2023 SUMMER

UNDERGRADUATE RESEARCH SYMPOSIUM

WEDNESDAY, JULY 26

10:00 a.m. - 2:00 p.m.

Jordan Hall of Science

Summer Undergraduate Research Symposium

Wednesday, July 26, 2023
10:00 a.m. - 2:00 p.m.
Jordan Hall of Science, Galleria and Room 105

Schedule

10:00 - 11:00 a.m.	Poster Session 1	Galleria	56 posters
11:00 - 11:15 a.m.	Break		
11:15 a.m. - 12:15 p.m.	Poster Session 2	Galleria	56 posters
12:15 - 12:30 p.m.	Break		
12:30 - 2:00 p.m.	3MT Competition	Room 105	13 competitors

Student Participants

There are 116 students presenting 112 posters representing 16 summer REU programs. Students conducted their summer research projects in collaboration with faculty in 4 colleges and 14 departments at the University of Notre Dame and Saint Mary's College. Thirteen (13) students are competing in the 3MT Competition representing 10 summer REU programs, 3 colleges, and 6 departments.

Summer REU Programs

Biological Sciences - Integrative Cell and Molecular Biology REU
Center for Innovative and Strategic Transformation of Alkane Resources (CISTAR) RET
Center for Innovative and Strategic Transformation of Alkane Resources (CISTAR) Young Scholars Program
College of Science - Summer Undergraduate Research Fellowships (COS-SURF)
Computer Science and Engineering - CSE Summer Enrichment Program
Engineering Summer Undergraduate Research Experience (E-SURE)
Glynn Family Honors Program
Graduate School - ND-PREP Program (GS-ND-PREP)
Graduate School - Summer Research Opportunities Program (GS-SROP)
Lucy Family Institute for Data and Society
Naughton Fellowship Program
ND Energy - Vincent P. Slatt Fellowship for Undergraduate Research in Energy Systems and Processes (Slatt)
NDnano Undergraduate Research Fellowship (NURF)
Saint Mary's College
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU
Wireless Institute (AWaRE)

College of Arts and Letters, Notre Dame

Economics
History
Latino Studies
Political Science
Psychology

College of Engineering, Notre Dame

Aerospace and Mechanical Engineering (AME)
Chemical and Biomolecular Engineering (CBE)
Civil and Environmental Engineering and Earth Sciences (CEEES)
Computer Science and Engineering (CSE)
Electrical Engineering (EE)

College of Science, Notre Dame

Biological Sciences
Chemistry and Biochemistry

Saint Mary's College

Biology
Chemistry and Physics

UNIVERSITY OF NOTRE DAME

SAINT MARY'S COLLEGE NOTRE DAME, IN

10:00 - 11:00 a.m. Poster Session 1 (56 posters)

#	Name	Project Title	Program	Faculty Advisor
1	Bryan Bermúdez Agosto	Self-Assembly Peptides: From Fundamental Design to Type 1 & Type 2 Diabetes Therapeutic Applications	GS-SROP	Matthew Webber, CBE
2	Anna Araujo	Increased Proliferation in Response to Acute Damage in Zebrafish Photoreceptor Mutants	GS-SROP	David Hyde, Biology
3	Andrew Arcidiacono	Visualizations of Simulated Atmosphere and Particle Data	E-SURE	David Richter, CEEES
4	Sophia Baker	Role of Cannabinoid Signaling in Zebrafish Kidney	COS-SURF	Rebecca Wingert, Biology
5	Jordan Basabanda	Enhancing Admissions Processes Through Storytelling With Evidence: An Investigation of an Innovative Application	CSE	Ron Metoyer, CSE
6	Dan Boice	ß-Cyclodextrin Crosslinker Increases Longevity in Polymer Membranes	SMASH Engr	Ruilan Guo, CBE
7	James Boumalhab	Optimizing Sensor Network Performance: Adaptive Filtering with Innovation Check for Efficient Data Processing	NURF	Yih-Fang Huang, Ningyuan Cau, EE
8	Brigid Burns	Investigating the Impact of Processing Approaches on Hurricane Dropsonde Data	E-SURE	David Richter, CEEES
9	Antonia Castro	Yap or Taz: Understanding the Divergent Roles of the Hippo Pathway Coactivators in Nephrogenesis	GS-SROP	Rebecca Wingert, Biology
10	Sam Chen	Polymer Gel Electrolyte in Next Generation Rechargeable Battery	Slatt	Jennifer Schaefer, CBE
11	Dorrian Cohen	The Last of Fung-Us: Evaluating the Antifungal Activity of a Synthetic Enterocin Peptide Library	COS-SURF	Shaun Lee, Biology
12	Aliyah Collins	Defining the Vacuolar Protein 8 of the Pathogenic Yeast Cryptococcus Neoformans as a Good Therapeutic Target	Biology	Felipe Santiago-Tirado, Biology
13	Lydia Csaszar	Generating Genomic Contigs with Migrating Threads in Python	E-SURE	Peter M. Kogge, CSE
14	Ultan Fallon	Exploration of Pneumatic Exosuit Bands with Desirable Mechanical Property Changes	Naughton	Margaret Coad, AME
15	Adora Goodluck	Characterization of Ionic and Electronic Conductivity of PEO-LiTFSI Electrolyte and Sulfur Copolymer Cathode in Solid-State Lithium-Sulfur Batteries	SMASH Engr	Jennifer Schaefer, CBE
16	Dominique Gramm	Functional Analysis of Vascular Networks in Stem Cell Organoids	GS-ND-PREP	Donny Hanyaja-Putra, AME
17	Richard Hernandez	Differential whiB6 Promoter Activation in Response to Changes in Growth Environment in Mycobacterium Marinum	Biology	Patricia Champion, Biology
18	Grace Johnston	Extreme Temperatures Reduce Strike Success in Smallmouth Bass Feeding	Saint Mary's	Katrina Whitlow, Biology
19	Kayla Kellner	The Role of Youth and Mother's Familism on Youth Mental Health in Mexican Families	GS-SROP	Kristin Valentino, Psychology
20	Paityn Krout	Hydrogel-enabled 3D Cell Culture for HTHC Janus Particle Immunodetection of Exosomes	SMASH Engr	Yichun Wang, CBE

10:00 - 11:00 a.m. **Poster Session 1** (56 posters)

#	Name	Project Title	Program	Faculty Advisor
21	Brían Lawlor	Studying the Effect of Cancer-associated Fibroblasts on Glioblastoma Cell Stemness	Naughton	Meenal Datta, AME
22	Sarah Leddy	Developing a Trifluoromethylation Strategy of Alcohols and Amines for the Synthesis of New Therapeutics and Agrochemicals	Saint Mary's	Elsa M. Hinds, Chemistry/Physics
23	Scott Leeper	Differences of Perceived Suicide Stigma Among Veterans Across Regions of the United States	GS-SROP	Brooke Ammerman, Psychology
24	Fatima Maciel	Voting Rights and Federalism: Understanding the California Voting Rights Act	GS-SROP	Luis Fraga, Political Science
25	Gabriela Meléndez Martínez	Identification of Biofilm Forming Microbes in CAUTIs in Mice through Amplification and Sequencing of the 16s Region	GS-SROP	Ana Lidia Flores-Mireles, Biology
26	Bethany McKittrick	Visualising ATP Detection by Electrochromic Sensors	Naughton	Kaiyu Fu, Chemistry
27	Kailee Mendiola	Characterizing and Controlling Calcium Signaling Dynamics in Lymphatic Endothelial Cells	SMASH Engr	Donny Hanjaya-Putra, AME
28	Juan Leal Mendoza	Ensuring Gracefulness in Withdrawals: The Dynamics of the Early 1970s American Withdrawal from South Korea	GS-SROP	Eugene Gholz, Political Science
29	Reid Metoyer	Smart Shopper: Healthy Food Choices with a Multi-level Hierarchy and Recommendation Algorithm	GS-SROP	Ronald Metoyer, CSE
30	Dhemi Mislenkov	Optimizing the Synthesis of Tetra-2-pyridinylpyrazine and its Iron Complexes for Use in Redox Flow Batteries	Saint Mary's	Michael Drummond, Chemistry/Physics
31	Jennifer Morones	Improving Network Inference for Protein Structural Classification	CSE	Tijana Milenkovic, CSE
32	Nadia Muniz	The Role of Nephronectin in Cell Fate Determination During Retinal Regeneration in the Adult Zebrafish	Biology	David Hyde, Biology
33	Ryan Murray	Modeling 5G Interference on Weather Radiometer	AWaRE	J. Nicholas Laneman, EE
34	Nga Nguyen	Enhancing Liquid-Liquid Phase Separation through Confinement and Crowding	SMASH Engr	Jonathan Whitmer, CBE
35	Daniel O'Connor	Tuning Amine-based Polymer Catalyst for CO_2 Conversion through Structural Modification via Quaternization	Slatt	Casey O'Brien, CBE
36	Angel Ortiz Emmanuel De La Paz	Automatic Characterization of Software Exploits	E-SURE	Taeho Jung, CSE
37	Mónica Leal Palma	Nanoparticle Mediated Reprogramming of Cells to Fight Cancer	NURF	Meenal Datta, Ryan Roeder, AME
38	Elizabeth Power	Nanoscale Formulation of Corrective Hormones for Bblood Glucose Control	NURF	Matthew Webber, CBE
39	Gleniarys Rivera	Donnan Dialysis for the Recovery of Metal Ions utilizing EDTA as a Complexing Agent	SMASH Engr	Merlin Bruening, CBE
40	Johnathan Robinson	Simulated Hydrogen Gas Adsorption in Soft Porous Coordination Polymers	SMASH Engr	Yamil Colón, CBE

10:00 - 11:00 a.m. **Poster Session 1** (56 posters)

#	Name	Project Title	Program	Faculty Advisor
41	Dorielis Rodríguez	Microenvironmental Effects on the Mechanical Behavior of Cancer Cells	SMASH Engr	Meenal Datta, AME
42	Peter Schimpf	Increasing Safety in Lithium-Ion Batteries with Gel Polymer Electrolytes by Modeling Thermal Runaway	NURF	Jennifer Schaefer, CBE
43	Bennett Schmitt	Investigating Rare Earth Element Mineralization Within Fenite Alteration Zones	Slatt	Antonio Simonetti, CEEES
44	Julia Schutz	Efficient Synthesis of N-(2-picolyl)picolinamide Ligand and Application in Organometallic Transformations	Saint Mary's	Elsa Hinds, Chemistry/Physics
45	Patrick Schwartz	NASA FLOATing DRAGON Challenge: Autonomous Navigation of a Parafoil from a High-Altitude Balloon	AWaRE	Scott Howard, EE
46	Sarah Shibuya	Regulation of Synaptic Activity through a CB1 Receptor-Dependent Mechanism in Fragile X Syndrome Induced Neurons	Biology	Christopher Patzke, Biology
47	Parker Tamucci	Optimizing Dosage of VRK-1 Inhibitory Drugs for Inducing Cellular Senescence	Biology	Kevin Vaughan, Biology
48	Ximena Tobon	College Students' Collectivism, Financial Wellbeing, and Future Retirement	GS-SROP	Karen Richman, Latino Studies
49	Rubén Torres	Measurement of Wide Band Gap Semiconductor Power Devices	Slatt	Patrick Fay, EE
50	Railyn Webster	Characterization of Candida spp. Clinical Isolates Pathogenesis in the Catheterized Bladder	GS-ND-PREP	Ana Flores-Mireles, Biology
51	Jasmine White	Familial Support: An Examination of the Relationship Between Low Income and Depression	GS-SROP	Theodore Beauchaine, Psychology
52	Bella Wiebelt-Smith	Investigating UTX in Kabuki Syndrome Inhibitory Neurons	Biology	Christopher Patzke, Biology
53	Alex Williams	Defining the Concentration and Presence of RNA Binding Proteins in Extracellular Vesicles Released From Mycobacteria Infected Macrophages	Biology	Jeffrey Schorey, Biology
54	Kelly Williams	Graph Embedding in Quantum Computers	E-SURE	Peter Kogge, CSE
55	Evan Wood	Selective Ion Transport Through Copolymer Membranes Functionalized with Imidazole Ligands	Slatt	William Phillip, CBE
56	Jose Zentella	Examining DA Algorithm Matching Outcomes in Markets Where Agents' Preferences are Determined by Degree of Similarity	GS-SROP	Maciej Kotowski, Economics

11:00 - 11:15 a.m. **Break**

11:15 a.m. - 12:15 p.m. **Poster Session 2** (56 posters)

11:15 a.m. - 12:15 p.m. **Poster Session 2** (56 posters)

#	Name	Project Title	Program	Faculty Advisor
1	Thomas Adams	PIM-COOH 1,6 Hexanediol Crosslink with Amine Conversion	CISTAR RET	Casey O' Brien, CBE
2	Mikey Anderson	Temporal Variation in Environmental DNA Export at a Pond-stream Interface	Biology	Jennifer Tank, Biology
3	Kayla Anderson	Characterization of the Atypical Transporter PDR2 in the Pathogenic Yeast Cryptococcus Neoformans	GS-ND-PREP	Felipe Santiago-Tirado, Biology
4	Alan Avalos y Arceo	Cellular Reconstruction of Somatosensory Vertebrate Circuitry and Synapsing Interneuron Population	GS-SROP	Cody Smith, Biology
5	Tori Banda	Leveraging Data Science and Machine Learning to Combat Inequity in Digitally Mediated Gig Work	CSE	Toby Li, CSE
6	Reinhard Bartsch	Novel Ruthenium Carbene Complexes	Slatt	Vlad Iluc, Chemistry
7	Nila Beamon	Fabricating Desalination Membranes using the Molecular Layer-by-Layer Method and Characterizing the Films using Electrochemical Impedance Spectroscopy	SMASH Engr	Jennifer Schaefer, CBE
8	Addisyn Camadeca	Development of an Effective Synthesis of Bis(2-pyridinylcarbonyl)amine Ligand	Saint Mary's	Elsa Hinds, Chemistry/Physics
9	Gilberto Cerda III	Temporal Foraging Tendencies of Micropterus Salmoides in the Northern Temperate Region of the United States	GS-SROP	Stuart Jones, Biology
10	Alijah Chalas	The Effects of Age and Time Spent in the United States on the Cultural Values of Adults of Mexican Origin	GS-SROP	Jenny Padilla, Psychology
11	Samuel Clough	Development of GaN IMPATT Diodes as High Power Millimeter Wave Sources	AWaRE	Patrick Fay, EE
12	Maria Isabella Corcoran	Hyperdimensional Computing Based In-sensor Side-channel Attack Detection	Naughton	Ningyuan Cao, EE
13	Ana Corcoran	Progress Towards Understanding the Fate of Ampicillin in Soil	Saint Mary's	Christopher Dunlap, Chemistry/Physics
14	Charlie Desnoyers	Development of an Aptamer Based Gold Nanoparticle Biosensor for the Quantification of Kanamycin	NURF	Kaiyu Fu, Chemistry
15	Bridget Donovan	Synthesis of Tridentate Ligands and their Iron Complexes for use in Redox Flow Batteries	Saint Mary's	Michael Drummond, Chemistry/Physics
16	Noelle Dorvault	The Role of AMT in Embryonic Development and Nephrogenesis	COS-SURF	Rebecca Wingert, Biology
17	Lauren Farrell	Exploring the Reactivity of Nucleophilic Iridium Complex with Electrophilic Carbon Compounds	Slatt	Seth Brown, Chemistry
18	Brisny Rodriguez Flores	Materials-Driven Application-Level Analysis of Emerging Workloads	CSE	Micheal Niemier, CSE
19	Michael Garza	Total Synthesis and Chemical Stability of Pseudouridimycin and its Analogues	GS-SROP	Juan Del Valle, Chemistry
20	Gabe Goertz	Synthesis of Nanocrystal Surface-Bound Transition Metal Complexes	Slatt	Emily Tsui, Chemistry

11:15 a.m. - 12:15 p.m. **Poster Session 2** (56 posters)

#	Name	Project Title	Program	Faculty Advisor
21	Juliana Gonzalez	Using Source Code Summarization to Eliminate User Necessity	CSE	Collin McMillan. CSE
22	Adrian Gonzalez	Improving the Quality of Diffusion Cell Experiments using 3D Printing and Automation	GS-SROP	William Phillip, CBE
23	Sofia Granieri	Construction and Characterization of Functionalized HEMA Membranes for Biocompatible Sensors	NURF	William Phillip, CBE, Kaiyu Fu, Chemistry
24	Aisling Hanrahan	Exploring the Functionality of iPSC Derived Lymphatic Endothelial Cells using Metabolite-assisted Growth Factor Differentiation Protocol	Naughton	Donny Hanjaya-Putra, AME
25	John Howe	Synthesizing Gold Hexagonal Nanoplates under Different Lighting Conditions	NURF	Svetlana Neretina, AME
26	Tyler Kopf	Investigating the Role of Enah in Dorsal Root Ganglia Invasion of the Spinal Cord	Biology	Cody Smith, Biology
27	Aisling Kruger	Elucidating the Role of Iroquois Transcription Factor 4a in Kidney Development	COS-SURF	Rebecca Wingert,Biology
28	Evangelina Louis	Investigation of Apolipoprotein L1 Function in Zebrafish Pronephros Development	Glynn Honors	Rebecca Wingert, Biology
29	Lauren Martin	Energy Transfer in Lead Halide Perovskite-Molecular Hybrid Assemblies for Light Harvesting Applications	Slatt	Prashant Kamat, Chemistry
30	Kutemwa Masafwa	Poly(propylene carbonate)-based Composite Polymer Electrolyte for Solid-state Lithium-ion Batteries	SMASH Engr	Jennifer Schaefer, CBE
31	Darragh McAndrew	Estimation of Socket-stump Pressure in Transfemoral Amputees Combining Electronic Fabrics and Pressure Models	Naughton	Edgar Bolívar-Nieto, AME
32	Simon McElroy	Exploring Sea Turtle Locomotion Mechanics for Biomimetic Robotic Design	Naughton	Yasemin Ozkan-Aydin, EE
33	Nia McGee	Mechanical Deformation Induced By Tumor Progression Analyzed In Patient MRIs	SMASH Engr	Maria Holland, AME
34	Joshua Moeller	Characterizing the Effects of Ethanol in Zebrafish Embryonic Nephron Development	Biology	Rebecca Wingert, Biology
35	John Moore	Charge-Functionalized Nanofiltration Membranes Exhibit Multi-Valent Ion Rejection	Slatt	William Phillip, CBE
36	Omar Muñoz	Animating Construction Process of Modular Lapped Reinforced Concrete Connections to Accelerate Nuclear Building Project Schedules	Slatt	Yahya Kurama, CEEES
37	Maximilian Niebur	Understanding the Interactions Between Non-Equilibrium Plasma and Nanomaterials in a Fluidized Gliding Arc	NURF	David Go, AME
38	Allison O'Brien	Graph Embedding in Quantum Computers	E-SURE	Peter Kogge, CSE
39	Axaraly Ortiz	Land and Cultural Loss: Touristic Development and Neoliberal Reforms in the Yucatán Peninsula	GS-SROP	Jaime Pensado, History
40	Derek Pepple	Constructing Heterogeneous Systems with Migrating Threads	E-SURE	Peter Kogge, CSE

11:15 a.m. - 12:15 p.m. **Poster Session 2** (56 posters)

#	Name	Project Title	Program	Faculty Advisor
41	Molly Pooler	Analyzing a Hands-On Project-Based Data Science Course Impact on Students' Own Attitudes and Engagement Within the Field	Lucy Institute	Ying (Alison) Cheng, Psychology
42	Edgar Andrés León Rivera	Design of Peptide-Based Macrocycles for Discovery of Novel Glucose Binders	SMASH Engr	Matthew Webber, CBE
43	Laura Rodriguez	Knockdown of Cathepsin B Protein in Mammalian Epithelial Cells Affect Cell Proliferation during ECM-detachment	Biology	Zachary Schafer, Biology
44	Mario Ruiz-Yamamoto	The Effects of Oxidation and Reduction on a Platinum-Tin Alloy on Silica and Models of Physical Properties	CISTAR YS	William Schneider, Jason Hicks, CBE
45	Delaney Ryan	Characterization of Tributyl Phosphate Radicals by Electron Spin Resonance	Slatt	Ian Carmichael, Chemistry
46	Reed Snedeker	Cortical Thickness Patterns in Developing Fetal Brains with Spinal Bifida	E-SURE	Maria Holland, AME
47	Karolek Suchocki	Lagrangian Cloud Model Validation and the Effects of Aerosol Count	E-SURE	David Richter, CEEES
48	Molly Sullivan, Juan Pablo Rubero, Confidence Nawali, Farah Aburokba	A Mobile App for Guided Human-Computer Interaction Fuzz Testing of Small Uncrewed Aerial Systems	CSE	Jane Cleland-Huang, CSE
49	Angela Taglione	Micro-Organoids Generation by a Gel Droplet Platform for Cancer Drug Screening	NURF	Donny Hanjaya-Putra, AME
50	Frances Ubogu	PGAM5, a Regulator of Cancer Cell Survival	Biology	Zach Schafer, Biology
51	Allen Jeremy Uy	Machine Learning Methods for Spectrum Occupancy	AWaRE	Michael Lemmon, EE
52	Emily Volpe	Amia Calva Show Extensive Chewing to Reposition Prey before Swallowing	Saint Mary's	Katie Whitlow, Biology
53	Rebecca Warren	The Effect Of Repeated Experimental Design Parameters on the Alignment Between Top-Down Attentional Control and Volitional Control	GS-ND-PREP	Bradley Gibson, Psychology
54	Marissa White	A Novel Graphical User Interface for Rapid Deployment of Multi-Drone Missions for Emergency Response	CSE	Jane Cleland-Huang, CSE
55	Jeffrey Yang	High-Frequency Response of Thermoelectrically Coupled Nanoantennas	NURF	Gergo Szakmany, EE
56	Wenjun (Anya) Zhao	Mechanobiological Interactions of Macrophages and Cancer Cells in Glioblastoma Models	E-SURE	Meenal Datta, AME

12:15 - 12:30 p.m. Break

12:30 - 2:00 p.m. 3MT Competition (Room 105)

12:30 a.m. - 2:00 p.m.   3MT Competition

Contestant #	Name	Program	Faculty Advisor, Department
1	Sam Chen	Slatt	Jennifer Schaefer, CBE
2	Dorrian Cohen	COS-SURF	Shaun Lee, Biological Sciences
3	Lydia Csaszar	E-SURE	Peter M. Kogge, CSE
4	Ultan Fallon	Naughton	Margaret Coad, AME
5	Grace Johnston	Saint Mary's	Katrina Whitlow, Biology
6	Gabriela Melendez Martinez	GS-SROP	Ana Lidia Flores-Mireles, Biological Sciences
7	Kailee Mendiola	SMASH Engr	Donny Hanjaya-Putra, AME
8	Reid Metoyer	GS-SROP	Ronald Metoyer, CSE
9	Peter Schimpf	NURF	Jennifer Schaefer, CBE
10	Allen Uy	AWaRE	Michael Lemmon, EE
11	Bella Wiebelt-Smith	Biology	Christopher Patzke, Biological Sciences
12	Alex Williams	Biology	Jeffrey Schorey, Biological Sciences
13	Evan Wood	Slatt	William Phillip, CBE

THANK YOU FOR ATTENDING THE
2023 SUMMER UNDERGRADUATE RESEARCH SYMPOSIUM!

