclitaxel delivery to treat esophageal cancer.

Adversity During Multiple Periods of Development Does Not Influence Adult Parasite Loads in Wild Baboons

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Abstract:

Early life adversity has long-term effects on individual health and survival. Indeed, in long-lived primates, adversity is commonly linked to an increased likelihood of chronic inflammatory disorders and shorter lifespans. While these long-term effects are widespread and well-documented, few studies have directly compared how health in adulthood varies when social and environmental adversities occur during different periods of development. Our objective was to compare how health in adulthood varies when adversities occur during two key phases of development for the adaptive immune system: post-natal life and adolescence. We hypothesized that adversity occurring in the early post-natal period would have stronger effects than adversity during adolescence because postnatal environments are important for the immediate development of the adaptive immune system. Alternatively, adversity in adolescence could be stronger because it occurs closer in time to adulthood. We tested this hypothesis by analyzing parasite loads in wild, adult female baboons (Papio cynocephalus) living in Amboseli, Kenya. Specifically, we quantified the fecal parasite loads of known individual baboons by counting the number of Trichuris trichiura, Strongyle, Streptopharagus pigmentatus, and Abbreviata caucasica eggs, as well as the total number of species present. We also identified five sources of adversity: death of the mother, drought, social isolation, large group size, and low maternal rank. We created a cumulative adversity index by adding up the total number of adversities that each individual experienced at each critical period during the early postnatal period and adolescence. We found no significant relationship between cumulative adversity scores and any measure of parasite load during either critical time period. However, we did find that other factors in the baboon's environment during the sample collection time were significant predictors of parasite loads. Specifically, older individuals and individuals whose samples were collected during the dry season had higher parasite loads. While our analyses do not reveal a link between adversity during the immune system's critical periods and adult parasite loads, it is possible that this null result is an artifact of selection bias. In our analysis, we only included samples of baboons who lived through both critical periods, meaning that all individuals who did not survive to adulthood were automatically excluded from the analysis. It is possible that those baboons who died before reaching adulthood had poor or under-developed immune systems which contributed to their early death. In contrast, all baboons who did survive to adulthood and were included in this analysis, must have had well-developed and resilient immune systems. This selection bias may explain why it was difficult to identify a relationship between adversity during development and parasite loads in adulthood.

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