10:00 – 11:00 A.M.
POSTER SESSION 1

ABSTRACTS

Self-Assembly Peptides: From Fundamental Design to Type 1 & Type 2 Diabetes Therapeutic Applications

Bryan Bermúdez Agosto
Graduate School (SROP)

Faculty Advisor:
Matthew Webber, Chemical and Biomolecular Engineering
College of Engineering

Mentor:
Weike Chen, Graduate Student

Diabetes has become a worldwide public health issue. Approximately 37.3 million or 11.3% of the U.S. population are diabetic with over 1.7 million new cases diagnosed in 2012. Among them, over 90% of adult diabetic cases are type 2, making important the development of new therapeutics to treat type 2 diabetics (T2D). In 2017, diabetes was the seventh leading cause of death in the United States. Lower limb amputation, kidney failure, heart attacks, blindness and strokes are some major causes of diabetes. Recently, glucagon-like peptide-1 (GLP1) analogues have been developed as new class of diabetic drugs with therapeutic potential to treat T2D, due to its stimulation of insulin release and inhibition of glucagon release to lower blood glucose level and reduce body weight. However, the clinical application of GLP1 is limited by its short two-minute half-life, owing to its rapid in vivo clearance and vulnerable enzyme degradation. To advance the next generation of GLP1 delivery, supramolecular chemistry has been leveraged to design functional biomaterials to achieve desired delivery profiles. By precisely tailoring molecular motifs used in the self-assembled materials, one can generate materials with dynamic behaviors that can control the mechanical properties to modulate the enzymatic stability and release kinetics of encapsulated drug. In this study, we synthesized a series of modified GLP1 analogues and tune the mechanical properties of biomaterials used for their delivery to control and prolong release of the active therapeutics.

Increased Proliferation in Response to Acute Damage in Zebrafish Photoreceptor Mutants

Anna Araujo
Graduate School (SROP)

Faculty Advisor:
David Hyde, Biological Sciences
College of Science

Mentor:
Maria Iribarne, Senior Researcher

Chronic degeneration of retinal photoreceptors is the cause of many vision-related disorders in humans, including Retinitis Pigmentosa and Ciliopathies. While humans lack the ability to regenerate retinal neurons, zebrafish can regenerate all retinal cell types following an acute damage due to the reprogramming and proliferation of the resident Muller glia cells (MG). However, zebrafish cannot regenerate neurons following chronic retinal degeneration. It is unclear if chronic degeneration mutants are either unable to regenerate lost neurons or if the chronic damage confers a resistance to regenerate. To address this question, we examined two different chronic degeneration mutants, one that results in a chronic loss of rod photoreceptors (rho) and one that exhibits a chronic loss of cone photoreceptors (cep290). We induced an acute damage, either light to kill the remaining photoreceptors or NMDA to destroy inner retinal neurons, to determine if the chronic mutants retain the ability to regenerate lost neurons.

We used immunohistochemistry to stain for expression of the cell proliferation marker PCNA to identify proliferating cells in the retina of rho and cep290 zebrafish lines. Subsequently, we use confocal microscopy to image these immunostained retinas and quantified proliferating retinal cells.

We observed an increase in the number of PCNA-positive cells in the outer nuclear layer of the retina in rho mutants at 0 hours post-NMDA injections compared to wild-type (WT) retinas, indicating an increased number in rod progenitor cells in the rho mutant without acute damage, suggesting that there was regeneration of rod photoreceptors from the rod progenitor cells, but not the resident MG. At 72 hours post-NMDA injection, there were increased numbers of PCNA-positive MG, demonstrating that the chronic rho mutant possessed the ability to regenerate lost retinal neurons, but required an additional stimulus (NMDA damage) to do so. In contrast, there was no difference in the number of PCNA-positive cells between cep290 and WT fish at 0 hours of acute light damage, confirming that there was no regeneration response due to the chronic loss of cone photoreceptors. Additionally, we observed a significantly fewer PCNA-positive MG in cep290 mutant retinas at 72 hours of light damage relative to WT fish. This may be due to the cep290 mutant fish having fewer photoreceptors to lose due to light damage than WT fish and therefore, required a small regeneration response.

Taken together, these data suggest a differential, amplified response to acute damage in chronic photoreceptor mutants compared to WT zebrafish. Understanding zebrafish mutant retinal regeneration, compared to WT regeneration, allows for more translatable results to human retinal disorders. Future research is needed to investigate cell fate and regenerative capacity of zebrafish photoreceptor mutants.

Visualizations of Simulated Atmosphere and Particle Data

Andrew Arcidiacono
E-SURE

Faculty Advisor:
David Richter, Civil and Environmental Engineering and Earth Sciences
College of Engineering

Understanding how hurricanes and tropical storms form and intensify is an important part of predicting and therefore preparing for them. For many variables, such as the total water mass in the air from ocean spray, it is not fully known how they affect these storms. Our research simulates sections of the atmosphere above the ocean to better understand the effect these processes have. My section of this project focuses on taking the atmosphere and particle data from these simulations and creating compelling and easy to understand images and animations. VAPOR, a 3D rendering software used for atmospheric research, was used to create these visualizations. VAPOR, however, does not support the data format of the output of our simulations, so the data needed to be rewritten into supported formats. This reformatting was accomplished by writing MATLAB scripts to read in the variables we wanted to visualize from the raw data and translating them into a data file that VAPOR can understand. The particle data were translated in this way into netCDFs, which organize the variables such as the number of particles and the position of these particles into labeled dimensions. Similarly, the atmospheric flow data were translated into binary files, which just contain a chain of values, with BOV (Brick of Values) header files to give VAPOR all the necessary information on how to arrange these values. In this way, the data is fully prepared to be rendered in VAPOR, and detailed images and animations can be created. This process has allowed us to generate images and simple animations of a 3D view of these data. As this project continues, we will create longer and smoother animations and a wider variety of visual representations of the data. Additionally, we plan on using Python to set up and run the renders to avoid needing to open the VAPOR GUI, which will make creating the visualizations quicker and easier.

Role of Cannabinoid Signaling in Zebrafish Kidney

Sophia Baker
COS-SURF

Faculty Advisor:
Rebecca Wingert, Biological Sciences
College of Science

Mentor:
Thanh Khoa Nguyen, Graduate Student

Cannabinoid receptors are located throughout the body and are part of the endocannabinoid system. Endocannabinoids bind to G protein-coupled receptors in the central nervous system (CNS), as well as the peripheral nervous system, which includes the kidneys. However, there is still very little known about the role of cannabinoid receptors, and their role within the kidneys. Our goal is to observe the role of cannabinoid receptors, specifically CB1, in multiciliated cells (MCCs) within zebrafish kidneys. We have recently shown that CB1 agonism of mature MCC markers results in a decrease of MCC numbers, but progenitor cell markers do not seem to produce an effect. Through the use of CB1 agonists, Methanamide and Anandamide we have observed decreased MCC counts that is consistent with our hypothesis that CB1 receptors play a role in MCC development. Additionally, live imaging of drug treated zebrafish embryos at 24, 48, and 72 hour-post-fertilization (hpf) revealed that MCC deficiency produced morphological changes such as edema and curved bodies. We also implemented the use of a splice-targeting morpholino of the cnr1 gene, which also exhibited a decrease in MCCs, further supporting our original findings with agonist treatment. Interestingly, the treatment with antagonists AM-281 and AM-251 produced different results. The number of MCCs decreased significantly with treatment of AM-251, but not AM-281. The morphological changes that were associated with agonist treatment were also seen with antagonists. These results provide promising direction for future studies, including characterization of CB1 receptor by crn1 genetic loss of function with th3e use of CRISPR Cas9 to create a stable CB1 mutant line of zebrafish for further experimentation.

Enhancing Admissions Processes Through Storytelling With Evidence: An Investigation of an Innovative Application

Jordan Basabanda
CSE Summer Enrichment

Faculty Advisor:
Ron Metoyer, Computer Science and Engineering
College of Engineering

Storytelling is a powerful tool that offers valuable insights into applicants' unique experiences, perspectives, and abilities. In an era of increasing competitiveness in higher education admissions, finding effective methods to sort and filter out students based on specific criteria is crucial for admissions officers. However, due to the nature of the admissions process and time constraints on these reviewers, storytelling is often overlooked as during an applicant's evaluation. This research aims to address this issue by exploring the potential of an innovative application that incorporates interactive storytelling elements to enhance the standard admissions processes.

In the current landscape of college admissions, the evaluation of applicants is typically focused on academic achievements, standardized test scores, and extracurricular activities. While these factors provide valuable information, they often fail to capture the important holistic factors of an applicant's story. The nature of the current admissions process, along with the large number of applications to review, leaves little time for equal and strong consideration for each and every one of the applicants personal narrative.

Recognizing this limitation, the research investigates the use of a storytelling admissions application to overcome these challenges. A critical part of storytelling in the admissions process is the ability to capture and recall evidence that supports or challenges a potential candidate's qualifications, experiences, and personal qualities.By integrating narrative elements and a visually appealing platform, the application provides a way for applicants to have their unique journeys, aspirations, and motivations analyzed qualitatively. In this case, admissions officers are able to make informed decisions about the suitability of an applicant for their academic community.

The resulting prototype is functional and appropriate for running controlled lab experiments to understand the impact of the evidence collection of narratives. We ran initial pilot experiments with the prototype. We found that participants can successfully use the prototype to capture evidence and construct holistic narratives about the candidates and that those stories are richer in content and more factual than stories told without the tool.

ß-Cyclodextrin Crosslinker Increases Longevity in Polymer Membranes

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Polymer-based gas separation membranes are a promising alternative to other thermally-driven separation methods, as they are comparatively inexpensive to create and require much less energy to operate. In a polymer membrane separation system, the membrane is used as a filter to allow desired gasses to pass through the membrane while other gasses are blocked from passing through- the amount of gas and what gasses are allowed through the membrane depends on the particular membrane's permeability and selectivity. Despite the benefits of polymer membranes, their industrial applications are limited due to challenges such as physical aging, wherein the polymer's permeability decreases over time. A polymer experiencing aging has its free volume decrease as the polymer chains relax towards a thermodynamic equilibrium leading to more compact chain packing. Polymer of intrinsic microporosity-1 (PIM-1) is noted for having high fractional free volume and rapid aging time, making it an ideal candidate for studying methods to mitigate the physical aging process. Previous studies using PIM-1 have performed modifications to restrict polymer chain motion using crosslinking, where polymer chains bond together at random junctions along the polymer backbone. While effective at reducing aging, random crosslinking severely decreases permeability in the membrane. In our work, we instead aim to use the conical and hollow crosslinker ß-cyclodextrin to connect partially hydrolyzed PIM-1 chains together in order to maintain a high degree of free volume within the membrane to mitigate losses to permeability after crosslinking. Specifically, we have developed protocols to reliably produce hydrolyzed PIM-1 with >70% hydrolysis degree in less than 72 hours, allowing us to quickly create test-ready membranes via esterification reaction between ß-cyclodextrin crosslinker and hydrolyzed PIM-1. We are currently undergoing film characterization and testing. We anticipate that the ß-cyclodextrin crosslinked PIM-1 membranes will maintain high permeability after crosslinking and showing significantly improved resistance toward physical aging.

Optimizing Sensor Network Performance: Adaptive Filtering with Innovation check for Efficient Data Processing

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Sensors are all around us, collecting data from the environment and transmitting it to various destinations. However, continuous data collection by traditional sensors, especially in stable environmental conditions, can lead to unnecessary processing utilization and higher power consumption. In this research, we propose an alternative approach that integrates an adaptive filtering algorithm into sensor systems to address these limitations. By employing the set-membership normalized least mean square (SM-NLMS) algorithm, we aim to enhance the efficiency and effectiveness of sensor systems by reducing the number of unnecessary updates. To evaluate our proposed approach, we implemented the SM-NLMS algorithm using MATLAB programming software. Simulated sensor scenarios were created by generating random data, parameters, and noise, emulating real sensor measurements. The algorithm was iteratively applied over a fixed number of iterations, and an error value was calculated between the artificial data and the predicted output. To improve the algorithm's efficiency, we incorporated an innovation check to detect deviations from normal environmental behaviors, triggering updates only when necessary. Our evaluation showed promising results. The Mean Squared Error (MSE) and Normalized Mean Squared Error (NMSE) metrics demonstrated the convergence of the system's parameters towards the desired values. Additionally, we observed a significant improvement in efficiency, with up to a 35% reduction in the number of unnecessary updates due to the innovation check. These results indicate that employing the SM-NLMS algorithm with an innovation check can enhance overall performance and efficiency in the process of data collection within sensor networks. In conclusion, our research highlights the benefits of integrating adaptive filtering algorithms into sensor systems with selective use of sensor data. The presented approach offers reduced processing utilization and improved efficiency, resulting in a more optimized sensor network system. These findings contribute to the advancement of sensor technologies and their practical applications.

Investigating the Impact of Processing Approaches on Hurricane Dropsonde Data

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A dropsonde is a meteorological instrument equipped with sensors for measuring atmospheric parameters. It is used to collect atmospheric data in weather forecasting and research. These sondes are deployed from aircraft to collect data during severe weather events, such as tropical cyclones.

The Hurricane Research Division (HRD) of the National Oceanic and Atmospheric Administration (NOAA) maintains an archive of these sondes. Each storm in the archive contains multiple types of data formats, including both the raw and processed data. However, the files processed by NOAA have not been uniformly processed. The aim of this experiment is to investigate the potential effects of different processing approaches on the raw data.

To ensure consistency in processing, this project generated two additional datasets by manually processing the raw data using ASPEN. ASPEN (Atmospheric Sounding Processing Environment) is software specifically designed for the analysis and quality control of sounding data. The first dataset was processed without adjusting any of ASPEN's quality control parameters, while the second dataset was processed with the adjustment of the Dynamic Correction quality control parameter.

The dropsondes in each of the three datasets are used to create average velocity profiles with respect to height. These profiles enable the estimation of surface stress, a crucial quantity in a hurricane environment. Moreover, these dropsondes can be utilized to estimate the relationship between u* (the friction velocity) and u10 (the wind speed at a height of 10m). Both u* and u10 are linked to Cd, the drag coefficient associated with the atmosphere and ocean's surface. After processing approximately 100 storms and over 45,000 sondes, significant differences are observed in the values of the average velocity profiles, u*, and u10, when initial processing methods differ. These differences in estimates using various processing methods would indicate a lack of robustness of the method and a large degree of uncertainty in the estimated values.

Yap or Taz: Understanding the Divergent Roles of the Hippo Pathway Coactivators in Nephrogenesis

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Podocytes are specialized cells vital to maintaining overall renal health. Podocytes form a crucial component of the filtration apparatus in the nephron working units of the kidney, which function to clean the blood. The Hippo pathway, a conserved signaling pathway within vertebrates involved in organ size control, tissue homeostasis, and regeneration, has emerged as a key regulator of podocyte function and integrity. Yes-associated protein (YAP) and the transcriptional coactivator with PDZ-binding motif (TAZ) are transcriptional coactivators within the Hippo pathway, both are significantly expressed in the podocyte nuclei. Previous studies demonstrated that silencing YAP leaves podocytes significantly more vulnerable to apoptosis, whilst TAZ deletion has been shown to affect the morphology of the podocytes and impede their function. Research has demonstrated the importance of Hippo pathway components in podocyte development and integrity, however, the mechanisms of how this occurs are not yet fully understood. In this study, we investigated the roles of yap1 and taz(wwtr1) in zebrafish and podocyte development through their effects on the expression of podocyte markers, nephrin, wt1a, and wt1b. Interestingly, our data indicate a role for yap1 in early podocyte formation and warrant future studies to explore the emergence of podocyte progenitors and the dynamic processes of podocyte differentiation and maturation. These findings contribute to the growing body of evidence supporting the intricate role of the Hippo pathway in mediating podocyte development. By expanding on the existing knowledge in the field we may better understand the potential of the Hippo Pathway as a therapeutic target for kidney diseases.

Polymer Gel Electrolyte in Next Generation Rechargeable Battery

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Due to environmental concerns and limitations of fossil fuel resources, society is shifting towards cleaner and renewable energy sources such as solar and wind energy. One concern of such a shift is how to store those forms of energy when they are not accessible, thus, resulting in a higher demand for high-capacity and rechargeable batteries. However, liquid electrolytes in commercialized lithium-ion batteries are highly volatile and flammable. My project aims at understanding the electrochemical properties of gel-polymer electrolytes and taking advantage of their unique characteristics, such as improved safety and binding of anions to improve lithium transport properties. Research conducted by Dr. DeSimone's group at the University of Stanford suggested the great potential of perfluoropolyether (PFPE) materials as candidate components for nonflammable and highly conductive gel polymer electrolytes. Previously, I tested the conductivity performance of different compositions of perfluoropolyether diacrylate (PFPEDA) based electrolytes for lithium-ion batteries. Among all compositions, the gel polymer electrolyte based on PFPEDA and lithium sulfonyl (trifluoromethane sulfonyl) imide methacrylate (MTFSiLi) in combination with organic carbonate solvents excels in comparison with other formulations. It was found that to avoid electrolytes' self-polymerization, the monomer materials must not exceed 10 percent of the total electrolyte by mass. The organic solvent is a mixture of ethylene carbonate (EC), ethyl methyl carbonate (EMC), and dimethyl carbonate (DMC) with a ratio of 3:3:4 to dissolve the monomers while maintaining potential stability. This summer, the impact of the mass ratio between PFPEDA and MTFSiLi on battery performance was further studied. The lithium transference number was measured for different electrolyte compositions using potential electrochemical impedance spectroscopy. Linear scan voltammetry was done to investigate the oxidative (upper voltage) stability of the electrolyte. A stepwise potential stability test was also performed to provide information about electrolytes' electrochemical stability at various potentials. To further understand how well the electrolytes perform, PFPEDA-based batteries were cycled at various charge/discharge rates, and their charge/discharge capacities were recorded.

The Last of Fung-Us: Evaluating the Antifungal Activity of a Synthetic Enterocin Peptide Library

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The antimicrobial peptide (AMP) circularized bacteriocin enterocin AS-48 produced by Enterococcus sp. exhibits broad-spectrum antibacterial activity via dimer insertion into the plasma membrane that forms pore structures. A specific alpha-helical region of enterocin AS-48 is responsible for the membrane-penetrating activity of the peptide. The canon syn-enterocin peptide library previously generated by the Lee Lab using rational design techniques to have ninety-five synthetic peptide variants from the truncated, linearized enterocin AS-48 was screened against three clinically relevant fungal strains: Cryptococcus neoformans, Candida albicans, and Candida auris. In screening, twelve peptides exhibited activity against C. neoformans, and two peptides exhibited activity against C. albicans. None of these fourteen peptides showed cytotoxicity to an immortalized human keratinocyte cell line (HaCats). Four peptides were identified with minimum inhibitory concentrations (MICs) below 8 µM against C. neoformans. One of these four peptides, peptide 24, has previously been shown to be effective against gram-negative and gram-positive bacteria and another one of these peptides, peptide 19, has previously been shown to be effective against the protozoan parasite Leishmania donovani. Early fungistatic/fungicidal tests show that three of the four peptides, 24, 32, and 40, are fungicidal. In 36-hour cell growth tests with these fungicidal peptides, peptide 32 exhibited C. neoformans cell counts slightly below those of the antifungal medication fluconazole and peptides 24 and 40 exhibited C. neoformans cell counts below those of vehicle control. These findings demonstrate that naturally derived AMPs produced by bacteria can be engineered and modified to exhibit potent antifungal activity. Our results will contribute to the development of new treatment alternatives to fungal infections and lend themselves to direct implications for possible treatment options for C. neoformans infections.

Defining the Vacuolar Protein 8 of the Pathogenic Yeast Cryptococcus Neoformans as a Good Therapeutic Target

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Cryptococcus neoformans is an opportunistic fungal pathogen commonly found in the environment, leading to frequent exposure. Immunocompetent individuals rarely experience symptoms, while immunocompromised individuals may develop life threatening cryptococcal meningitis. The World Health Organization recently released their first Fungal Priority Pathogens List which identified C. neoformans as the most threatening pathogen due to its increasing incidence and high mortality rates. The similarity between yeast and mammalian cells makes treatment of fungal infections challenging with often severe side effects. Therefore, it is essential to identify new antifungal drugs that effectively target yeast cells while limiting their effect on human cells. One potential target is the yeast vacuole. Studies in the nonpathogenic fungus Saccharomyces cerevisiae have shown the importance of vacuolar protein 8 (Vac8) in multiple vacuole fusion, vacuole inheritance, and autophagosome formation, among other cellular processes. To determine the importance of Vac8 in C. neoformans virulence and fitness, we deleted VAC8 using CRISPR Cas9. We are also using the same system to create a fluorescently tagged VAC8 strain to confirm Vac8 localization to the yeast vacuole. Comparison of C. neoformans's wildtype and vac8□ strains reveal deletion of Vac8 leads to aberrant vacuolar morphology. Additionally, vac8□ also exhibited slight decreases in growth when exposed to various cell wall stressors and the antifungals fluconazole and amphotericin B. Using an in vivo Galleria mellonella wax worm model we hope to further explore the role of Vac8 in fungal virulence. Understanding the role the vacuole plays in the overall fitness of pathogenic fungi is essential for controlling these deadly infections. The unique structure and importance of Vac8 makes it an optimal target for possible therapeutic intervention.

Generating Genomic Contigs with Migrating Threads in Python

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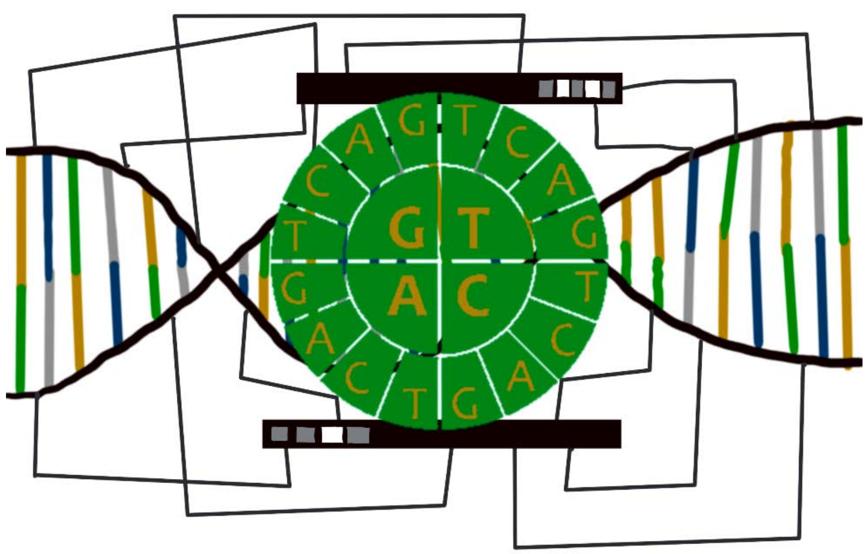
The de novo genome assembly problem in computational biology focuses on the current challenges of processing large sets of individual Deoxyribonucleic Acid (DNA) strands as input, and the original DNA sequence is to be assembled. There are a handful of algorithms that attempt to solve the problem but suffer scalability problems when run on conventional distributed memory systems, this includes accuracy issues and burdensome time and resource consumption. The ideal solution to this problem will assemble DNA sequences of a target genome of unknown origin while not compromising time. It will accomplish this by taking multiple DNA fragments as "reads" and, after traversing the reads, find prefixes and suffix pairs that match Kmers substrings and "prune" repeated matching pairs to generate a final set of contigs. This project presents a novel enhancement to a previously proposed solution by Dr. P Ghosh et al. in their paper PaKman: A Scalable Algorithm for Generating Genomic Contigs on Distributed Memory Machines. This project uses the pseudocode presentation in the paper translated to Python, which allows us to take full advantage of the language's simplicity in parallel threading and allow threads to migrate as needed, removing the need for inter-node messaging code stacks. Utilizing Python also opens the potential to apply the algorithm to accelerator hardware to reduce computational time without sacrificing accuracy, creating a dual-action solution to two major computational problems facing computer scientists' research in this area.



Exploration of Pneumatic Exosuit Bands with Desirable Mechanical Property Changes

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William Butler Yeats, a famous Irish poet once commented, ‘Education is not the filling of a pail, but the lighting of a fire’. This quote accurately describes my time that I have spent in Notre Dame’s IRIS Lab. The variety of topics that I have learned about in the field of soft robotics has sparked my growing interest in this field, as I can clearly envision its applications in years to come in my field, Biomedical Engineering, along with other disciplines such as the Military and beyond.

My supervisors have been both Katalin Schäffer, PhD student, and Dr. Margaret Coad, head of the Notre Dame IRIS Lab. They’ve been exceptional mentors, aiding me by incrementally broadening my understanding of soft robotics and specifically assisting my project, which is the exploration of pneumatic exosuit bands with desirable mechanical property changes. The ultimate goal of this research was to develop the understanding of physical human-robot interaction.

Exosuits such as this are vital to recovering stroke patients, people with Parkinson’s disease and even late-stage Diabetes. Discovering the cases of late-stage diabetes’ effect on arm mobility proved extremely compelling to me, as a type 1 diabetic myself. These exosuits allow movement in the arm and wrist for people with limited movement and in turn gives them the freedom to perform vital everyday tasks.

The primary challenge of this project is to create a pneumatic sleeve that was superior to commercial fabric sleeves. The requirements were that the sleeve would shrink to fit all who would wear it, acting as an anchor for the wrist exosuit to aid its holding force without slipping and hence avoid failure. This can be completed by considering beneficial mechanical property changes that the use of pneumatics exerts on different actuators.

I investigated the viability of fabric pneumatic artificial muscle (fPAM). This is a novel use of this actuator in a pneumatic sleeve, with the fPAM material’s light weight, its single layer threaded fabric makeup and its air-tightness initially displaying its feasibility. This actuator is unique as it contracts to 70% of its original length when filled with air to sufficient pressure. When used in a pneumatic sleeve, this compresses the sleeve onto the arm, consequently enabling the sleeve’s anchorage.

The design and execution of numerous experiments was one of the most interesting components of my project. The resulting data was appropriately used in altering my design, improving the performance of my pneumatic sleeve. These tests include conclusive tests on compressional force, holding force and stretching on three sleeve designs. These experiments proved the fPAM’s superiority to other actuators.

Characterization of Ionic and Electronic Conductivity of PEO-LiTFSI Electrolyte and Sulfur Copolymer Cathode in Solid-State Lithium-Sulfur Batteries

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The creation of sustainable, non-toxic energy infrastructure is crucial to environmental health. Batteries are necessary for sustainable energy systems as a replacement for fossil energy sources that generate toxic emissions. Lithium-sulfur batteries (LSB) are environmentally benign and due to the abundance of elemental sulfur reserves on Earth, they are inexpensive, making them a promising candidate for the future-generation battery. Solid-state electrolytes (SSEs) avoid the leakage and flammability hazards of organic liquid electrolytes, reducing the combustibility of the battery. SSEs are resistant to self-ignition, reduce the risk of thermal runaway as good heat conductors, and have good mechanical strength. Achieving a favorable ionic conductivity with a SSE, compared to organic liquid state electrolytes present in commercial lithium-ion batteries, would be a reliable solution to the hazards caused by the liquid-state. A solid-state electrolyte with high ionic conductivity is essential to a high-performing solid-state lithium-sulfur battery. Attaining a good electronic conductivity for efficient electron transport through the cathode is just as important because sulfur, the LSB cathode, is a poor electrical conductor. In this study, we constructed two cell set-ups to measure the ionic and electronic conductivity of the solid sulfur cathode and polymer electrolyte. Polyethylene oxide (PEO) is not electronically conductive and has high mechanical strength alone, so LiTFSI is added to increase the amount of lithium ions in the PEO, forming a thin-film electrolyte capable of relatively high ionic conductivity and efficient lithium-ion transport throughout the cell. The cathode active material consists of carbon nanotubes (CNT) and a sulfur copolymer, polysulfur-r-styrene-r-PEG styrene (PSSPS), that rests on a thin sheet of carbon nanofibers (CNF). CNFs are utilized as a current collector and supporting structure to hold the sulfur copolymer active material. CNTs allow electrons to flow from the CNF current collector to the sulfur regions of the electrode, increasing the electronic conductivity of the cathode material. We performed differential scanning calorimetry (DSC) and measured the ionic conductivity at four temperatures via the Broadband Dielectric /Impedance Spectrometer of both the PEO and PEO-LiTFSI films. We measured the electronic conductivity of samples of cathode material via the PARSTAT Potentiostat, with varying ratios of CNT: S. Attaining a dependable ratio of CNT:S to efficiently increase the electronic conductivity of the cathode material, and of LiTFSI: PEO to increase the ionic conductivity of the electrolyte is necessary in the study toward constructing a high performing SSE LSB that can potentially be used to store cleaner and more sustainable energy.

Functional Analysis of Vascular Networks in Stem Cell Organoids

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This project aims to investigate the functionality of blood vessels formed by lymphatic endothelial organoids embedded within norbornene modified hyaluronic acid (NorHA) hydrogels. The objective is to analyze the sensitivity and diffusion capabilities of the vessels sprouted around the organoid by employing a combination of experimental and mathematical modeling approaches. The understanding of blood vessel function in organoids has significant implications for advancing knowledge of vascular biology and its applications in regenerative medicine and tissue engineering.

The study will involve the cultivation of embryoid bodies (EB) within NorHA gels, supplemented with growth factors, such as vascular endothelial growth factors (VEGF), to induce the differentiation of lymphatic endothelial organoids. After an incubation period of one week, dyes will be introduced to assess the live-dead distribution and analyze the sensitivity of the vessels within the organoid. Additionally, a mathematical model will be developed to simulate and validate the diffusion of the dye into the organoid, serving as an indicator of efficient transport through the blood vessels.

Expected results of the live-dead analysis anticipate the production of fluorescent signals predominantly inside the blood vessels of the organoids, demonstrating their functional nature. While the dead dye accumulation is expected in the central region due to restricted oxygen availability. Controlled experiments will be performed by comparing organoids cultured without VEGF supplementation. Confocal microscopy will capture images of the live-dead stained organoids, and statistical analysis, such as t-tests and ANOVA tests, will be conducted to determine the differences between the experimental conditions. It is anticipated that the live-dead stained organoids will exhibit more organized vascular branches and increased contrast of colors compared to the controlled experiment.

Secondary Metabolites in Mushrooms at Saint Mary's Campus

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Pathogenic mycobacteria share a conserved secretion system (ESX-1) which allows them to lyse the phagosome of host macrophages, and is essential for virulence. The core membrane components of the ESX-1 system exert transcriptional control over the production of ESX secreted substrates via three transcription factors, which all bind to the same promoter. The first of these, WhiB6 serves as a self activator, as well as an activator for ESX-1 substrates. The second, EspM, is divergently transcribed from and serves as a repressor of WhiB6, by binding to the whiB6-espM intergenic region. The final, EspN, serves as a secondary activator of WhiB6, binding to this same intergenic region. However, in vitro experiments have shown that it only has this capacity in the absence of EspM. The mechanism dictating which transcription factor has priority for binding to this intergenic region, the whiB6 promoter, is still unknown. Moreover, the exact role each of these transcription factors play in the fine tuning of the ESX-1 system is still unknown. Here we aimed to determine whether environmental signals which might be present in host macrophages (eg. pH or host specific carbon sources) lead to differential activation of whiB6 promoter. We demonstrate that acidic conditions can restore ESX-1 dependent red blood cell lysis in specific non-hemolytic mycobacterial strains. Additionally, we used a fluorescent reporter construct to monitor transcription levels of EspM and WhiB6 in different pH conditions as well as in the presence of various carbon sources. We employed flow-cytometry to measure transcriptional activation of the whiB6 promoter at the level of individual cells. Finally, we hypothesize that PhoPR, a pH responsive kinase-transcription factor pair, is responsible for the restoration of lytic capabilities of the specific non-hemolytic strains.

Extreme Temperatures Reduce Strike Success in Smallmouth Bass Feeding

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Successful feeding is critical to survival in fish. Particularly in fish that eat elusive prey, strike success is heavily dependent on the predator's kinematics. Temperature drastically impacts swimming and bioenergetics in ectothermic animals, as muscle performance both increases with temperature and is strongest within a narrow homeostatic range, dropping off at extreme temperatures. Temperature also affects the behavior of fishes, though the mechanisms behind the observed shifts are less clear. This experiment investigates how different temperature treatments affect striking kinematics and success in Micropterus dolomieu (Smallmouth Bass). Smallmouth Bass are a species of fish native to the Great Lakes and the Mississippi River Basin that live in a wide variety of environments. They preferentially occupy colder waters and are predicted to be more vulnerable to increasing global temperatures relative to other local fish species. Previous knowledge on their kinematics and bioenergetics, as well as their importance ecologically and economically, make them a prime candidate for study. Bass were acclimated to temperature treatments ranging from 15°C-30°C, fed live prey, and filmed using a high-speed Edgertronic SC1 camera. Film was analyzed in ImageJ and is under analysis in DeepLabCut. Preliminary findings suggest that extreme temperature treatments of 15°C and 30°C result in more missed strikes in bass, as well as colder treatments making the bass less prone to strike. The gape size of the mouth and the velocity of its opening also appears to increase with warmer temperature treatments. Further analyses will examine the motion of the body and fins, striking distance, and role of prey response across temperatures.

The Role of Youth and Mother's Familism on Youth Mental Health in Mexican Families

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Background: The Latinx population is the largest and fastest growing minority population in the United States. Additionally, Latinx individuals experience a variety of stressors, such as discrimination, as well as a variety of protective and promotive factors, including familism and peer support. Familism is an important Hispanic cultural value that emphasizes family loyalty and interdependence within the family. Interest in familism has increased in recent decades due to its potential to prevent negative mental health outcomes, as prior research suggests that youth familism values are associated with positive mental health outcomes. However, when maternal familism values are considered, findings are mixed, with some studies suggesting that high levels of maternal familism may exacerbate mental health concerns for Mexican youth. The purpose of this study is to examine whether maternal perspectives of familism moderates the association between youth familism and internalizing symptoms.

Methods: Using Wave 1 data from a larger longitudinal study, 344 Mexican-descent families in Indiana with children ages 12-15 years were interviewed. Both mothers and youth reported on their personal familism values and on youth internalizing symptoms using questionnaires.

Results: After conducting correlation and regression analyses, the regression results illustrate that after controlling for youth age and gender, youth reported familism accounts for a significant proportion of variance in youth reported internalizing symptoms, $\beta = -.134$, $p<.05$, such that familism is related to fewer internalizing symptoms. In this model, maternal familism was not a significant predictor, and maternal familism did not moderate the association between youth familism and youth internalizing. In contrast, after controlling for youth age and gender, mother-reported familism accounted for a significant proportion of variance in the mother report of youth internalizing symptoms $\beta = -.21$, $p<.05$, such that mother-reported familism was related to fewer internalizing symptoms. In this model, youth reported familism was a nonsignificant predictor, and consistent with the first model, there was no significant interaction of youth and mother reported families on mother-reported youth internalizing symptoms.

Discussion: These results support prior findings that familism is protective for youth mental health, and it reveals that it is protective from both the youth and mother perspectives. This is valuable as we consider mental health interventions for Mexican-descent youth. Encouraging familism in youth can potentially protect against negative mental health outcomes. However, future research needs to explore how familism is transmitted between generations while also considering how differing levels of familism within a family may impact family dynamics and youth mental health.

Hydrogel-enabled 3D Cell Culture for HTHC Janus Particle Immunodetection of Exosomes

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Mentor:
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Three-dimensional (3D) cell cultures have been utilized as a growing tool in drug screening by mimicking the complex tissue microenvironment and allowing for better cellular communication than traditional 2D cell culture. 3D cellular spheroids have gained tremendous attention as tumor models for drug screening as they closely resemble the natural structural organization and drug resistance mechanisms. Hydrogels, gel-like crosslinked networks of polymers, are promising biomaterials with excellent biocompatibility, tunable porosity, and strength that can provide a platform to enable diverse 3D cell cultures. Here we take advantage of alginate-based hydrogels to develop a 3D cell culture platform for tumor spheroid culture, which can be scaled up for high-throughput high-content (HTHC), and can be integrated with a conventional microwell plate, allowing for both traditional assays and novel solution-based biosensing techniques. The aim of this work is to develop a 3D HTHC hydrogel culture system for tumor spheroid culture and integrate it with Janus particle immunodetection to overcome the difficult detection and analysis of exosomes, potential cancer markers, for drug screening. By combining Janus particle-based immunodetection, 3D hydrogel cell culture, and high-throughput high-content screening, this research will contribute to a dynamic exosomal detection platform and work towards advancing the efficiency of drug screening for clinical testing.

Studying the Effect of Cancer-associated Fibroblasts on Glioblastoma Cell Stemness

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Glioblastoma is an aggressive malignancy of the central nervous system in which the median patient survival time is about 20 months. Glioblastoma primary tumours display significant cellular heterogeneity including glioblastoma stem cells, vascular pericytes, cancer-associated fibroblasts and immune cells such as macrophages. Cancer-associated fibroblasts serve key roles in the tumour microenvironment, particularly in deposition of extracellular matrix as well as contributing to the proliferation and invasion of cancer cells. Their presence and function have been well understood in a number of extracranial tumours but are limited in tumours of the central nervous system. In regards to the origin of glioblastoma cancer-associated fibroblasts, given our previous findings, we hypothesize that glioblastoma stem cells may give rise to cancer-associated fibroblasts through mesenchymal differentiation. The possibility of cancer-associated fibroblasts originating from mesenchymal differentiation of glioblastoma stem cells is supported by studies which have shown that vascular pericytes that are closely related to fibroblasts, are also generated through differentiation of glioblastoma stem cells.

Through a series of in vitro experiments, we attempt to uncover and describe the origin of cancer-associated fibroblasts and their role in maintenance of the cancer stem cell niche in glioblastoma. Cancer stem cells are a subpopulation of malignant cells with self-renewal and differentiation capabilities and an immune-evasive phenotype. In glioblastoma, cancer stem cells are responsible for anti-cancer therapy resistance and tumour recurrence. Cancer stem cells within GBM tumours are therefore promising therapeutic targets. Hence, understanding the mechanisms by which these cells arise and are maintained is invaluable information in the design and selection of novel therapeutics.

Developing a Trifluoromethylation Strategy of Alcohols and Amines for the Synthesis of New Therapeutics and Agrochemicals

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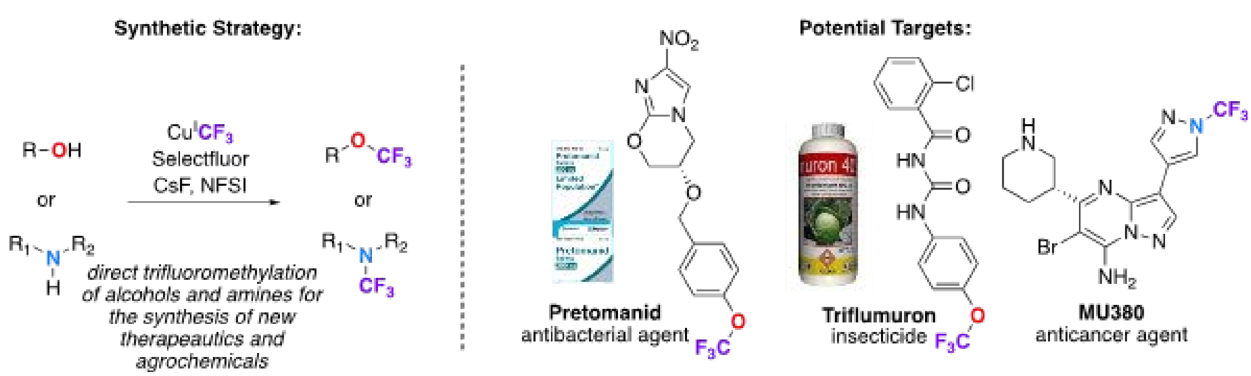
Trifluoromethylation is a prominent topic in the field of organic chemistry due to the abundance of the trifluoromethyl motif (CF3) in pharmaceuticals, agrochemicals, and other promising targets such as Pretomanid, Triflumuron, and MU380. The presence of these motifs results in heightened bio-reactivity, lipophilicity, and metabolic stability for these compounds. The addition of a trifluoromethyl group to an alcohol or amine can be used to affect the molecules properties, such as changing polarity, pKa, and bonding interactions. This can be useful when trying to make fine-tuned changes to a compound, such as during drug design. New methods for incorporating the CF3 group will allow for a wider range of access to these compounds. While there are several methods for trifluoromethylation, many have issues due to harsh reaction conditions, limited availability of reagents, low efficiencies, and limited scope. The goal of this project is to develop a methodology for the synthesis of trifluoromethyl ethers (ROCF3) and trifluoromethyl amines (R2NCF3) that is cost effective, safe, and applicable to a wide variety of compounds. The proposed method involves reacting CuICF3 with a variety of alcohols and amines to form the trifluoromethyl ethers and trifluoromethyl amines, respectively. Before exploring the trifluoromethylation reactions, the CuICF3 reaction was examined to ensure and optimize its formation. It was determined that to reliably synthesize the CuICF3 the reaction required a completely inert atmosphere in the glovebox. From there, an initial substrate screen was run for the alcohols and amines. Of these substrates, only the crude product mixtures for the secondary amines showed signs of potential product by 19F NMR spectroscopy. The compounds in these crude reaction mixtures were then isolated and analysis is ongoing. Based on the results of this analysis, the reactions with these secondary amines will undergo optimization through changes to reagents, equivalents, temperature, time, and solvents in order to achieve the desired product in high yield. Following this, the reactions with the alcohols and primary amines can be optimized while also determining the scope of these transformations. In the future, this method can then be used to access bioactive compounds more effectively while also promoting the development of new pharmaceuticals and agrochemicals.



Differences of Perceived Suicide Stigma Among Veterans Across Regions of the United States

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As suicide continues to increase for many demographics, stigma surrounding suicide continues to exist. Evidence suggests that stigma surrounding suicidal thoughts and behaviors (STBs) is higher within the veteran population compared to the civilian population. Researchers have examined the comparison of levels of STB stigma between veterans that live in rural environments and veterans that live in urban environments. Evidence suggests higher levels of STB stigma in rural environments. However, research examining the difference in levels of STB stigma between regions has not been conducted. The current study investigated potential differences in STB stigma between the regions of the United States, as well as different population sizes within each region. Additionally, we examined potential differences in STB stigma between veteran (n=253) and civilian (n=247) populations. We ran a moderation model to examine whether a region would moderate the relationship between veteran status and stigma. The model was not significant ($p = .497$); the pattern of results did not change when controlling for age or gender. We also ran a moderation model to examine whether the population would moderate the relationship between veteran status and stigma. The model was not significant ($p = .435$); the pattern of results did not change when controlling for age or gender. Findings suggest no difference in STB stigma between veterans and civilians, as well as no difference in stigma based on region and population. This is contrary to our hypotheses and prior research suggesting a difference in stigma between rural and urban environments. This could be due to our measure of stigma or the population that we surveyed which was willing to participate in a study regarding suicidal thoughts and behaviors. Further research is needed to explore updated measures for suicide stigma, as well as obtaining a sample that includes participants less willing to talk about suicide.

Voting Rights and Federalism: Understanding the California Voting Rights Act

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While Latino and minority populations in California continue to grow, their representation in elected government positions fails to reflect this growth. The disconnect between the two signifies the urgency and importance of having conversations regarding apportionment and equal representation among these communities. Since the passing of the California Voting Rights Act in 2002, over 88 cities across the state have been mandated under law to change their at-large elections to single-member district elections; in hopes of extending minority groups' protection from voter dilution while simultaneously increasing their voter turnout. The CVRA was created with the intent to expand voting rights protections provided under the Federal Voting Rights Act by altering existing forms of electoral systems to enhance the voting power of minority voters in local government elections. Per CVRA advocates, at large elections have historically reflected racially polarized voting that has prioritized the preferences of the white majority and left non-white minority voters at a systematic disadvantage. While cities continue to be placed under intense scrutiny and litigation threats for failure to change their electoral systems, debates as to whether such a change makes a significant difference in increasing minority voter turnout and representation at the local level concur equally. This research project aims to uncover and fill in the gap in knowledge regarding the relationship between the switch from at-large elections to district elections and their effect on minority voters and representation.

Identification of Biofilm Forming Microbes in CAUTIs in Mice through Amplification and Sequencing of the 16s Region

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Hospitalized patients have a higher risk of acquiring healthcare-associated infections, including Urinary Tract Infections (UTI). Of these nosocomial infections, 75% of UTIs are Catheter-associated Urinary Tract Infections (CAUTI) and nearly 25% of hospitalized patients require a urinary catheter, meaning that this type of infection is one of the most common. When a catheter is introduced into the bladder, it causes inflammation and damages the tissue. The body's healing response results in accumulation of host serum proteins, specifically Fibrinogen (Fg), in the bladder which deposit onto the catheter surface. Microorganisms present in the bladder utilize these deposited proteins as a scaffold for binding and as a nutrient source, allowing them to form a biofilm. The subsequent infection can eventually spread to the kidneys and bloodstream, resulting in a systemic infection. CAUTIs are typically treated with antibiotics and the temporary removal of the catheter. However, we have found that the longer the catheter remains in the bladder, the greater the microbial accumulation as well as the diversity of the present microbiome, making treatment more difficult. To manage the microbial accumulation, it is necessary to first identify the microorganisms responsible for the biofilm formation. For this, microorganisms were isolated from the bladders, kidneys, and spleens of infected mice 3, 7 or 14 days after infection. The DNA of the isolated microbes was then extracted. Afterwards, polymerase chain reaction was used to amplify the 16s region of the genome which were sent for sequencing and the microbe was identified using this sequence.

Visualising ATP Detection by Electrochromic Sensors

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Accurate and rapid point-of-care sensing is crucial for disease prevention, particularly in the context of hospital acquired infections, such as sepsis. Aptamer-based electrochemical biosensors offer a reliable means of detecting various biomarkers. The use of aptamers allows the binding to a target molecule with high specificity, facilitating direct sensing without the need for separation. In particular aptamer-based biosensors can be integrated into closed bipolar electrode (CBE) architectures as they allow coupling of electrochemical actuation with highly sensitive colorimetric readouts. Upon a specific target binding event, the resulting change in aptamer conformation changes the electrochemical response of the analytical cell, providing high selectivity, sensitivity, and robustness. Changes in the analytical cell are then translated to a change in the optical readout, providing a quantitative readout, using electrochromic sensing. This facilitates high level, accurate sensing whilst enabling RGB analysis using a smartphone and easy-to-use software.

In this project, our goal is to design and engineer an aptamer based electrochemical sensor for adenosine triphosphate (ATP) detection which can be integrated as the analytical cell in a CBE structure. First, we electrochemically deposit gold on indium tin oxide (ITO) electrodes, to generate an immobilization platform for thiol linked aptamers, by electrolyzing chloroauric acid solution. To validate the effectiveness of these methods, cyclic voltammetry and square wave voltammetry scans were conducted and gold deposition was confirmed by electrochemical reduction of gold oxide on the ITO surface. Subsequently, ATP selective aptamer (43-7) was immobilized onto the gold surface and square wave voltammetry experiments, for varying target concentrations, were performed. The presence of the target molecules led to significant decreases in peak current, indicating successful binding between the aptamer and the target molecule. This serves as a proof-of-concept experiment for the detection of ATP using an aptamer based analytical cell.

Overall, the closed bipolar electrode device, when connected in an analytical and readout cell configuration, holds significant potential for point-of-care applications, offering direct and efficient sensing without the need for complex sample separation, potentially finding important implications for rapid and reliable diagnostics.

Characterizing and Controlling Calcium Signaling Dynamics in Lymphatic Endothelial Cells

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Cell-to-cell communication is important to maintain blood and lymphatic vascular hemostasis and regeneration. Unlike in blood vasculatures, little is known about the role of calcium (Ca2+) signaling dynamics in lymphatic endothelial cells (LECs) under different physiological conditions. Here, we characterize Ca2+ signaling dynamics on LECs under different ranges of physiological shear stresses. Then, we use ion-exchange membrane (IEM) modules to deplete/enrich extracellular Ca2+ to control the cellular action potential. Activation of mechanotransduction pathways in the cells is achieved by introducing flow through a microfluidic pump system. Live imaging of the LECs during the experiments showed synchronous Ca2+ spiking within the cells. Characterization of the Ca2+ dynamics has shown simultaneous spiking during ion depletion and sequential synchronistic signaling after cell morphology has been physically altered. Comprehending how extracellular potential and stress stimuli influence the patterns of Ca2+ signaling provides a deeper understanding of the cellular communication needed for controlled lymphangiogenesis and future applications in tissue regeneration.

Ensuring Gracefulness in Withdrawals: The Dynamics of the Early 1970s American Withdrawal from South Korea

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The Nixon administration's partial withdrawal from South Korea in 1971 was an unprecedented act for American peacetime foreign policy in East Asia. It can be partially attributed to Nixon's ambition to implement the Nixon Doctrine, Congressional inclination to do some military cuts, and America's quasi-isolationist mood during the latter stages of the Vietnam War. Regardless of the cause, its successful implementation and eventual support from South Korea were also unprecedented, yet, a matter with little coverage in American foreign policy.

Through research of government documentation (particularly that of the Nixon Library and the History of the Foreign Relations of the United States [FRUS] database), academic analyses, and an understanding of the greater regional patterns going on at the time, this research found that the withdrawal's success came from a combination of effective American posturing (insofar as objectives, consulting and aid offered to South Korea to make up for the withdrawal), poor South Korean negotiation tactics, and greater political pressures going on at the time (originating from the Nixon doctrine's goals and the US congress). Hence, South Korea's initial hostility towards the withdrawal gradually shifted towards reluctant acceptance and compliance.

Barring a few exceptions, the United States got what they wanted from this withdrawal, while South Korea was forced to ease up their demands until the final agreements were shaped in a way that favored the US all the way down to diction choices. In turn, "graceful" peacetime withdrawals by large states from their allies are possible through robust planning, credible pre-existing motivators, and "carrot-and-stick" tactics that compel allies to comply and participate. However, it is difficult to ensure that allies agree with every detail of a "graceful" withdrawal and/or may attempt to push back when in disagreement with said details. Finally, these same factors again shaped US withdrawal attempts from Korea in 1978 and 1991.

Smart Shopper: Healthy Food Choices with a Multi-level Hierarchy and Recommendation Algorithm

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Sustaining a healthy and affordable diet is a challenge for many Americans who must balance their nutritional needs against costs. This balancing act is a challenge due to the amount of information one must consider (e.g. pricing, sales, nutritional value, nutritional goals) to make the best possible choice. In this project, we treat this problem as an optimization problem over all possible product selections. Using this approach, one strategy to improve eating habits is to replace particularly unhealthy food items with healthier and/or less-expensive options. To achieve this automatically through a recommendation algorithm, we required an organized, traversable data structure containing all possible products. Thus, we developed a multi-level food hierarchy to support efficient search for suitable substitutions. The hierarchy is based on the five MyPlate food groups which are then broken down into more specific categories, allowing recommendations to be made at different levels of specificity. The hierarchy and recommendation algorithm work in tandem to offer potential substitutions to a user's grocery items that can range from healthier versions of the desired product to items in an entirely different food group. While the decision of which product to choose is ultimately up to the user, we strive to design our application to provide relevant information and support their agency. We plan on conducting interviews with local students to understand the suitability of the substitutions recommended by our algorithm. By asking participants to evaluate the quality of our system's recommendations, we will be able to clarify the strengths and weaknesses of the algorithm's current iteration and make pertinent alterations to improve it.

Optimizing the Synthesis of Tetra-2-pyridinylpyrazine and its Iron Complexes for Use in Redox Flow Batteries

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As the United States implements more renewable energy sources, a new problem is introduced: the storage of energy between times when it is generated and needed on the grid. Redox flow batteries (RFBs) have shown promise as a part of the solution. RFBs have their electroactive materials remain fully dissolved in solution throughout the entirety of the charging and discharging cycles in comparison to a battery such as lithium-ion, where at least one electrode is a solid metal species. Prototype flow batteries have used a water-based electrolyte solution, but there are limitations that prohibit the large-scale implementation and usage of these batteries, namely operating temperatures and maximum energy densities. Water is electrochemically stable across ~1.5 V, whereas organic solvents have much larger stability windows. For example, acetonitrile is stable across ~5 V. Therefore, the push to develop a flow battery in non-aqueous solvents, such as acetonitrile could be beneficial, allowing for increased battery energy density. However, in order to accomplish this, soluble electrolytes must be developed that have extremely high or extremely low reduction potentials. Our lab sees metal coordination complexes of the ligand tetra-2-pyridinylpyrazine (tppz) as a promising candidate for non-aqueous flow batteries (NARFBs) due to previously reported complexes with very high oxidation potentials, and a redox-active ligand. Our current work seeks to increase the yield of the tppz from a new synthetic route involving copper. Initial reactions and characterization have been performed to complex tppz with earth-abundant metals, and explore its potential as an electrolyte for NARFBs.

Improving Network Inference for Protein Structural Classification

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A protein is a sequence of amino acids that folds into a 3D structure. Protein structure networks (PSN) are powerful models of 3D structures. In a PSN, nodes are amino acids, and edges are spatial proximities between the amino acids in the 3D fold. A well-established computational task when studying PSNs is protein structural classification (PSC), which involves categorizing proteins into pre-defined structural classes based on their sequence, 3D structural, or PSN features. State-of-the-art PSC approaches are PSN-based. However, traditional PSN approaches for PSC model the 3D structure of a protein as a static PSN, disregarding the dynamics of the protein folding process. Recently, our lab published a novel approach that captured the dynamics, by modeling a protein 3D structure as a dynamic rather than static PSN, which resulted in improved PSC accuracy [1].

A dynamic PSN is constructed as follows [1]. Given a protein sequence and its 3D structure, incremental sub-sequences of the protein are defined, with the first sub-sequence containing the first k amino acids of the entire sequence, the second sub-sequence containing the first 2k amino acids of the entire sequence, the third sub-sequence containing the first 3k amino acids of the entire sequence, etc. Then, each sub-sequence is modeled as a network snapshot. Collection of all snapshots forms the dynamic PSN for the given protein. Then, the analysis of changes in network structure between the different dynamic PSN snapshots is meant to capture the dynamics of the protein folding process. In the published study, the value of the network inference parameter of five (i.e., k=5) was used.

To test the hypothesis whether dynamic PSNs would yield higher PSC accuracy than static PSNs, an evaluation was conducted on 72 PSN datasets encompassing ~44,000 PSNs [1]. The PSN labels (i.e., structural classes) used for classification are based on CATH and SCOPe protein domain categories (e.g., alpha, beta, or alpha-beta) that the PSNs belong to. PSC accuracies were measured via misclassification rate, for both dynamic and static PSNs, and for each PSN dataset. Dynamic PSNs outperformed all existing static PSN approaches on 58 out of the 72 the datasets.

In our newest work, we (specifically Jennifer Morones) build upon this published study. First, we replicate the published dynamic PSN results using the exact evaluation. This includes k=5 for the network inference parameter. We compare the 72 PSC accuracy scores (corresponding to the 72 PSN datasets) obtained from the replicated analysis to the published ones, to ensure a correct reproduction. Indeed, the results match.

Second, and more importantly, we extend the published study by evaluating additional values of the network inference parameter (k=4, 6, 10, 15), to test the effect of this parameter on PSC accuracy. At the time of abstract submission, results are pending and will be discussed during poster presentation. Beyond our analyses, dynamic PSNs have the potential to guide future PSC method development and also provide insights into protein folding.

[1] https://doi.org/10.1002/prot.26349

The Role of Nephronectin in Cell Fate Determination During Retinal Regeneration in the Adult Zebrafish

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Mentor:
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Retinal degenerative diseases are the leading cause of irreversible vision loss, affecting approximately a billion people worldwide. These conditions are often progressive and irreversible because humans do not possess an innate regenerative capacity in the central nervous system. However, some vertebrates, such as the zebrafish, have a robust capability to regenerate any retinal cell type following damage. This regeneration involves the resident Müller glia responding to injury by reprogramming and reentering the cell cycle to produce neural progenitor cells (NPC) that proliferate and differentiate into the lost cell types. Because humans also possess Müller glia, there is the potential to stimulate a regeneration response in humans. While much attention has been paid to understanding the intracellular mechanisms of retinal regeneration, the role of the extracellular environment remains poorly understood. The extracellular matrix (ECM) plays crucial roles in retinal development and homeostasis and should influence the regenerative process, which recapitulates retinal development. One ECM component that is upregulated in expression following retinal injury is nephronectin (NPNT). To study its role, we performed in vivo morpholino-mediated gene knockdown to repress NPNT expression, and observed the ensuing changes in regeneration and the cell types produced by the NPCs.

We dark-adapted albino zebrafish for 14 days, followed by exposure to constant bright light for 4 days, effectively killing photoreceptors, after which the fish were kept under normal light conditions for 7 days. EdU, a thymidine analogue which is incorporated into the DNA of proliferating cells, was injected intraperitoneally at either 72h or 96h of light damage, or at 1 day recovery, to label proliferating cells. Following tissue collection, the retinas were cryosectioned, immunolabeled for EdU and cell-specific proteins, and analyzed by confocal microscopy. Knocking down NPNT expression leads to decreased numbers of EdU+ cells relative to controls, consistent with our previous data showing decreased NPC proliferation. Moreover, there is a significant decrease in the proportion of HuC/D+ amacrine and ganglion cells generated at 72h light damage in the npnt-morphant retinas. These data suggest that NPNT regulates proliferation, as well as cell fate, during regeneration. Investigating NPNT and other ECM components will allow us to further understand the ECM’s role in regeneration and its future potential for human therapeutics.

Modeling 5G Interference on Weather Radiometer

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Organizations such as NOAA and NASA use sensitive weather radiometers to measure meteorological data such as water vapor in the atmosphere. The weak signals located within the 23.6-24 GHz band which the radiometers detect require the equipment to be extremely sensitive, in turn making the radiometers vulnerable to outside interference. The recent introduction of 5G to the 24.25-27 GHz band has raised concern in NOAA and NASA since the comparatively much stronger 5G signals are likely to interfere with the measurements of the radiometers. This interference on the radiometers would result in less accurate meteorological predictions with some sources saying the interference sets the technology back to the equivalent of the 1980s. However, limiting the power of the 5G signals to avoid interference could result in signals that are too weak to transmit data effectively.

To understand how 5G interference affects radiometers, I created a model based off the Joint Polar Satellite System Advanced Technology Microwave Sounder, a multichannel radiometer used by NOAA, where the first channel of the JPSS ATMS measures at a center frequency of 23.8 GHz, close to the 5G band. With the target signal and interference having different center frequencies and bandwidths, I introduced the interference to a Dicke radiometer model using realistic values and tracked how the interference changes the power throughout all stages of the radiometer. I finally found the output power of the radiometer with this interference based on 5G signals. These findings can provide the basis for a complete interference protection criteria which finds the best ways to limit harmful interference.

Enhancing Liquid-Liquid Phase Separation through Confinement and Crowding

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Liquid-liquid phase separation is a phenomenon that underlies the formation of biomolecular condensates such as membrane-less organelles inside the cytosol of living cells. In this research, we conducted molecular dynamics simulations to investigate complex coacervation --- the process of liquid-liquid phase separation of polyelectrolytes (here representing the charged polymers in cells) --- with a specific emphasis on their behavior under confinement and in the presence of crowding agents. In this model, the system was confined within a box, containing both oppositely charged polyelectrolytes and solvent components. We currently are working on the addition of a crowding agent to better represent the cytosol environment. The computational system was constructed by assembling 400 polyelectrolyte chains, each composed of 10 monomers, with scaled charges ranging from 1.50 to 3.0. These chains were immersed in a solvent containing 44,000 atoms. The polyelectrolyte chains were modeled using the Kremer–Grest bead–spring model with the modifications of Stevens and Kremer for polyelectrolyte simulation, while the interactions between the solvent and polymers were described using the Lenard-Jones potential. Charged interactions are computed using the particle–particle—particle–mesh (P3M) algorithm for long-ranged interactions. The simulations were carried out within the NVT ensemble, employing a Langevin thermostat to control the system's temperature. The system was analyzed with order parameters of density profiles and radial distribution functions. The results show that at lower values of q (corresponding to effectively higher temperatures), the system exhibited a gas-like behavior, characterized by the diffusion of polyelectrolytes across the system. However, as the charge density increases, the polyelectrolytes condense, and form a dense liquid or arrested solid. Sufficient decrease in the charge density of polyelectrolytes ultimately results in a uniform distribution of them in solution, as anticipated for fluids which pass through a critical temperature. In the end, we extracted the lower and upper bounds of polyelectrolytes densities by a fitting step function. This enabled us to construct the phase diagram of the polyelectrolytes to determine the critical point through the phase transition from a liquid or gas phase to a solid phase. These findings provide insight into understanding liquid-liquid phase separations in cells.

Tuning Amine-based Polymer Catalyst for CO 2 Conversion through Structural Modification via Quaternization

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As global temperatures continue to rise, reducing the Carbon Dioxide concentration in the atmosphere becomes an increasingly prominent global concern, with current sorbent-based methods for removing CO2 from the atmosphere being inefficient and energy intensive. Developing a catalytic membrane that can integrate CO2 capture and conversion into a single unit process has the potential to offer a more energy efficient and cost-effective alternative for reducing the CO2 concentration in our atmosphere. Through previous work, poly(4-vinylpyridine) (P4VP) based membranes have shown to be permeable and selective for CO2 separation from mixed gases and are catalytically active for cyclic carbonate synthesis at mild temperatures. The quaternization of P4VP with alkyl halides can tune CO2 separation performance and catalytic activity. This work focuses on how different alkyl halides as well as structural modification of the P4VP samples affect the catalytic activity of P4VP for the model reaction of cyclic carbonate synthesis from CO2 and epichlorohydrin (ECH). P4VP samples with varying chain lengths and halide groups were tested within batch reactions for their catalytic activity in dry and wet conditions. A concern stemming from these experiments was the stability of longer chained quaternization samples, which out preformed shorter chained samples with respect to cyclic carbonate production at the cost of being more soluble. To tackle this challenge various crosslinked quaternization samples with varying chain length and halide group were created and tested in dry and wet conditions. Wet conditions continued to reduce productivity due to the halogen shielding the functional group from water, limiting its ability as a hydrogen bond donor. Catalyst samples using a halogen located below the previously tested halogen in the halogen group column enabled higher production even in wet conditions, and by utilizing the crosslinking quaternization samples were found to be less soluble, which is ideal for their implementation into membranes. Findings from this work gives insight into the development of more efficient membranes for the capture and conversion of CO2 as well as contribute to the further tuning of amine-based polymer catalysts.

Automatic Characterization of Software Exploits

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For vendors whose software systems have been affected by vulnerabilities, it is important to know the exploitation code that exposes the consequence of the issue as well as to provide an indication of the vulnerable part of their code that can be exploited. By knowing this, software vendors can be more prepared to counteract potential attacks. Along with these exploits, software vendors also need a textual description that explains the steps to reproduce the security breach, and other metadata, such as vulnerability type. To do so, software vendors typically search for such executable exploits and their metadata in online databases, mailing lists, or issue tracking systems. Even though the information obtained from these sources is valuable and valid, it is not organized in a standardized way that could be easily searchable.

Thus, this ongoing research project aims to investigate the use of NER (Named Entity Recognition) to extract exploit-related metadata. The goal is to create an accurate database that can be used to replicate vulnerabilities. To achieve this goal, we retrieve exploits from a variety of online sources, such as mailing lists, issue tracking systems, and exploit databases. Subsequently, we create a labeled dataset of annotated exploits to train a machine learning model to recognize this metadata.

Our contributions throughout the summer include deciding which entities/metadata we want the project's NER model to identify, looking into related works to find what is currently out there when it comes to NER and cybersecurity, and contributing to the project's research paper. When deciding which NER entities we could use we extracted links that were organized by domain, we looked through around 100 examples of each domain and what they contained. If a certain piece of metadata had a constant factor within that domain group it would be added to the Excel sheet. Issues did arise since different domains use different words to describe the same thing, one website might have a “description” section while another has one that is called “Overview” which led to some redundancies in the sheet.

Nanoparticle Mediated Reprogramming of Cells to Fight Cancer

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Mentors:
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Fibroblasts are important for maintaining the structure and function of tissues, but when cancer signals are present, they can adopt an activated phenotype marked by the expression of biomarkers such as fibroblast activation protein alpha (FAPα) and alpha smooth muscle actin (αSMA). These cancer-associated fibroblasts (CAFs) are an abundant component of the tumor microenvironment (TME) in many solid tumors, and are known to promote tumor progression, metastasis, immunosuppression, and treatment resistance. However, a subset of CAFs (e.g., CAV1high CAFs) are also known to promote anti-tumor activity. Nanoparticles (NPs) have been used to target cells due to enhanced targeting specificity, high payload, protection of delivered biomolecules and imaging capabilities. The objective of this study is to investigate fluorescein isothiocyanate (FITC) labeled silica (FITC-SiO2) NPs as a platform for engineering fibroblast-specific antibodies to enable targeting and reprogramming of CAFs into a tumor-restraining state.

FITC-SiO2 NPs, were synthesized using a modified Stöber method. FITC-SiO2 NPs exhibited unchanged hydrodynamic size of ~132 nm and fluorescence intensity for a week in water, indicating aqueous stability and sufficient fluorescence for longitudinal imaging. Proof of concept antibody conjugation was demonstrated by functionalizing FITC-SiO2 NPs with COOH groups and subsequently conjugated with immunoglobulin G (IgG) antibody using EDC/NHS chemistry. Antibody bioconjugation was confirmed by visible agglomeration when mixing IgG conjugated FITC-SiO2 NPs with protein A biobeads. In contrast, NPs without IgG and mixed with protein A biobeads exhibited the fluorescent of NPs without any agglomeration.

FITC-SiO2 NPs conjugated with FAP antibody are being investigated for their ability to target and reprogram TGF-β-transformed CAFs in vitro. NIH3T3 murine fibroblasts were cultured and treated with human recombinant TGF-β. The activation of the murine fibroblasts following TGF-β treatment were evaluated by qPCR and immunofluorescence staining. A pilot study to investigate the biodistribution of NPs and evaluate their performance in vivo is ongoing.

Nanoscale Formulation of Corrective Hormones for Bblood Glucose Control

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Recent medical advances have highlighted the efficacy of Glucagon-like peptide 1 (GLP-1) analogs as a treatment for type 2 diabetes (T2D). This hormone lowers glucose levels by promoting insulin secretion, suppressing the release of glucagon, and sustaining satiety by slowing gastric emptying leading to increased control of blood glucose levels and a decrease in BMI. However, the pairing of GLP-1 treatments with other blood-glucose-lowering therapeutics has been shown to significantly increase an individual's risk of hypoglycemia. To address the need for glucose-dependent potency of GLP-1 therapeutics, we have incorporated mechanisms to enable activity to be shut off when function is not needed, thereby lowering the risk of hypoglycemia. Accordingly, by modifying the sequence and chemistry of GLP-1 variants, our design is intended to suppress functional activity at low blood glucose. Structurally, GLP-1 is composed of two alpha helices linked by a short linker region. We identified modification sites near the C-terminus, N-terminus, or within the linker region, that were determined not critical for receptor activation or binding based on alanine scanning studies. We verified successful synthesis of the peptide through mass spectroscopy and developed assays to determine glucose-responsive structural and functional properties. Circular dichroism testing was done to verify the alpha-helical structure of the peptide, and further tests were done at varying glucose concentrations in order to observe how the molecule changes conformationally when glucose is present. Success in producing a glucose-responsive GLP-1 analog would introduce a safer therapeutic for individuals with T2D dependent on insulin therapy, allowing for improved glycemic control and satiety without fear of hypoglycemic incidents.

Donnan Dialysis for the Recovery of Metal Ions utilizing EDTA as a Complexing Agent

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Lithium-ion batteries may contain a range of metals including Co, Mn, Cu, Ni and of course Li (Backhaus, 2021). Production of these metals through mining and purification may lead to long-term ecological damage (Jacoby, 2019).Recycling of metals in batteries could decrease need for mining of these materials. Unfortunately, most recycling methods will likely include dissolving the battery components to create a complicated mixture containing metal ions. Thus, recycling will require a method for isolating the desired ions. This work explores whether can separate metals such as Cu2+, Ni2+, Co2+, Mn2+, and Na+. Prior studies showed that Donnan Dialysis through cation-exchange or anion-exchange membranes can effectively separate ions (Bruggen, 2018). This research explored using ion transport through Nafion N-115, a widely used cation-exchange membrane to separate the metal ions with the same charge. However, the Nafion membrane itself shows little selectivity for separating ions with the same charge. To achieve selectivity, ethylene diamine tetraacetic acid (EDTA) was added to the solutions to selectively bind to specific metal ions. Complexation with deprotonated EDTA will create a metal ion-EDTA complex that is negatively charged so the complex will not pass through the cation-exchange membrane. In initial experiments, the Nafion membrane separated a source phase containing equimolar copper (II) nitrate and sodium nitrate from a receiving solution containing nitric acid, with the objective of passing Na+ through the membrane while rejection Cu2+. Without the addition of EDTA, Cu2+ and Na+ moved through the membrane at approximately rates. After replacing the sodium nitrate with the EDTA disodium salt, the selectivity for Na+ over Cu2+ transport was 20. The same process was applied to a second feed solution containing manganese (II) chloride and cobalt (II) chloride, with a receiving solution containing hydrochloric acid. As EDTA selectively binds Co2+ over Mn2+, these experiments aimed to achieve selective Mn2+ transport. The same phenomenon occurred with the selectivity for Co2+ over the Mn2+ in the solution, which increased after the addition of the complexing agent. Without EDTA, the Mn2+/Co2+ selectivity was around 1. These experiment clearly show that the addition of a negatively charged complexing agent can lead to selective dialysis, which may lead to methods for purifying transition metals during battery recycling.

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Simulated Hydrogen Gas Adsorption in Soft Porous Coordination Polymers

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Mentor:
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Adsorption, the accumulation of molecules at the surface of materials, is a process that has applications in drug delivery, separations, and energy storage. Soft porous coordination polymers (SPCPs) are a class of material that demonstrates the ability to adsorb due to their porous nature. SPCPs are a new material of interest and therefore there is a need to identify and characterize their molecular qualities before any experimental trials. Here we report hydrogen gas adsorption intake quantities as well as pore size, volume, and surface area for select SPCPs. Simulations show that crystalline structures exhibit higher intakes than amorphous structures. This is in part due to the crystalline structures possessing larger pore size, volume, and surface areas. Temperature and pressure also play an important role in intake quantities; data shows at lower temperatures and higher pressures, SPCPs adsorb better. The connectivity between polymer chains also influences simulation results. The connection or linker types displayed consistent results for crystalline structures until cryogenic temperatures. However, for the amorphous structures, these temperatures did not affect the hydrogen gas adsorption trends. These results portray key material characteristics that are vital to progression in real-world applications. The assessment of hydrogen gas adsorption ability is extremely important for SPCPs potential use in the hydrogen energy economy. For future research, a new area of interest is the relationship between a molecule's crystalline and amorphous structures under fluctuating pressure.

Microenvironmental Effects on the Mechanical Behavior of Cancer Cells

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Mentor:
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The impact of the host environment on cancer cells has been extensively studied. However, the biophysical and mechanical components of the metastatic cascade, e.g., of breast cancer cells to the brain, is poorly understood. In this study, we investigated the effect of different environments on invasive and aggressive cancer cells through conditioned media cultures with human normal and cancerous cell lines, shear stress assays, live imaging, and digital image correlation to understand the mechanical differences between brain and breast cancer cells under varying environmental conditions and how these differences influence their mechanical properties. We hypothesized that cancer cells would acquire mechanical properties resembling those of the environment they are exposed to. To test this, we cultured brain cancer cells (U87, glioblastoma) in a normal breast cancer environment (conditioned media from MCF10A mammary epithelial cells) and breast cancer cells (MBA-MD-231, triple-negative breast cancer) in a normal brain cell environment (conditioned media from SV40T astrocytes). The cells were subjected to conditioned media for 24 hours prior to assessing their mechanical properties within their respective environments. Subsequently, a shear assay method was employed to apply stress to the cells and observe their response and resistance. Digital image correlation and data analysis was performed using DaVis and MATLAB softwares. The results were utilized to visualize cell deformation and to characterize their mechanical properties. Notably, the cells exhibited responses to the different environments, indicating changes when placed in unfamiliar conditions. Surprisingly, even cells of the same type cultured in the same environment exhibited varying responses, indicating intra-cell-line heterogeneity.

This study sheds light on the dynamic nature of cancer cells and their ability to adapt to different microenvironments. By understanding how cellular mechanical properties are influenced by the host environment, we gain valuable insights into cancer and its complex mechanisms. Further research in this area is crucial for advancing our understanding of metastasis and developing innovative diagnostic and therapeutic approaches.

Increasing Safety in Lithium-Ion Batteries with Gel Polymer Electrolytes by Modeling Thermal Runaway

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As the climate continues to be affected by anthropogenic greenhouse gas emissions, it is necessary to design power systems with low emissions in mind. Rechargeable battery systems are desirable due to low emissions when charged with low-carbon generated electricity, but they sacrifice the high energy density offered by fossil fuels. High energy density is a critical factor in designing viable systems that produce significant power without being too large for portable use. Lithium-ion batteries are favorable due to their high energy density when compared to other rechargeable batteries. However, the common use of organic liquid electrolytes in lithium-ion batteries puts these systems at risk of undergoing thermal runaway triggered by overuse, external heating, short circuits, or other factors. Thermal runaway is the cause for many safety concerns, which may shift public opinion away from widespread use of rechargeable battery systems as power sources. The use of gel polymer electrolytes has been studied to increase the safety of lithium-ion batteries by decreasing the risk of triggering thermal runaway. To understand this process and qualify how gel polymer electrolytes contribute to the safety of lithium-ion batteries, COMSOL Multiphysics was used to create a simplified model of thermal runaway in lithium-ion batteries. The model uses Arrhenius-type equations factoring in heat generated from the degradation of the electrolyte, anode, and cathode. The model was initially made to be two-dimensional and only based on thermal equations. The simplified model will be used to study the effect of various polymer distributions within gel polymer electrolytes on thermal runaway. The study will focus on a lithium-ion battery with a gel polymer electrolyte composed of polymerized polyethylene glycol diacrylate (PEGDA) suspended in a liquid electrolyte comprised of $LiPF_6$ in ethylene carbonate, dimethyl carbonate, and ethyl methyl carbonate (EC:DMC:EMC). Once the simplified model is validated against lab experiments, it can be expanded to more complicated systems and varied electrolyte compositions. The expanded model will include coupled electrochemical and thermal reactions as well as a more detailed, three-dimensional version of the battery makeup to include the separator and solid-electrolyte interface.

Investigating Rare Earth Element Mineralization Within Fenite Alteration Zones

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Rare earth elements (REEs) play a critical role in the expansion of clean energy technology. These elements form key components of batteries for electric vehicles and other next-generation energy storage devices, but their low concentration throughout Earth's crust requires inefficient, energy-intensive extraction processes. In the last few decades, carbonatites—a carbonate-rich subset of igneous rocks—have been shown to harbor the most abundant REE deposits in the world. Carbonatite complexes have been studied extensively, but little attention has been given to the nearby rocks that are chemically altered by the intrusion of carbonatite magma. These rocks, known as fenites, may show a similar REE enrichment and represent an untapped reservoir of key elements and REE-bearing minerals that can help to accelerate the transition to a clean energy future.

Here, we investigate the movement and concentration of REEs in three carbonatite complexes in China (Miaoya, Maonuiping-Dagudao, and Bayan Obo) and their spatially associated fenite alteration zones. Combining bulk rock, solution-mode trace element and isotopic analyses obtained via multicollector-inductively coupled plasma mass spectrometry (MC-ICP-MS) with in-situ analyses obtained via laser ablation (LA) MC-ICP-MS, we can investigate both the petrogenetic relationship between the fenites and their associated carbonatites and the partitioning of trace elements in minerals dominating the bulk rock (calcite, amphibole, clinopyroxene).

Bulk rock analysis of fenite samples from the Maonuiping-Dagudao deposit has revealed extreme light REE enrichment, with certain areas of the fenite alteration zone exhibiting nearly sevenfold enrichment—as measured by total REE concentration—compared to the associated carbonatitic intrusion. The bulk rock trace element results also validate analogous data obtained by LA-ICP-MS for calcite, amphibole, and clinopyroxene, which provide insight into the phases controlling the REE budget in these fenite alteration zones and carbonatite complexes. For all three minerals, chondrite-normalized REE profiles are similar and show variable degrees of REE enrichment, with calcite controlling the mass budget for light REEs, while amphibole and clinopyroxene show heavy REE enrichment.

In-situ Pb isotope ratios obtained from the studied complexes indicate open system behavior, involving metasomatism and/or crustal contamination. For both Maonuiping-Dagudao and Bayan Obo, in-situ Pb isotope ratios for amphibole are distinct from those for corresponding whole rock and other phases (clinopyroxene, calcite). Future work will involve obtaining in-situ Sr isotope ratios of the different minerals, as well as the δ11B (‰) isotope compositions of fenites and associated carbonatites, to better distinguish between the roles of metasomatic activity and crustal contamination in the petrogenesis of the carbonatite complexes. Through the juxtaposition of bulk rock and in-situ trace element analyses, we have been able to gain a heightened understanding of the distribution of REEs between the fenites and their associated carbonatites, thus providing valuable insight into the future use of these complexes as reservoirs of economically and technologically critical elements.

Efficient Synthesis of N-(2-picolyl)picolinamide Ligand and Application in Organometallic Transformations

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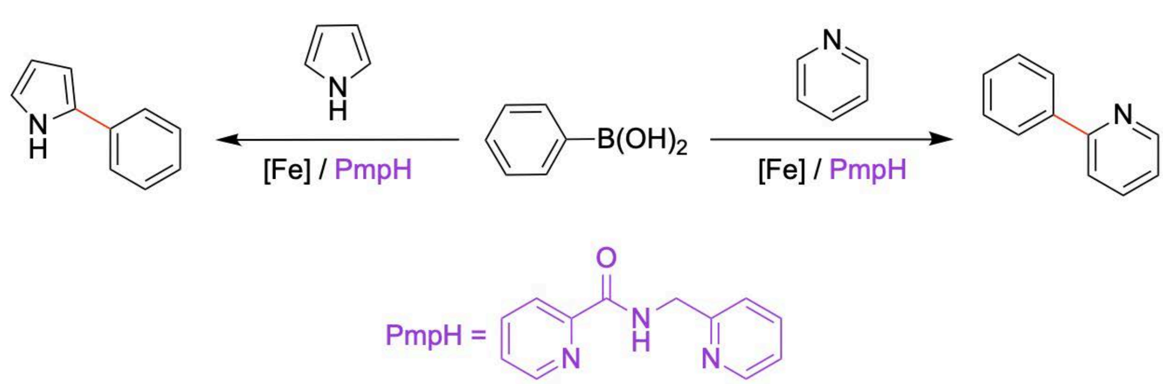
The use of tridentate ligands in organic catalysis is a promising area of organic chemistry with virtually infinite scope. Tridentate ligands feature three atoms that can coordinate to metals to form metal complexes and. Once formed, metal-catalyzed synthetic transformations use these metal complexes to make new bonds such as carbon-carbon bonds. The goal of this research is primarily to assess ways in which N-(2-picolyl)picolinamide (pmpH) can be used in organic catalysis to form new bonds or improve existing chemical syntheses. Applications of the pmpH ligand in organic catalysis may lead to the creation of novel synthetic processes that could be safer, more environmentally friendly, and more atom-efficient. An effective synthesis of pmpH was carried out and optimized before assessing the ligand in organometallic reactions. The pmpH ligand was synthesized most successfully using 2-picolylamine, ethyl 2-picolinate, and a catalytic amount of glacial acetic acid at 120–150 °C for 4 hours. The procedure does not require a solvent, is time-efficient, and is relatively straightforward. 1H NMR spectroscopy as well as IR spectroscopy indicated that pmpH was synthesized successfully in moderate yield (50-80%). This research's initial complexations were focused on pmpH coordinated with iron (III) sources. An iron-mediated procedure for the arylation of pyridine and pyrrole was adapted to use pmpH. The results show that there has not been a successful arylation up to this point. Optimization of these reactions is ongoing and will include purification of starting materials and recrystallization of pmpH. If successful, this application of pmpH would create a new route to the synthesis of biaryl compounds, which have a wide range of use in the assembly of pharmaceuticals, natural products, and agrochemicals.

Current Organometallic Application of PmpH[2]



NASA FLOATing DRAGON Challenge: Autonomous Navigation of a Parafoil from a High-Altitude Balloon

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High-Altitude Balloons (HABs) are a method of collecting large amounts of scientific data in the atmosphere. The data collected can sometimes be too much to be transmitted back from the balloon, so data vaults must be dropped from the balloons. A system for targeted delivery of these data vaults is necessary in order to mitigate the risks associated with dropping an uncontrolled package from 120,000 ft. NASA put out a design competition called FLOATing DRAGON (Formulate, Lift, Observe, And Testing; Data Recovery And Guided On-board Node) for universities to design a system capable of completing this task. The system designed by the University of Notre Dame team was selected as a finalist in January and construction of the system began. This summer, the system was finalized and tested, and it will be launched in Fort Sumner, NM by NASA on August 9.

The system consists of a deployer and a node. The deployer is permanently mounted to the gondola and it holds the node in place until it is time to release. When the deployer receives a signal from the gondola of the HAB, it releases the node. Upon release, a parachute deploys to control the initial part of the descent. After the node reaches an altitude where the air density is high enough, and the winds are low enough, it will transition to a parafoil and begin the steered part of the descent. The parafoil is steered by two servo motors that pull the brake lines of the parafoil causing it to bank and turn in the desired direction. The servos are controlled by the flight computer, which consists of a Raspberry Pi and Arduino Nano.

Regulation of Synaptic Activity through a CB1 Receptor-Dependent Mechanism in Fragile X Syndrome Induced Neurons

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Fragile X Syndrome (FXS) is a rare inherited developmental disorder that leads to learning disabilities in affected individuals. FXS is caused by a trinucleotide CGG repeat mutation following the promoter region of the Fragile X Messenger Ribonucleoprotein 1 (FMR1) gene. Methylation of the promoter due to this repeat mutation inhibits the transcription of the FMRP protein, which influences neural plasticity and cognitive development. We have previously found decreased activity of the Cannabinoid Receptor Type 1 (CB1R) in FXS neurons, causing an increase in cyclic adenosine monophosphate (cAMP) and a subsequent increase in the protein kinase A mediated phosphorylation of synapsin-1 (syn1), leading to decreased recruitment of synaptic vesicles to the presynaptic terminal. Therapeutics designed to correct the CB1R pathway such as reduction of cAMP levels by overexpression of phosphodiesterase (PDE) or a Gi-DREADD, CB1R activation by THC and WIN55, and protein kinase A inhibition by H89, are predicted to restore levels of phosphorylated synapsin-1, cAMP, and synaptic vesicles in FXS induced neurons, rescuing the wildtype phenotype. We have found through preliminary confocal imaging of Pink Flamindo (a fluorescent reporter for cAMP levels) and western blot analysis for phospho-syn1 levels that, in a singular trial using low cell-density coverslips, PDE may not restore concentrations of cAMP and phospho-syn1 levels in FXS iNs. Further experiments using higher cell-density coverslips will be completed with PDE involving both FXS and corrected human neurons. To supplement our study, FMR1 and CNR1 will be individually knocked out in wildtype iPS cells and neurons derived thereof via CRISPR/Cas9. These investigations will contribute to further studies involving the CB1R pathway and its relation to FXS.

Optimizing Dosage of VRK-1 Inhibitory Drugs for Inducing Cellular Senescence

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Pancreatic ductal adenocarcinoma (PDAC) is a rare cancer that has a very high mortality rate and poor treatments. The NIH estimates 64,050 new cases and 50,550 deaths in 2023. The median survival rate even with treatment is 10-12 months. The current standard of care for PDAC is gemcitabine. Gemcitabine disrupts DNA replication which induces apoptosis and violent cell death.The violent cell death caused by Gemcitabine is hypothesized to lead to the harmful side effects of treatment. Gemcitabine, although the current standard of care, is very toxic and often causes more damage to the patient than good. We believe that if cellular senescence is induced rather than apoptosis the side effects to treatment can be mitigated. Cellular senescence is the state in which a cell permanently stops dividing but does not die. If senescence can be induced in cancer cells then the cancerous cells will stop dividing and allow the immune system to start clearing out the tumor. The Vaughan lab has discovered that disrupting lamina induces a blebbing phenotype which in turn causes senescence. Nuclear blebbing is a protrusion of the nuclear membrane usually due to disruption of nuclear envelope proteins.. We are inhibiting VRK-1 with VRK-IN-1 and Luteolin in order to cause the blebbing phenotype which drives senescence. VRK-1 is a kinase that phosphorylates barrier-to-autointegration factor (BAF) which activates BAF and allows for proper nuclear envelope formation. When BAF is not phosphorylated the nuclear envelope is weakened due to the misregulation of VRK-1 and the blebbing phenotype occurs. This weakened nuclear envelope is hypothesized to allow DNA to leak out into the cytoplasm. This activates Cyclic GMP-AMP Synthase to activate which in turn activates Stimulator of interferon genes (STING) which has been directly linked to cellular senescence. The VRK-1 inhibitory drugs have been found to cause cell death at higher concentrations rather than the desired cellar senescence. So, finding the optimal dosage at which senescence occurs at a high rate and minimal apoptosis occurs is very important. Our research is optimizing the dosage at which VRK-1 inhibitory drugs to cause the highest level of senescence with the least amount of violent cell death possible.

College Students' Collectivism, Financial Wellbeing, and Future Retirement

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The purpose of this study is to determine if a relationship exists between collectivist and individualistic attitudes, financial literacy, and retirement planning among college students in the United States. American society prioritizes the independent individual and the economic system in turn expects the individual's financial self-reliance. But the American population is growing from immigration by people who value collectivism and economic cooperation over individualism. The idea of retirement - who is responsible for supporting people when they are no longer productive and earning an income - is one of the crucial sites for the conflict between economic individualism and collectivism in America. The years spent in college can be the most formative time for Americans as it is a rite of passage into adulthood - for financial and personal independence. College students today are more diverse (as minorities, immigrants, and children of immigrants) than previous generations (Pew Research Center 2020) and a significant percentage of them find their collectivist obligations in conflict with mainstream values. All college students today also face new challenges of financial literacy in a society with easy access to money and debt through digital technology (Richardson 2022). Many take on debt to finance their education or homes, while there is an uncertainty about what the economic future holds, especially after the COVID-19 pandemic (Rutledge 2018). Results from this research illustrate how collectivism vs. individualism impacts college students' attitudes and behavior generally and on their financial literacy, specifically, ideas about debt and saving for retirement. Recommendations suggest more effective and culturally competent financial education on campuses that acknowledge the collectivist norms of a significant portion of a diverse study body. While, efforts such as support groups focussed on financial wellbeing are also recommended to promote the financial and retirement security for all of society.

Measurement of Wide Band Gap Semiconductor Power Devices

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The importance of semiconductors in our daily life is more significant than we often think. Since these devices, put in a simplified way, help conducting the energy that electronic devices need, and do so in an efficient and secure way. These electronic devices range from phones, to computers, to cars, and even to industrial controllers. Nearly every device that uses energy in some way, takes advantages of semiconductor devices for operation. As technology progress and innovates, semiconductors are being designed and created smaller. The reason for this is to have more efficient devices. In this research we are focusing on semiconductors that are power devices based on wide band gap semiconductors. The target application for these devices are for circuits requiring operation at higher voltages and temperatures. In this project, pn junction rectifiers (diodes) based on GaN with different areas that range from 35, 70, 160, 325 and 550 um (micrometers) in diameter were measured and assessed in terms of performance. In particular, we have been investigating the reverse recovery transient and charge storage effects in vertical GaN pn junctions. The measurements have been performed using the Keysight B1530 plugin in conjunction with a Keysight B1500 semiconductor parameter analyzer, connected to a probe station for making electrical contact to the devices. We have found that using short cables is essential to minimize ringing or interference that adversely impacts the accuracy of the measurement.

Characterization of Candida spp. Clinical Isolates Pathogenesis in the Catheterized Bladder

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Fungal pathogens like Candida spp. are responsible for many costly and deadly infections and diseases. The most common Candida spp, C. albicans, can be found in different morphologies yeast, pseudohyphae, and hyphae. Hyphae formation is one of the main virulence mechanisms of this fungal species that contributes to biofilm formation. These biofilms can form on medical devices like urinary catheters. Since most hospital patients and nursing home residents will receive urinary catheters, there is an increased concern with the development of these biofilms and infections in these environments. Catheter-associated urinary tract infections, or CAUTIs, are a result of these biofilms, and they are responsible for 150 million infections per year. This is a major health concern as the current treatments are expensive and ineffective. While a majority of fungal CAUTIs are caused by C. albicans, there has been an increase in other Candida spp in the catheterized bladder environment. However, there is not enough known about these fungal pathogens and conditions required for their infections to persist. In this project, we are aiming to characterize multiple clinical Candida spp. isolates pathogenesis in the catheterized bladder environment. To accomplish this, we will assess their growth in urine through CFU enumeration analysis in addition to cell morphology via microscopy. Additionally, we will quantify and visualize biofilm formation of the strains in urine conditions after 48 hours. Lastly, we will use our in vivo mouse model of CAUTI to determine these clinical species' ability to cause infection and disseminate to other organs. Characterizing these strains will give a better understanding of the pathogenesis of varying Candida spp. in the catheterized bladder environment, providing insights for the development of alternative treatment options.

Familial Support: An Examination of the Relationship Between Low Income and Depression

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Depression is one of the most common mental health concerns in the United States; 16.8% of middle-aged adults reporting symptoms in the past two weeks (CDC, 2019). Adult depression also presents a large economic burden, costing the U.S. economy an estimated $236 billion in 2018 alone (Greenburg et. al., 2021). It is imperative to understand risk factors for depression to better treat it. Low income, low levels of family support, and non-White racial identity are associated with increased depressive symptoms (Bailey et. al., 2019). Racial identity affects income and family support, but research must elucidate associations among these factors (Hodgkinson et. al., 2017). We examine effects of family support on relation between income and depression, and whether race (White vs. non-White) moderates any effect.

Participants ($N = 576$) were middle-aged adults (mean age = 42.8 years, $SD = 9.8$) who participated in 1995, 2004, and 2013 in the Midlife in the United States (MIDUS) survey, a longitudinal study of health and well-being. Participants were 54.7% female ($n=315$) and 92% White ($n=534$). Household income and participant demographics were measured at T1, family support was measured at T2, and depression was measured with the Mood and Anxiety Symptom Questionnaire (MASQ) at T3. A moderated mediation model was used to test 1) whether family support mediates the longitudinal relation between income and depression, and 2) whether race (White vs non-White) moderates the relation between income and family support.

The moderated mediation model had good fit ($CFI > 0.9$, $RMSEA < .08$). A significant direct effect of low income on depression was found ($c' = .17$, $p < .001$). A negative effect of low-income on family support was found ($b = -0.09$, $p < .01$), and conditional effect testing revealed a stronger effect of low-income on family support for non-White families ($b = -0.142$, $p < .05$). Furthermore, we found a negative effect of family support on depression ($b = -0.467$, $p < .001$). The indirect effect of low income on depression via family support was only observed for non-White participants ($b = .066$, $p < .05$). Given the direct effect of income on depression, this suggests a partial mediation effect of family support for non-White families.

In accordance with previous research (Tracy et. al., 2008), results emphasize the importance of family support for low income, non-White individuals. Family support could be a useful focus of treatment when working with non-White populations. Further research is needed to understand relations among family support, race, and income; the current sample is disproportionately White and does not allow for a more nuanced analysis of racial backgrounds. Additionally, each variable was measured at one time point, limiting our ability to make longitudinal inferences. Future research should include more diverse samples to examine effects of specific racial identities and income on depression. Identifying factors contributing to family support, such as proximity, monetary support, and family size, may provide further insight into avenues for treatment of depression among low-income non-White patients.

Investigating UTX in Kabuki Syndrome Inhibitory Neurons

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Kabuki Syndrome is a rare neurodevelopmental disorder that causes facial deformation, developmental delay, and intellectual disability. This condition can be caused by a mutation in KDM6A (also known as UTX), encoding a histone-3 lysine-27 demethylase. Previous immunocytochemistry experiments on neural cultures from wild-type mice have demonstrated a potential localization of this protein at the synapse in addition to its already recognized location in the nucleus. In order to further investigate, we first constructed lentiviruses containing wild-type and mutant versions of UTX tagged with hemagglutinin (HA) to overexpress the protein in neuronal cell culture. Staining of cells infected with these viruses supports the proposed localization at synaptic puncta. Second, we created lentiviruses expressing fusion proteins to direct UTX to the presynapse, postsynapse, or nucleus. Infecting neurons with those viruses will enable us to analyze the location of UTX within the cell through a comparison to the non targeted overexpression model, in addition to the impact of the protein at these spots in the synapse. Future experiments include immunocytochemistry with neurons collected from UTX conditional knockout mice. Infecting cultures of neurons from these mice with our UTX lentiviruses will permit characterization of this protein without the interference of endogenous production of the protein. Comparison of stained neurons infected with a lentivirus encoding the wild type version of the protein to a virus with a catalytically dead mutant version will provide insight into its functional impacts at the synapse. Although initial results support the hypothesis that UTX is localized at both the nucleus and the synapse, further investigations will be required to definitively affirm that finding and to discover its functionality in this area of the neuron.

Defining the Concentration and Presence of RNA Binding Proteins in Extracellular Vesicles Released From Mycobacteria Infected Macrophages

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Tuberculosis (TB) is the second leading cause of death by an infectious organism and is responsible for approximately 1.5 million deaths annually. There are numerous reasons for why we have failed to control this deadly disease, but a major factor is that the diagnostic tools available for TB have significant limitations. One potential diagnostic approach is the use of Extracellular Vesicles (EV's). EV's are crucial for intracellular communication in multicellular organisms and play a key role in the ability of the immune system to detect pathogens. Recent studies have revealed that bacterial RNA is present in EVs released from mycobacteria infected macrophages and this could serve as a potential biomarker of infection. While the mechanism for how bacterial RNA enters these EV's remains unknown, it is hypothesized that host RNA binding proteins may be involved. This study compared the concentrations and the presences of RNA binding proteins in EVs released from uninfected and infected cells. EV's from M. avium and M. bovis BCG infected RAW264.7 cells were isolated through ultracentrifugation and their concentrations were determined by particle tracking using a NanoSight detection system. For detection of the RNA binding proteins, EVs previously generated in the laboratory that were isolated from uninfected and M. tuberculosis infected RAW264.7 cells were used. Three RNA binding proteins were detected by western blot: HNRNPA2B1, HNRNPK, and MVP/LRP. Results indicated that the concentration of EVs were higher in uninfected cells compared to M. avium and BCG infected cells. Western blot analysis revealed that the three RNA binding proteins were present in higher concentrations in EVs from M. tuberculosis infected compared to uninfected cells. These findings suggest that mycobacterial infections modulate both the amount and content of EVs released from macrophages and have implications for both the biology of EV biogenesis and EVs as diagnostic markers for mycobacteria/TB infections.

Graph Embedding in Quantum Computers

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E-SURE

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Many graph problems are NP-complete or harder, making the discovery of efficient quantum algorithms for them of significant value. Thus, how such graphs can be “embedded" in an array of qubits in a quantum computer, and how many such qubits will be needed to embed the graph are interesting questions. This poster documents an organized attempt to at least partially answer these questions through experimentation. It reviews the currently known embedding algorithms, and applies them in a controlled fashion to a variety of graphs with specific characteristics. Multiple topologies for qubit couplings are considered, first idealized and then with the presence of faulty qubits. The minorminer, clique, and layout-aware algorithms are used to embed complete, fixed uniform degree, random degree, and power law graphs into the D-Wave Chimera, Pegasus, and Zephyr topologies for various graph sizes and percentage of faulty qubits. Each embedding is evaluated for accuracy, time to completion, the number of qubits used in the embedding, and the size and diameter of the resulting “qubit chains.” Results show that clique embedding is by far the fastest algorithm, but requires the greatest number of qubits and is limited to complete graphs. The layout-aware algorithms yielded the highest percentage of valid embeddings for complex problems. Minorminer, the industry standard embedding algorithm, prevailed in nearly every other case.

Selective Ion Transport Through Copolymer Membranes Functionalized with Imidazole Ligands

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Mentor:
Jonathan Ouimet, Graduate Student

Recycling Lithium-Ion battery waste is increasingly important in order to stabilize supply of valuable metals such as cobalt and lithium. As important is the need to safely dispose of the estimated 500,000 tons of Lithium-Ion battery waste produced per year. Nanofiltration membranes can purify liquid-based feeds by separating small molecules in an energy-efficient manner. Particularly, these membranes could replace complex and waste-intensive solvent extraction methods used in Lithium-Ion battery recycling processes to separate valuable metals (cobalt, nickel, manganese, and lithium) from each other. However, nanofiltration membranes have not yet been developed to separate similarly-sized and similarly-charged ions from each other. This project uses imidazole ligands to selectively partition a target metal into a copolymer membrane–through ligand-metal complexes–while excluding metals with which the ligand has a lesser affinity.

The imidazole ligand was successfully attached to the membrane through a Copper-Catalyzed Azide Alkyne Coupling reaction and was confirmed using Fourier-transform infrared spectroscopy. X-Ray fluorescence was used to demonstrate the ligand's preference to complex with copper over cobalt. Ultraviolet-visible spectroscopy was used to confirm both the ability of the ligand to complex with the metal and the ligand to metal ratio present in complexes. Diffusion Cell experiments demonstrated that the current membrane system was dominated by the free diffusion of ions and as such, no separation of cobalt and copper had been accomplished. Future work must be done on altering the strength of the ligand-metal interaction as well as engineering the pore sizes to effectively exclude unbounded metals from entering the pore.

These membranes could greatly improve hydrometallurgical processes involved in Lithium-Ion battery recycling and outcompete the alternative pyrometallurgical smelting processes that are extremely energy intensive.

Examining DA Algorithm Matching Outcomes in Markets Where Agents' Preferences are Determined by Degree of Similarity

Jose Zentella
GS-SROP

Faculty Advisor:
Maciej Kotowski, Economics
College of Arts and Letters

D. Gale and L. S. Shapley (American Mathematical Monthly, 1962) introduced the "stable matching problem." In such a market, there are two sets of agents (be they buyers and sellers, students and universities, men and women, etc.). Agents from one side of the market seek to match with agents on the other side of the market; moreover, agents from either side of the market have preferences over whom they match with. In this problem, it is desirable that a resulting matching be stable. A matching or assignment is said to be stable if there are no two agents who would prefer to match over being paired with their assigned partner. Though not obvious, Gale and Shapley proved that a stable matching of agents always exists. They demonstrated this fact by introducing the Deferred Acceptance (DA) algorithm, in which they describe a matching protocol that generates market arrangements by assigning each side of the market the role of either making proposals to match or responding to incoming proposals in accordance with their preferences. The DA algorithm may terminate in one or multiple rounds of proposals depending on the particular preferences and responses of the agents composing the market. This research project studies the assignments the DA algorithm generates under the assumption that agents on both sides of a two-sided market prefer to match with agents that are most similar in some quantifiable characteristic (e.g., height, income, weight, etc.) We find that the degree to which the values of both sides of a market overlap systematically affects the number of proposal rounds taken to evaluate a matching. Furthermore, we examine cases with minor inconsistencies in the distribution of associated characteristic values among the populations using arbitrary tie-breaking in markets with perfect indifference in preferences between agents of opposing markets and find that slight alterations to characteristic values can greatly increase the number of proposal rounds taken to evaluate a stable matching in markets where resolving the matching problem would have taken many fewer proposal rounds. We believe these findings may shed light on the operation and inefficiency of real-world markets, in particular those in which participating agents adjust their preferences in response to expectations of other agents on both sides of the market having highly homogeneous preferences, and expose avenues for reducing the total number of rounds needed to produce stable arrangements in particular markets via alternative matching protocols.

11:15 A.M. – 12:15 P.M.
POSTER SESSION 2

ABSTRACTS

PIM-COOH 1,6 Hexanediol Crosslink with Amine Conversion

Thomas Adams
CISTAR RET

Faculty Advisor:
Casey O' Brien, Chemical and Biomolecular Engineering
College of Engineering

Mentor:
Cynthia Chen, Graduate Student

Currently, CISTAR researchers are attempting to develop processes to address carbon footprints related to fossil fuel consumption and refinement. One area of interest is the development of a polymer intrinsic microporosity membrane for the purpose of the separation of light hydrocarbons such as paraffin and olefin, which are products of petroleum refinement. While these polymers show potential, evidence shows that the permeability of these membranes are impacted by an aging process. Perhaps experimental crosslinking and amine conversions can have an impact on the effects of polymer membrane aging. In addition, the presenter, a high school math and physics teacher, will attempt to bring this experimental process to his students with an emphasis on the scientific method and engineering design principles.

CISTAR
NSF Engineering Research Center
Center for Innovative and Strategic Transformation of Alkane Resources

Temporal Variation in Environmental DNA Export at a Pond-stream Interface

Mikey Anderson
Biological Sciences REU

Faculty Advisor:
Jennifer Tank, Biological Sciences
College of Science

Mentor:
Elise Snyder, Graduate Student

Sampling genetic material shed into the environment by an organism (i.e., environmental DNA, hereafter eDNA), allows us to detect populations of invasive, endangered, and/or rare aquatic species using water sampling. While eDNA is an efficient, cost effective, and less destructive method of organismal detection compared to traditional sampling (e.g., netting, electrofishing, trapping), our understanding of eDNA transport is still limited. As such, a positive detection is confounded by upstream-downstream, unidirectional flow. Most eDNA research has been conducted in lentic systems, such as ponds and lakes, where it has been successfully used to estimate population location and density. However, there are still gaps in our understanding of the fate of eDNA once it has been shed into flowing water lotic systems (i.e., streams and rivers) due to downstream transport. There are also other environmental factors that impact eDNA removal from the water column, such as temperature and microbial degradation. Limited understanding of these factors limits our predictions about the density and location of target organisms using eDNA approaches. To explore eDNA dynamics in a small stream, we previously attempted to measure the transport of ambient eDNA generated by lentic species in a small pond, but unexpectedly discovered temporal variation in the concentration of the source eDNA as it moved from pond outlet to stream. To address this, we collected water samples over time from the outflow of Lawler Pond into a first order stream at the Fort Custer Training Center, and quantified eDNA concentrations for two pond fish species (Bluegill and Largemouth Bass). During each temporal sampling, we collected a 250 mL water sample every 15 minutes over a span of two hours, over four seasons (spring, summer, winter, and fall). The signature of eDNA export during the fall sampling showed temporal variation among samples taken across a two hour time period. With additional seasonal sampling, we predicted that eDNA concentrations would exhibit greatest temporal variation during the summer when there is expected to be the most fish movement. We also expected that total eDNA concentrations will be the highest during the spring and fall while fish remain active, but eDNA decay due to microbial activity is lower due to cooler temperatures. This work will enhance our understanding of eDNA removal dynamics at the interface of lentic and lotic systems, which will advance the use of eDNA as a monitoring tool for aquatic organisms.

Characterization of the Atypical Transporter PDR2 in the Pathogenic Yeast Cryptococcus Neoformans

Kayla Anderson
GS-ND-PREP

Faculty Advisor:
Felipe Santiago-Tirado, Biological Sciences
College of Science

Mentor:
Robbi Ross, Graduate Student

Fungal infections are a neglected but serious health threat worldwide. A leading cause of these infections is Cryptococcus neoformans, an environmental yeast that can live latent in the body after an initial respiratory inhalation, but that under certain conditions can disseminate and infect the brain, causing cryptococcal meningitis (CM). CM can be a fatal disease to immunocompromised individuals and is often difficult to treat due to inappropriate/inaccessible treatments and resistance to current antifungal drugs. C. neoformans has multiple virulence factors that aid in infection and its mechanisms to avoid the immune system are incompletely understood. Therefore, investigating known and putative virulence factors is important to inform and develop potential new drugs and therapies for CM. We are currently studying a group of genes that encode for atypical ATP binding cassette (ABC) transporters. These are known as the PDR sub-family of ABC transporters, and C.neoformans has 10 of them, most of which are uncharacterized or have yet to be thoroughly studied. Some of them, like PDR6, have been shown to have a role both in antifungal resistance and host interactions. Others, like PDR2, are completely uncharacterized yet, based on homology, might have a role in or contribute to the virulence of C.neoformans. In order to study this gene, we will generate a deletion strain of PDR2 (pdr2Δ) and analyze it through experiments compared to the wild type. In vitro experiments will include antifungal susceptibility testing and growth under stress conditions such as oxidative media. The pdr2Δ strain will also be exposed to phagocytic cells and imaged to analyze how the cells are recognized and killed. Additionally, we will do in vivo experiments in an invertebrate model (the Greater Wax moth) to determine if there are effects in pdr2Δ's virulence in an actual host with an immune system. Survivorship and fungal burden will be measured and compared against those infected with the wildtype strain. Through this study, we will understand more about how the PDR genes work in C.neoformans and may be able to use this information to guide future research and treatments.

Cellular Reconstruction of Somatosensory Vertebrate Circuitry and Synapsing Interneuron Population

Alan Avalos y Arceo
Graduate School (SROP)

Faculty Advisor:
Cody Smith, Biological Sciences
College of Science

Sensory neurons and their processes are critical to relay external stimuli to the brain. Our understanding of the sensory neuron circuitry relies upon knowledge of its connectivity and interactions with neighboring neuronal populations. However, a detailed description of sensory circuitry in vertebrates and the underlying mechanisms of such information acquisition and transmission needs deeper investigation. Here, we reconstructed vertebrate dorsal root ganglia somatosensory neurons using serial block electron microscopy of the zebrafish spinal cord to understand the neuroanatomical features of a vertebrate sensorimotor circuit. We first manually skeletonized the somatosensory neurons and then utilized automated approaches to reconstruct all the synaptic connections of the somatosensory neurons. Skeletonized tracing of the somatosensory neurons demonstrated their stereotypical bifurcation inside the central nervous system. We show that these neurons extend multiple hemisegments in the spinal cord, with few secondary branches extending from the primary bifurcated neuron. While in the peripheral nervous system, our reconstructions show the close association that somatosensory axons have with the underlying radial glia limitans. By following the synapsing interneuron populations, the relationship between afferent and efferent exchange in the spinal cord complements our understanding of sensory-motor integration processes. As we reconstructed sensory axon projections and spatial mapping of these synaptic sites we present quantifications essential to our understanding of a somatosensory neuron's features. This contribution to the larval zebrafish connectome, combined with previous reconstructions of simpler wiring diagrams, such as those in Drosophila, and C. elegans, better allows us to interrogate the foundational neuroanatomical features that impact vertebrate behavior.

Leveraging Data Science and Machine Learning to Combat Inequity in Digitally Mediated Gig Work

Tori Banda
CSE Summer Enrichment

Faculty Advisor:
Toby Li, Computer Science and Engineering
College of Engineering

Mentor:
Brianna Wimer, Graduate Student

The rise of digitally mediated gig work has transformed the labor landscape in recent years, but concerns regarding worker inequity persist. This research project addresses the issue by utilizing data science and developing an innovative app that leverages real-time data and intelligent assistants to maximize the benefits received by gig workers, while considering their personal preferences.

The research project utilizes both an experimental and analytical approach through development and testing of an app prototype in addition to combining data analysis and machine learning techniques to analyze the large 300M dataset centered around gig work, which is then used to derive key insights to inform the app's decision-making process. As this research project handles large scale data analysis and app development, it relies on data science software and tools, such as Python and a multitude of relevant libraries and modules, TensorFlow, and Tableau. The employment of the software was necessary for my contribution to the project, which includes data preprocessing and cleaning, hypothesis testing, interpretation of data, and predictive machine learning algorithm development. My contribution to this project included developing and evaluating a predictive machine learning algorithm, a linear regression model, that would predict the fare (earnings) of the driver for a rideshare trip using key features such as the length of the trip in miles and the time of the trip as independent variables to estimate and predict our fare, which acted as our dependent variable. An additional contribution included introducing additional data to determine what things might play a role in the fare of a trip (such as demographics of pickup and drop off community areas that could determine biases and the likeliness of the driver to take the job).

Ultimately, the research work unveils valuable insights into digitally mediated gig work. Observations include the identification of key factors influencing gig worker earnings. Machine learning algorithms provide predictive models for gig worker earnings and, in the future, will allow for targeted interventions and improved decision-making. Observations include the identification of key factors influencing gig worker earnings, those being length in miles and the time of the trip. It was determined that trips that are longer in miles are more likely to have a higher fare/fare per hour compared to shorter trips. Additionally, it was determined that trips that are extremely short in length, such as 0.1 – 2 miles, have a higher fare/fare per hour compared to trips ranging from 2 – 50 miles in length. The use of the linear regression model provides predictions for gig worker earnings and, in the future, will allow for targeted interventions and improved decision-making. The research has determined that by effectively analyzing and validating data, testing hypotheses, and developing accurate machine learning models, we can generate evidence-based recommendations to combat inequity and enhance gig worker experiences, and continued efforts in data analysis, validation, and machine learning algorithm development will contribute to a more transparent, fair, and sustainable gig work ecosystem.

Novel Ruthenium Carbene Complexes

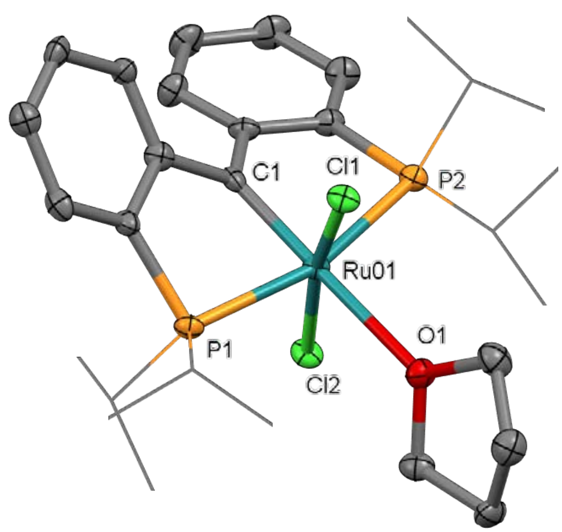
Reinhard Bartsch
ND Energy - Slatt Fellowship

Faculty Advisor:
Vlad Iluc, Chemistry and Biochemistry
College of Science

Mentor:
Zachary Lincoln, Graduate Student

Olefin metathesis is a synthetic organic reaction that has found a variety of uses in industry and academia. The reaction employs transition metal catalysts that regulate the formation of polymers and other organic compounds. Ruthenium carbenes have emerged as the most common catalysts used, however ruthenium is naturally scarce and can be toxic. This means that ruthenium catalysts require substantial amounts of money and energy to produce, isolate, and extract. The Iluc group is interested in overcoming these challenges by designing catalysts with earth-abundant elements for more sustainable synthesis. Recently, the Iluc group synthesized a paramagnetic iron (II) carbene that shows promise in moving towards iron catalyzed olefin metathesis, (Hoffbauer et al., 2021). However, since the compound is NMR-silent, I have been attempting to synthesize a NMR-active ruthenium analog for the iron carbene. Furthermore, I hope to contribute to the field of olefin metathesis by isolating and characterizing the first metathesis active ruthenium metallocyclobutane, a critical intermediate in understanding the mechanism behind olefin metathesis. Shedding light on the mechanism for this reaction is important because designing better catalysts requires one to understand all of the pieces of the mechanism. In this case, understanding the mechanism for the ruthenium system could lend valuable insight to the iron system and contribute to future work on iron catalyzed olefin metathesis. This could lead to the development of more metathesis active iron carbenes, which would bring about greater energy efficiency and reduce harmful waste production in synthetic processes that require olefin metathesis.

Utilizing the same PCH2P ligand as in the iron carbene I was able to synthesize a ruthenium (IV) carbene [(PC(sp2)P)Ru(Cl)2(L)] (L = THF, py, NCtBu), which I reduced to form a ruthenium (II) carbene [(PC(sp2)P)Ru(L)2] (L = PMe3). To test the metathesis activity of my ruthenium carbene, it will be reacted with different olefins. Given its structural similarities to common ruthenium catalysts, it is likely it will undergo a [2+2] cycloaddition, forming a metallocyclobutane intermediate. The pincer ligand in my carbene has a stabilizing effect that has helped with the isolation of otherwise reactive palladium and platinum carbene species in the past, so it may confer stability to the intermediate, possibly allowing for isolation and characterization of a ruthenium metallocyclobutane.



Fabricating Desalination Membranes using the Molecular Layer-by-Layer Method and Characterizing the Films using Electrochemical Impedance Spectroscopy

Nila Beamon
SMASH Engineering REU

Faculty Advisors:
Jennifer Schaefer, Chemical and Biomolecular Engineering
College of Engineering

Mentor:
Jizhou (January) Jiang, Graduate Student

When purifying water, membrane-based separation will require 90% less energy than distillation. Traditional reverse osmosis membranes are crosslinked polyamides that are prepared with two monomers, such as, 1,3,5-benzene tricarbonyl trichloride and m-phenylenediamine, using interfacial polymerization (IP). IP membranes are made by dissolving the monomers in two separate solutions which immiscible with each other and the diffusion between them will generate a film at the interface. Because the IP process creates randomized films, characterizing the membranes becomes difficult and the unevenness of the films does not fit the criteria needed for rigorous investigations of structure-property relationships. To overcome these limitations, in this study the polyamide films are formed using the molecular layer-by-layer (mLbL) method onto a gold substrate. The mLbL in theory builds the polymer one monomer layer at a time for a more controllable fabrication approach that forms a uniform and smooth surface allowing the usage of various characterization techniques to fill the knowledge gap existing in polyamide separation membranes. However, there is limited information obtained from prior electrochemical study on mLbL film. Here we utilize electrochemical impedance spectroscopy (EIS) to gain a better understanding of film properties. EIS measures films' resistivity and capacity, which can provide more information about the film's structure and ion transport. We prepared a series of films by the mLbL method, determining their thickness by ellipsometry. First, we established the methodology of EIS on a bare gold electrode to determine the potential, amplitude, and rest time that is necessary for adequate measurements from the films. Then EIS has been applied to a variety of membrane-coated gold electrodes consisting of different thicknesses. The resistivity and capacity have been analyzed to reveal the inhomogeneous growth during the mLbL process. The effect of pH of the electrolyte and monomer chemistries is also investigated. This study demonstrates the potential of electrochemical impedance spectroscopy (EIS) for investigating the growth of the mLbL process, surface charge, and local ion interactions in polyamide films.

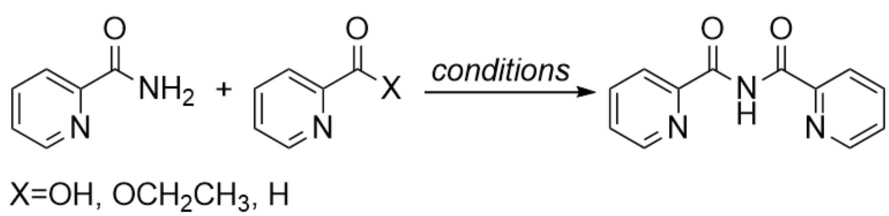
Development of an Effective Synthesis of Bis(2-pyridinylcarbonyl)amine Ligand

Addisyn Camadeca
Saint Mary's College

Faculty Advisor:
Elsa M. Hinds, Chemistry and Physics
Saint Mary's College

The synthesis of bis(2-pyridinylcarbonyl)amine (Hbpca) was pursued for its use as a ligand in metal-catalyzed transformations. The synthesis of novel ligands allows for exploration of bonding with metals to form metal complexes. Metal complexes are utilized in metal-catalyzed and -mediated synthetic transformations to create new bonds, such as carbon-carbon bonds. For example, many reactions can be explored such as oxidative cross-coupling and other metal-mediated or catalyzed procedures. Hbpca has been synthesized previously, but literature syntheses were not operationally safe, efficient, or descriptive. Hbpca must be synthesized because it is not easily able to be purchased. In this project, multiple syntheses were attempted, with all of the attempts reacting 2-picolinamide with other carbonyl starting materials including 2-pyridyl carboxylic acids, esters, and aldehydes. Reactions with 2-picolinic acid resulted in recovery of 2-picolinamide, and reactions with ethyl 2-picolinate resulted in recovery of both starting materials after silica column chromatography, likely because of the lack of reactivity of amides as a nucleophile. Amides are quite stable and unreactive because the nitrogen donates electrons to the carbonyl group through resonance. Amidation reactions of 2-picolinaldehyde so far have resulted in no conversion of starting materials, and a polymeric substance was formed, likely due to decreased reactivity of the pyridine rings and unfavorable interactions that will be examined. Additionally, future directions in this project are to use other 2-picolinic carboxylic acid derivatives, such as acid chlorides. Following the synthesis of Hbpca, it will be used in metal-catalyzed reactions such as nickel-catalysis for amide N-arylation. The nickel-Hbpca complex will be used as a catalyst to form a bond between an aromatic ring and a nitrogen atom of an amide to form new substituted amides.

General Synthesis



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Temporal Foraging Tendencies of Micropterus Salmoides in the Northern Temperate Region of the United States

Gilberto Cerda III
Graduate School (SROP)

Faculty Advisor:
Stuart Jones, Biological Sciences
College of Science

Mentor:
Camille Mosely, Graduate Student

Fisheries are important to the economic and biological health of many areas of the world. Largemouth Bass (Micropterus salmoides) are a keystone predator found in many lakes in the northern temperate region and are a popular sport fish. Largemouth Bass are known to have a varied diet consisting of many different organisms. It is uncertain exactly how or why largemouth bass select the prey they do. One idea is that largemouth bass are opportunistic foragers that will primarily forage upon abundant prey populations, while another idea is that bass are capable of being specialized foragers. When water temperature increases during the late spring, fish produce offspring through an external reproductive process known as spawning. Density dependent effects associated with spawn can affect bass diet. It is important to understand the diet choices and patterns of largemouth bass to ensure that fisheries remain healthy and fishable for anglers that wish to catch largemouth bass. As competition increases, there is a decrease in prey availability. A foraging strategy calls for the consumption of any available prey items, while a specializing strategy involves the consumption of specific diet items despite increased competition for the items. Because of increased density dependent effects after spawn, we hypothesized that a bass population practicing specialized foraging rather than opportunistic foraging will see a decrease in common year round prey items, such as crawfish, in their stomach contents. Research angling took place during the summers of 2021 and 2022 to assess diet changes across time as part of a whole lake experiment at the University of Notre Dame Environmental Research Center. We collected fish diet biomass using gastric lavage from two lakes to compare biomass and prey proportions. We observed an increase in overall diet biomass collected during the post-spawn periods. These results suggest that there was not a major decrease in resources that could have limited the breadth of the bass diets. Our statistical tests found no significant difference in the diet item biomass proportions between pre-spawn and post-spawn time periods. This suggests that the bass in these lakes could be taking a more generalized approach to their foraging as they maintained their consumption levels of the same prey despite increased density dependent effects that could be lowering prey species populations. Future diet studies can be conducted to examine how individual differences in bass influence generalist or foraging preferences.

The Effects of Age and Time Spent in the United States on the Cultural Values of Adults of Mexican Origin

Alijah Chalas
Graduate School (SROP)

Faculty Advisor:
Jenny Padilla, Psychology
College of Arts and Letters

Mentor:
Adriana Miranda, Graduate Student

Immigration takes a significant toll on the minds of immigrants as it is a difficult process and often stems from a need to solve pre-existing issues such as financial strain, conflict and danger in their home country, or simply the opportunity for a better life. This is also true of the families of Mexican origin that we looked at in a southwest metropolitan area. This study investigates the effect that age and time spent in the United States have on the opinion that adults of Mexican origin have of their own ethnic group. This was investigated via survey in the participants (n = 246 families of Mexican origin) preferred language. The sections of the survey that were targeted for analysis include ethnic-racial identity, ethnic values, acculturation, and perceived discrimination. The sections of the survey that focused on ethnic values and ethnic-racial identity gauged how the adults fit into their ethnic group and how they felt about their ethnic group. The sections on acculturation and perceived discrimination showed the ways in which their membership of their ethnic group has affected their daily lives. Those that live in the United States longer are expected to score higher on sections about negative feelings towards their racial group, but lower on acculturative stress measures because they are likely to feel like their ethnic group defines them less. The reverse is expected to be true of those that have lived in the United States for a shorter time as their membership of their ethnic group is likely to play a larger role in their personal identity. This would enable us to highlight a significant psychological issue for immigrants and potentially develop effective points of interjection to better aid those that move to the United States to build new lives.

Development of GaN IMPATT Diodes as High Power Millimeter Wave Sources

Samuel Clough
Wireless Institute (AWaRE)

Faculty Advisor:
Patrick Fay, Electrical Engineering
College of Engineering

Mentor:
Zhongtao Zhu, Graduate Student

Impact ionization avalanche transit-time (IMPATT) diodes are some of the best sources of high power millimeter waves. These devices exploit properties of semiconductor device physics to produce negative differential resistance, which can be used in conjunction with resonant circuits to produce continuous wave high frequency signals. However, there are physical limitations governing the maximum performance of these devices, depending on the semiconductors used in the diodes. Gallium nitride (GaN) is a semiconductor that is especially well suited for high power, high frequency applications, as previous simulations have shown that GaN-based IMPATT diodes have the potential to perform at power/frequency levels up to 600 times better than existing devices.

This research focused on fabricating IMPATT diodes on GaN and determining how to maximize the device performance. In particular, we've worked to measure and reduce the contact resistivity present at the metal/semiconductor interfaces of the device. We measured the contact resistivity using circular transmission line model methods. From these measurements, we could record how the contact resistivity changed when we annealed test samples at different temperatures. We can then determine the ideal temperature to use during device fabrication in order to minimize the contact resistivity.

Hyperdimensional Computing Based In-sensor Side-channel Attack Detection

Maria Isabella Corcoran
Naughton Fellowship

Faculty Advisor:
Ningyuan Cao, Electrical Engineering
College of Engineering

Mentor:
Jianbo Liu, Graduate Student

Internet of things (IoT) devices, for example smart watches, or smart home appliances, collect a lot of information about us, and are becoming increasingly prevalent in all different aspects of our lives. They are not only increasing in popularity in the home or as wearables but also in the medical field, as security devices, or in industrial settings. As they integrate further into our lives and more of our personal data is being collected, data security is becoming an increasing issue. Hackers are always becoming more inventive, and as the market for IoT devices grows, consumer or otherwise, so does the number of competitors producing such devices - and not every company holds itself to the highest standards of security, especially if it means more cost and less profit! Due to the nature of IoT devices, a low-power, low-cost, area-efficient solution is necessary. Our goal is to develop this solution.

My research involves the design of a chip that will be used to develop a low power, low area side-channel attack detection system. The project involves a software/hardware co-design approach to design the system with minimal power and area footprint.

A side channel attack is a type of attack that capitalizes on the physical implementation of a cryptographic algorithm. There are different ways to do this; there are timing, electromagnetic and power analysis attacks for example. Our focus is on power-analysis side channel attacks. A hacker may attach a probe to a device with the goal of reading the variations in power consumed by the device, which gives information about internal processes (in this case, encryption and decryption of private information). When a probe is connected to the power net of our chip, we want to detect it.

My main focus was to assist in implementing cryptography standards such as AES128 & HMAC-SHA256 on-chip; I have written a hardware implementation of HMAC-SHA256 in Verilog, a hardware description language. These encryption modules are being integrated into the chip.

A machine-learning algorithm called ‘Hyper-Dimensional Computing’ will be integrated on chip, with the intention of determining when a side-channel attack is taking place. This algorithm is intended to learn in the way the human brain does, by transposing data to a high dimensional space. HDC can handle a large volume of information with lower computational demands than many conventional machine learning algorithms, making it highly suitable for on-chip integration. It is energy-efficient to train and area-efficient, and thus is suitable for low-power and area constrained devices, for example Internet of Things (IoT) devices.

HDC achieves its efficiency due to several factors. On the hardware side, HDC computations are highly parallelizable as the operations can be applied to the high-dimensional vectors simultaneously; this is the same why our brain is postulated to work. Algorithmically, manipulating the high dimensional vector data is simpler due to it often being more linearly separable, and often containing a lot of zero vectors which can be ignored in computation.

Progress Towards Understanding the Fate of Ampicillin in Soil

Ana Corcoran
Saint Mary's College

Faculty Advisor:
Christopher Dunlap, Chemistry and Physics
Saint Mary's College

As the use of antibiotics continues to rise, it is important to understand the environmental impacts of improper disposal and pollution. Antibiotic pollution leads to the loss of naturally occurring bacteria that are present in the environment and can affect the local habitat. Ampicillin, a commonly used β-lactam antibiotic, is used in veterinary practice and for human use in developing countries. The goal of this research is to better understand the fate of ampicillin in soil and to determine whether the pharmaceutical is being absorbed into the pores of the soil or being degraded over time. In order to model a natural system, solutions of varying concentrations of ampicillin between 10 and 100 µg/L were added to soil samples acquired from the organic farm on Saint Mary's College campus. The samples were then analyzed using liquid chromatography-tandem mass spectrometry (LC-MS/MS). It was determined that the concentration of ampicillin in the samples decreases consistently over the course of six hours. Ampicillin does not degrade in aqueous solution over that same time period. Initial experiments to release absorbed ampicillin from the soil by changing the pH of the solution or through sonication have proven unsuccessful. Further work is needed to fully determine what is occurring to the ampicillin when added to soil. This could be done by utilizing different soil agitation techniques to minimize the porous quality of the soil as well as adjusting the pH of the solutions to either force degradation to occur or remove the pharmaceutical from the pores of the soil.

Development of an Aptamer Based Gold Nanoparticle Biosensor for the Quantification of Kanamycin

Charlie Desnoyers
NDnano (NURF)

Faculty Advisor:
Kaiyu Fu, Chemistry and Biochemistry
College of Science

Mentor:
Grayson Huldin, Graduate Student

Development of sensitive and rapid biosensors is crucial to understanding patient-specific pharmacokinetics and creating effective point-of-care devices with good sensitivity and high specificity in a timely reading manner. One way of creating such sensors is by using aptamers, which are short chain oligonucleotides that bind to specific targets with tunable sensitivity. Ideally, the target will bind to the aptamer which leads to a structural conformational change of the aptamer. By attaching a fluorescent reporter to the distal end of the aptamer, a signal change (either ON or OFF) is generated when the conformational change occurs. To create a signal ON sensor when the target molecule is added, we propose a quenching mechanism that triggers the target-aptamer binding to light up and create a fluorescent signal. By using gold nanoparticles (AuNP) as a dynamic quenching agent, aptamers attached to the fluorescent dye can be conjugated to AuNP which allows for a sensitive and proportional signal to be seen as more target is added. I have developed an aptamer-linked gold nanoparticle (Apt-AuNP) biosensor that allows for the rapid quantification of kanamycin, an aminoglycoside antibiotic, via fluorescence measurements. I synthesize, characterize, and measure the Apt-AuNP to understand their behavior with and without the addition of kanamycin. Through UV-Vis spectroscopy and fluorometer measurements, the sensing mechanism, concentration of aptamer per AuNP, and fluorescence behavior is understood. This robust biosensing platform can prove useful to screening how various pharmaceuticals behave in vivo and has potential applications with understanding patient specific metabolism of various drugs.

Synthesis of Tridentate Ligands and their Iron Complexes for use in Redox Flow Batteries

Bridget Donovan
Saint Mary's College

Faculty Advisor:
Michael Drummond, Chemistry and Physics
Saint Marys College

Over the past decade renewable energy, solar and wind, has been on the rise. This has caused a need for new energy storage technology to capture the renewable energy as it is intermittently generated. One emerging technology to address these challenges are redox flow batteries (RFBs). A redox flow battery is an electrochemical cell where chemical energy is stored by two chemical components (electrolytes) that are dissolved in solutions that are pumped through the charging chamber on different sides of a membrane. While the two chemical components circulate in their separate spaces, ion transfer will occur across the membrane aiding the flow of electric current in the external circuit. As the battery is charged, the solutions are stored in tanks until the battery is ready for discharge. Since the posilyte and negolyte are separated into two different tanks, RFBs do not self discharge as fast as a regular battery, and have the potential to store energy for longer periods of time. The variables that determine the energy density in an RFB are electrolyte concentration, cell voltage, and number of electrons transferred. Water solvents have a very narrow electrochemical stability window (ESWs, ~1.5 V) which limits the cell voltage of aqueous redox flow batteries. However, many organic solvents have a wide range of EWCs, for example acetonitrile is stable across ~5 V. If electrolytes with extremely negative and positive potentials can be developed, they could be used in non-aqueous RBFs (NARBFs) without concern for solvent breakdown. Since higher cell voltage leads to higher energy density, NARFBs have the possibility to achieve these then aqueous RFBs. This work reports the synthesis of two types of quinoline-pyridine-based ligands that, when combined with iron salts, will form metal complexes that can act as candidates for NARFBs.

The Role of AMT in Embryonic Development and Nephrogenesis

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Nonketotic hyperglycinemia (NKH) is a rare metabolic disorder resulting from a mutation in the glycine cleavage system (GCS), which catalyzes the breakdown of glycine. The GCS employs four major proteins to convert glycine into one-carbon subunits. One of these proteins is aminomethyltransferase (AMT) which functions to transfer carbon-2 of glycine to tetrahydrofolate. Mutations in AMT are seen in ~20% of NKH cases, but the extent to which AMT is involved in development remains unclear. Only one mouse model of Amt deficiency has been examined to date, and the analysis focused on neural tube defects. Though current NKH models are also primarily focused on central nervous system (CNS) ontogeny and function, there is evidence that AMT is crucial in organogenesis elsewhere, such as the kidney. AMT is highly expressed in nephron progenitors and tubule precursors in the human embryonic kidney. Here, we developed an amt loss of function model in the zebrafish, which led to morphological phenotypes including elevated cell death, hydrocephalus, pericardial edema, cloacal cysts, seizures, and kinked tails. amt deficient zebrafish also exhibited decreased survivability compared to wild-type controls. Based on these preliminary observations, we hypothesized that amt-deficient zebrafish would display abnormal CNS and renal development. To investigate this further, we used techniques such as whole mount in situ hybridization and observed differential patterning in both the brain and embryonic kidney. Within the kidney, the nephron functional units in amt morphants displayed a normal length but possessed segmentation defects including longer proximal convoluted tubule lengths, longer distal early tubule length, shorter distal late tubule length, less distance or fused podocytes, and enlarged cloaca. These findings may provide insight into why NKH patients can experience kidney dysfunction. Due to high levels of conservation from zebrafish to humans, zebrafish will continue to provide an amenable model for investigations into the molecular and developmental basis of NKH, building a knowledge base for future therapeutic development.

Exploring the Reactivity of Nucleophilic Iridium Complex with Electrophilic Carbon Compounds

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One method that could potentially produce fuels from carbon dioxide is anchoring it to a metal, which would allow it to be reduced to methanol or another functional fuel. It has been noted previously that the bis(iminoxolene)iridium complex [(Diso)2Ir]— (Diso = 2,4-di-tert-butyl-6-(2,6-diisopropylphenyl)iminoxolene) forms strong bonds with carbon compounds and thus is an interesting complex to consider to hold on to carbon dioxide as it gets reduced to a fuel. In order to be able to actualize this with the bis(iminoxolene) iridium complex, its reactivity with electrophiles needs to be well understood. The iridium complex reacts with alkyl halides and benzyl halides, replacing the halide in a typical SN2 fashion. It follows the expectations of an SN2 mechanism in that it reacts the fastest with butyl iodide and slowest with butyl chloride—as the leaving group improves, the rate constant increases. However, it appears that it reacts faster with butyl halides over benzyl halides, which is not observed in typical SN2 reactions—benzyl halides typically react 105 times faster than butyl halides. This difference may be because of a change in mechanism or that the reactivity properties of this particular nucleophile are atypical; further study is required to determine what is causing this discrepancy. In contrast to alkyl electrophiles, the iridium anion does not react readily with carbon dioxide or carbon disulfide. Future studies include using co-activators to facilitate the interaction of the iridium complex with carbon dioxide and trying to forge iridium-carbon bonds with other oxidation states of carbon.

Materials-Driven Application-Level Analysis of Emerging Workloads

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Recommendation systems are Artificial Intelligence/Machine Learning algorithms that use collected data to give recommendations on areas such as movies, music, generic products or even housing opportunities. Due to the expected growth of customers when implementing a recommendation system for a product advertisement, or simply the improvement on user-friendliness of our applications, recommendation systems are found everywhere from big technological companies such as Google or Netflix, to simple browsers on our own phones. However, interest is based on what the recommendation system is needed for, with some groups preferring increased efficiency by reducing energy consumption, while others mainly focus on proficiency by maximizing the system's accuracy. Recommendation systems are not only reliant on the way code has been created, but also on the technology, circuits, architectures, and algorithms used to support said systems. On account of the importance of recommendation systems in our present environment, it is key to understand and explore the salient features and variables that affect and build a recommendation system.

Dr Michael Niemier’s Lab is interested in studying how emerging technologies and architectures can ultimately impact machine learning (ML)/artificial intelligence (AI) workloads like recommendation systems. While a recommendation system is a rather large/involved problem to study in the context of new technologies and/or architectures, problems/models such as few shot-learning with memory augmented neural networks (MANNs) can be a good “proxy” for said problems, as many of the technology-enabled solutions for MANNs can also be used in recommendation systems. In order to move toward more sophisticated benchmarking efforts, my worked aimed to capture and analyze the impact (on accuracy, energy, latency, etc.) when different technology-enabled solutions were applied to MANNs. This allows researchers to see the strengths and weaknesses of certain systems based on the materials devices, and architectures, used to support the models.

My first contribution focused on identifying trends between energy consumption, variation, and accuracy. I constructed infrastructure to easily visualize/analyze collected data across the aforementioned figures of merit given different technology-based solutions (which allows us to dynamically plot data associated with future technology-architecture-application-level studies). My second contribution focused on a customized variation of a dot plot, with its primary use to show the relationship between accuracy and different distance formulas, materials and architectures. Again, the contribution focused on the code to be dynamically adaptable to the number of trials, types of trials, types of methods, and increased variation of trials. A third contribution focused on the comparison of the strengths of certain graph algorithms using datasets from Wikipedia and Facebook. Different approaches were analyzed via a radar plot on the basis of proficiency and efficiency. Finally, the last contribution is related to the implementation of a single-shortest-path algorithm; this will be used to see how “tolerant” this algorithm is to variation that may arise from new memory technologies at the algorithmic-level. Data is still being collected for this thread.

Total Synthesis and Chemical Stability of Pseudouridimycin and its Analogues

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The discovery and development of broad-spectrum antibiotics is of high interest due to the widespread emergence of drug-resistant pathogens. Bacterial RNA polymerase (RNAP) is a validated bacterial drug target since viability of bacterial cells relies on RNAP-mediated transcription. Pseudouridimycin (PUM) is a naturally occurring C-nucleoside/dipeptide antibiotic isolated from Streptomyces albus. PUM inhibits bacterial RNAP in vitro in the mid-nanomolar range, with greater than 10-fold selectivity over human RNAP and does not exhibit significant toxicity to human cells. PUM also displays potent bacterial growth inhibition in vitro and in vivo. Despite this promise, PUM’s efficacy is compromised due to instability at physiological pH limiting its therapeutic potential. Our laboratory has previously identified two intramolecular decomposition pathways with a guanidine-assisted hydroxamate bond scission being the major pathway at physiological pH. To address this, we have synthesized hydroxamate and guanidine modified PUM analogues which seek to enhance chemical stability while maintaining biological activity. We further describe an expedited solid-phase synthetic approach utilizing a stable des-hydroxy PUM analogue to rapidly screen dipeptide modifications which seek to optimize the binding affinity and direct future analogue design. These studies will pave the way for novel synthetic analogues of PUM to be advanced toward the clinic.

Synthesis of Nanocrystal Surface-Bound Transition Metal Complexes

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Colloidal semiconductor nanomaterials introduce a new layer of customizability to the field of catalysis. Electric fields present on the surface of semiconductor nanocrystals, for example, may allow for alteration of the electronic landscape of bound ligands—in the case of a bound catalytically active species, the possibilities of adjustable reactivity and rate parameters are introduced.

In this work, we target syntheses of several transition metal complexes: salen and bipyridine ligands are used as electrically responsive backbones. These ligands are able to house both transition metal center and appended auxiliary groups, which may participate in a ligand exchange reaction where coordination to a CdSe nanocrystal would occur.

Using Source Code Summarization to Eliminate User Necessity

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Source code summarization is the process of translating segments of a programming language into a brief English summary. These summaries are utilized in documentation sites such as JavaDocs but are written by a user. Our lab is using large language models to eliminate the necessity for users to create a description and instead have it generated automatically.

My contribution to the lab is an interface that utilizes the source code summarization models they've established and makes it digestible and usable for the average user. With only a few files installed and commands executed, a user can traverse through a Java file and have short descriptions returned effortlessly without the need for extensive user input.

My program functions by using a Python script and the language model. The program runs by traversing each Java file in a specific directory and taking its components such as the method name, its code snippet, and any comments. This information is then sent to a Flask server which uses that information to create a concise, one-sentence description of what the method does. The program returns the generated description as a method comment, recognizes if a pre-existing comment block exists, places it inside if necessary, and places this information in a new file in a specified directory.

Looking ahead, my focus for the upcoming weeks will be on fine-tuning the pre-trained model using my datasets. The input takes a Java file with methods that do not have summary comments attached. The output is a Java file with added summary comments created by the language model. This process aims to enhance the efficiency and accuracy of the model, further improving the quality of the generated descriptions.

Improving the Quality of Diffusion Cell Experiments using 3D Printing and Automation

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Traditional thermal methods for chemical separations are energy-intensive, creating the need to find alternate energy efficient methods, such as membrane separations. The transport mechanism of the membrane, which can be studied through diffusion cell experiments, defines how well-suited a membrane is for its application. Diffusion cell experiments are key for identifying transport mechanisms and measuring membrane properties like diffusion coefficient. Current diffusion cell designs can provide difficulties such as hard and time-consuming assembling process, solution leaking out of the cell, and they do not provide a way to install a sensor in a fixed position for consistent readings. In addition, the experiments themselves can be time consuming, and data collected manually could represent big errors and inconsistencies. This work shows how the quality of diffusion cell experiments can be improved by using 3D printing and automation. The powerful technique of 3D printing allowed for the design of the diffusion cell to be customized and printed many times to create a prototype that can be assembled in an easy, fast, and reproducible way; is air-tight so there is no solution leaking out of the cell; and contains an integrated sensor for consistent measurements. Combining the optimal design of the diffusion cell with a proper code made it possible to improve the quality of the data collected by automating the experiment. The methods shown in this work improve the diffusion cell experiments, leading to time savings and better data quality. The collection of high data quality leads to a better analysis of the membrane properties and therefore, a possibility to create better membranes to address big societal challenges that require chemical separations, such as the production of fresh water and fuel generation in an energy efficient way.

Construction and Characterization of Functionalized HEMA Membranes for Biocompatible Sensors

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Biocompatible membranes can act as a barrier between the body and sensors, allowing for specific analytes to be measured while protecting the device from fouling caused by the deposition of material on its surface. Exposure to proteins and other molecules present in biofluids can non-specifically adsorb onto the sensor surface, reducing its performance. Studies have shown that membranes functionalized with compounds such as zwitterions exhibited antifouling characteristics by preventing protein adsorption. However, there is a need to develop a membrane that has these antifouling properties and is able to interface with a sensor. In this study we synthesized 2-hydroxyethyl methacrylate (HEMA) copolymer membranes and functionalized them with a zwitterion. Several measurements were performed on the membranes to characterize permeability and pore size. We found that the functionalized HEMA membranes had an averaged permeability of 0.3167 Lm-2h-1bar-1 which was considerably lower than the regular HEMA membranes that had an averaged permeability of 2.811 Lm-2h-1bar-1. The HEMA membranes had an estimated pore diameter of 4.5 nm. It was also shown that the absence of stirring in solution during rejection experiments using the HEMA membranes led to a decreased percent rejection due to concentration polarization of the solution. These results demonstrate that functionalizing HEMA with a zwitterion can affect the way the membrane interacts with solutions. To further investigate the effects of the functionalized HEMA, the membranes will undergo diffusion experiments with proteins such as fibrinogen and BSA to observe if there are noticeable antifouling properties. The mass transfer resistance of the membrane, which would negatively impact performance similar to the concentration polarization seen during experimentation, can be reduced by decreasing the thickness of the membrane. Thus, we have begun looking at spin coating as a way to both produce a thinner membrane and attach the membrane onto the device.

Exploring the Functionality of iPSC Derived Lymphatic Endothelial Cells using Metabolite-assisted Growth Factor Differentiation Protocol

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Induced pluripotent stem cell-derived lymphatic endothelial cells (iPSC-dLECs) are a valuable tool for developing lymphatic vascularized tissues and modelling lymphatic diseases such as lymphedema. Some of the methods of differentiating iPSCs into iPSC-dLECs include addition of growth factors such as vascular endothelial growth factor (VEGF) or transfection of transcription factors such as ETS2. These differentiation methods, however, suffer from low yield and reduced functionality compared to their native counterparts. A potential method to improve the efficiency is through addition of fatty acid oxidation (FAO)-related metabolites, which LECs use for histone acetylation of key lymphatic gene VEGFR3. In this study, we test the iPSC-dLEC derived using the FAO metabolite-assisted growth factor stepwise differentiation method to determine if the addition of metabolites produce functional dLECs.

We used an 8-day protocol to differentiate iPSCs into iPSC-dLECs by initially creating mesodermal cells and then further differentiating them to endothelial cells. They are made to be lymphatic specific by adding VEGF-C and sodium acetate, a precursor molecule for FAO-related metabolite, acetyl-CoA, for the final 4 days. We first confirm that the iPSC-dLEC express higher levels of common lymphatic markers with sodium acetate treatment by carrying out fluorescence-activated cell sorting (FACS) and qPCR. We then verify that the differentiated LECs mimic the functionality of primary LECs by testing their migration and network formation capacity which are crucial for their incorporation into engineered tissues.

Lastly, we explore the application of the metabolite-assisted differentiation in generating lymphatic vasculature-containing iPSC-derived organoids. We form iPSC organoids and differentiate them using optimized protocol in suspension culture for 9 days and embed them into various hydrogels to induce lymphatic vascularization. We test three materials: collagen-Matrigel, fibrin gel, and norbornene-modified hyaluronic acid, and analyze the resulting vascularization pattern and level of lymphatic marker expression in the vascularized organoids. Taken together, this study confirms that the metabolite-assisted differentiation method efficiently produces functional LECs in both 2D and 3D culture. Our findings also suggest that our lymphatic vascularized organoids can be formed in various animal-derived and synthetic hydrogels, which may be applicable in 3D in vitro drug screening or disease modeling applications.

Synthesizing Gold Hexagonal Nanoplates under Different Lighting Conditions

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Tunable and reliable nanostructure formation shows promising applications in remote sensing, nanoelectronics, and plasmonics. While it has been proven difficult to create processes that include tunable growth rates and array formation, recent developments in the Neretina Lab in the growth of gold nanoplates have allowed for further control over nanostructure growth. Specifically, previous processes of gold nanoplate synthesis using aqueous gold salt ($HAuCl_4$) and Brij-700 block copolymer solution on crystalline sapphire substrates have been shown to have high yields and excellent consistency (95%). Interactions between external light sources and Brij-700 based growth within these processes have also been observed, with external LED light sources causing accelerated growth rates. However, little is known about how different wavelengths or intensities of light affect Brij-700 solution-based growths.

Herein, we demonstrate that nanoplate growth rates are inherently reliant on light irradiation intensity as well as the wavelength(s) of the irradiating light, with smaller wavelengths of light, such as ultraviolet or blue light, inducing a faster growth rate than red light or green light, even when controlled for the same intensity. We also demonstrate certain solution aging techniques in the growth process, such as irradiating growth solution prior to exposing it to an array, can further affect the growth rate. This phenomenon hints at how different wavelengths of light might increase the rate of electron transfer between the Brij-700 and the gold salt, as well as which part of the synthesis process light directly and indirectly affects. Gold seed arrays, fabricated via nanoimprint lithography (NIL), are placed in reaction vessels and stirred constantly within low-light reaction chambers that are lined with reflective foil. Arrays are then exclusively subjected to single color LED irradiation with controlled intensity and duration while inside the isolated reaction chamber. In the separate aging process, growth solutions are irradiated before arrays are introduced to the solution, and arrays are then exclusively grown in the absence of light. The growths are periodically monitored through spectrophotometry in the UV and visible spectrums of light (UV-VIS) and imaged via Scanning Electron Microscopy (SEM). Individual plate height and angle of growth are determined through Atomic Force Microscopy (AFM). Overall, these experiments provide a fundamental insight into the effects of light on the growth of nanostructures with photochemically sensitive substances.

Investigating the Role of Enah in Dorsal Root Ganglia Invasion of the Spinal Cord

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The connection between the Peripheral Nervous System (PNS) and Central Nervous System (CNS) is essential for both sensory perception and motor control. To establish this connection, Dorsal Root Ganglia (DRG) axons must navigate to and enter the Dorsal Root Entry Zone (DREZ). DRG axons move through extracellular environments using finger-like processes composed of actin filaments to reach the DREZ. Injury to DRG axons in cases such as Brachial Plexus Avulsion sever the PNS to CNS connection leading to sensory and motor control loss, and clinical regeneration of DRG neurons remains unsuccessful. Through genetic screening, the Smith lab found the gene Enah, the zebrafish homolog of Enabled, to be essential for DRG invasion in zebrafish. CRISPR-mediated knockout of Enah in transgenic zebrafish revealed a reduction in DRG entry. The navigation of DRG axons relies on an extraordinarily complex and dynamic process to remodel the actin cytoskeleton. Enah is known to stabilize polymerizing actin filaments. We therefore asked whether the actin-stabilizing function of Enah facilitates DRG entry. We performed genetic experiments to show that loss of Enah reduces axon entry. This loss can be rescued by pharmacological treatments with actin-stabilizing drugs. Furthermore, we examined actin filament structure in Enah knockouts by timelapse imaging of live zebrafish larvae. Our data suggest that the actin-regulating functions of Enah are critical for DRG axon entry during CNS/PNS development.

Elucidating the Role of Iroquois Transcription Factor 4a in Kidney Development

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Chronic kidney disease is a very prominent problem in the US, impacting millions of Americans a year. In order to better address this issue, more advanced knowledge of kidney function and development is critical. The kidney is a vital organ responsible for both filtering waste from the blood, and balancing ion concentrations in the blood. These roles are carried out by the nephron, the functional unit of the kidney. The nephron consists of a glomerular blood filter attached to a segmented epithelial tubule, which is organized into functionally distinct domains. Although nephron development is vital to renal function, there has been limited research into the genetic mechanisms that regulate their formation. There are many genetic pathways that play crucial roles in the various components of kidney formation, one of which is the Iroquois (Irx) gene family of transcription factors. Of these, Iroquois transcription factor 4a (irx4a), is previously unstudied in regards to its role in nephrogenesis. The zebrafish is a useful model to study nephron development due to the high conservation in nephron composition with humans. Here, using whole mount in situ hybridization to assess spatiotemporal expression, we found that irx4a was expressed in the proximal straight tubule (PST) and distal early (DE) regions of the embryonic nephron. Interestingly, irx4a transcripts were first expressed at around the 12 somite stage (ss) in the renal progenitors which found these segment regions. Further irx4a+ cells exhibited a speckled expression pattern within the nephron, which suggests that it is likely a marker of either multiciliated cells (MCCs) or transporter cells. In the zebrafish kidney, MCCs are responsible for driving fluid flow through the kidney. We hypothesize that irx4a acts redundantly with irx2a, another member of the Iroquois gene family, because the two genes have very similar expression patterns. irx2a is expressed in MCCs, so it is believed that irx4a is expressed in MCCs as well. To examine whether irx4a is required for nephrogenesis, irx4a deficient embryos were created through the microinjection of a splice blocking morpholino. irx4a knockdown caused a significant decrease in the number of MCCs present in the nephron. This implies that irx4a plays a vital role in proper MCC formation. Future studies will examine the consequence of dual irx4a/2a deficiency on MCC ontogeny. Gaining insight into the function of genes such as irx4a will allow for greater understanding of how kidneys develop. This knowledge could provide critical insight into better understanding and eventually treating congenital and chronic kidney diseases.

Investigation of Apolipoprotein L1 Function in Zebrafish Pronephros Development

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Chronic kidney disease (CKD) is a significant health burden to approximately 15% of the United States population, and continued research to understand the onset of CKD is needed. Mutations in Apolipoprotein L1 (APOL1) have been linked to increased risk for kidney disease and failure in African and African American populations. APOL1 is a component of the cholesterol metabolism pathway, and APOL1 is highly expressed in various tissues of the mammalian body, including the kidney. However, little is understood about the role of APOL1 in these tissues. To investigate this gap in knowledge, we are using the zebrafish animal model. The zebrafish embryonic kidney, or pronephros, is an ideal model for kidney disease and development due to its high conservation with the mammalian kidney. In addition, the zebrafish is one of the few organisms to possess apol1 in its genome. We created an apol1 loss of function model using an antisense morpholino oligonucleotide (MO) and assessed renal development at critical stages, namely 24 hours post fertilization (hpf), 36 hpf, and 48 hpf. Whole-mount in situ hybridization (WISH) was utilized to examine the gene transcripts of cell populations involved in pronephros differentiation, development, and segmentation. Here, we show that the knockdown of apol1 significantly reduced the expression of podocytes, cells that are integral to forming the filtration barrier of the pronephros, lineage-based makers wt1b and nephrin. Further investigation of other podocyte progenitor markers is necessary to understand whether apol1 affects other factors of podocyte development. To do this, multiple WISH analyses will be performed using the early podocyte markers mafba and lhx1a at 15 somites, 24 hpf, and 36 hpf. Furthermore, our preliminary data suggests that the knockdown of apol1 by MO decreases the length of the distal early (DE) and increases the length of the distal late (DL) at 24 hpf, which we detected using the lineage markers slc12a1 (DE) and slc12a3 (DL). To confirm whether this phenotype is consistent across development, further WISH analyses will be performed using slc12a1 and slc12a3 at 36 hpf and 48 hpf. Taken together, our results demonstrate that apol1 may have a role in renal progenitor fate choice and proper development of the podocytes and distal tubule. Further investigation and the use of other gene editing tools are necessary to provide insight into apol1 in pronephros development. To this end, we are currently establishing a genetic apol1 knockout line to confirm these phenotypes across models. The long-term goal of these studies is to leverage the attributes of the zebrafish to gain novel insights into Apol1 function that can be used to inform research to delineate the roles of APOL1 in the mammalian kidney.

SEnergy Transfer in Lead Halide Perovskite-Molecular Hybrid Assemblies for Light Harvesting Applications

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In order to facilitate efficient energy capture and transfer in semiconductor nanocrystals, sensitizing dyes are applied to create assemblies that can capture photons over a wide range of visible and near-infrared regions. With proper tailoring, these assemblies can trigger nonlinear optoelectronic processes like triplet-triplet annihilation (TTA) and singlet fission (SF); processes that theoretically overcome power conversion efficiency barriers in traditional photovoltaic cells. In this work, we focus on CsPbI3 nanocrystals (NCs) as the sensitizer and the near-infrared tricarbocyanine dye (IR-125) as the acceptor molecule. The presence of functional groups on the IR-125 dye helps to bind strongly on the surface of the CsPbI3 NCs with an apparent association constant of Kapp = 2 x 105 M-1, facilitating energy transfer between the two species. Fluorescence quenching of CsPbI3 NCs and evolution IR-125 emission was observed upon increasing the concentration of IR-125 dye. The origin of IR-125 emission was investigated using photoluminescence excitation (PLE) spectroscopy. The contribution of CsPbI3 excitation in the IR-125 emission was observed from PLE spectra. The kinetic analysis of the energy transfer was achieved using photoluminescence (PL) lifetime and transient absorption spectroscopy. The PL lifetime of CsPbI3 decreased from 42.8 ns to 2.4 ns for 0 and 4.6 uM IR-125, respectively and had a calculated energy transfer efficiency of $\boldsymbol{\varphi ET}$ = 94.4%. Transient absorption spectroscopy further supported evidence of energy transfer through faster decay kinetics of CsPbI3 bleaching at 670 nm in the presence of IR-125 dye. Taken together, the evidence provided in this paper confidently supports the presence of a singlet energy transfer between CsPbI3 and IR-125 hybrid assemblies and the importance of tailoring sensitizing dye - semiconductor assemblies to optimize power conversion efficiency.

Poly(propylene carbonate)-based Composite Polymer Electrolyte for Solid-state Lithium-ion Batteries

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The need for renewable and efficient energy sources continues to increase with technological advancements, especially given the adverse impact of fossil fuels on the environment. Along with renewable resources like solar power, batteries provide readily available energy with better environmental outcomes. Lithium-ion battery technology is the focus of many efforts toward sustainable energy due to its significant advantages over other energy storage systems. Owing to the properties of the lithium ion, lithium-ion batteries deliver higher energy density by taking up smaller space with fast charging, along with long-lasting performance. However, the choice of electrolytes used in these batteries greatly affects their performance by regulating the flow of lithium-ions. Traditional liquid electrolytes are hazardous due to flammability, thermal instability, and leakage whereas solid electrolytes are a safer alternative with higher energy density and thermal stability. Solid-state composite polymer electrolytes (CPEs) are a class of solid electrolytes which combine ion conductive ceramics with flexible polymers for good interfacial contact with the electrodes; this makes them a viable option. In this study, the CPE consisted primarily of poly(propylene carbonate) (PPC), one of the few polymers stable at high voltage and flexible for good contact with excellent oxidative stability. This CPE was prepared by cross-linking polymers poly(ethylene glycol) diacrylate (PEGDA) and poly(ethylene glycol) methyl ether acrylate (PEGMEA) in the presence of PPC to increase the stability and mechanical strength of the polymer matrix. The lithium salt, lithium bis(trifluoromethane)sulfonimide (LiTFSI), was added to aid ion conduction through the polymer. The ceramic used was Li6.4La3Zr1.4Ta0.6O12 (LLZTO), which can enhance mechanical strength and ionic conductivity while maintaining flexibility. After preparing the CPE, it was characterized using various tools to understand its structure and properties better. Differential scanning calorimetry was used to study the material's thermal properties, and Raman spectroscopy was used to understand the ion states, as this impacts ion transport properties. Conductivity tests were also done to determine the performance of the CPE in a coin cell. All tests were performed on samples without and with 10 wt.% LLZTO to assess the effect of LLZTO particles on the polymer properties and performance. Based on the conductivity of LLZTO, the CPE's performance is expected to be better than that of previously studied solid polymer electrolytes. This study is anticipated to provide further insights into the structure-property relationship of new materials that can replace liquid electrolytes with safer solid electrolytes without sacrificing ionic conductivity.

Estimation of Socket-stump Pressure in Transfemoral Amputees Combining Electronic Fabrics and Pressure Models

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I. Introduction

Prosthetics and orthoses have significantly transformed the biomedical field, leading to numerous positive health outcomes. However, despite their considerable advantages, these devices can cause physical discomfort, including the development of pressure points resulting from the interaction between compliant human tissue and the rigid or padded structures. This project aims to address the knowledge gap in characterizing interface pressures in prosthetics and orthotics outside of clinical settings. By introducing innovative sensor designs and advanced algorithms, the project aims to enable precise and continuous measurement of interface pressure for extended durations in the user's natural environments. This is achieved by capitalizing on acquired pressure data from sensors and leveraging the initial geometry of the sensor array to establish a comprehensive pressure distribution map, facilitating the detection of pressure points.

II. Methods

After reading literature such as [1] it was concluded the methodology of recording pressure readings could be improved. A new sensing design was developed using computer-aided design (CAD) software and 3D printed. The design comprised two layers, one fixed and the other capable of movement in one direction, with a load distributor attached. Four bolts cantilevered off the inner layer that pass through the outer layer ensured the movement only occurred in the singular direction. This new design enhanced the normal loading of the sensor, resulting in more accurate data. In order to test how accurate the sensors are, a temporary lower limb model was constructed, seen in Fig. 1. The lower leg segment was created using an aluminium pylon to simulate the tibia and fibula, while the upper leg segment consisted of a 3D printed femur bone [2] and ballistic gel to mimic compliant tissue. Due to being in the building process of the experimental set up, no experiments have been conducted using the sensors yet. The goal before returning to Ireland in regards to testing is to place the sensor sleeve in between the ballistic gel and the prosthetic, with a force plate that will be positioned below the artificial lower limb to record ground reaction forces. Forces will be applied to the femur bone manually in various directions to simulate motion. Pressure and force readings will be recorded from both the sensors in the prosthesis and the ground reaction forces from the force plate. These readings will be compared and analysed

III. Expected Results

The expected results from a successful testing will depict that the sum of forces in each direction recorded from the force plate will closely match the sum of forces recorded by the sensors. These values if successful, will be within a small tolerance, indicating the effectiveness of the sensing design. It also portrays how the sensing design could be effective in the natural environment of the prosthesis user.

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Exploring Sea Turtle Locomotion Mechanics for Biomimetic Robotic Design

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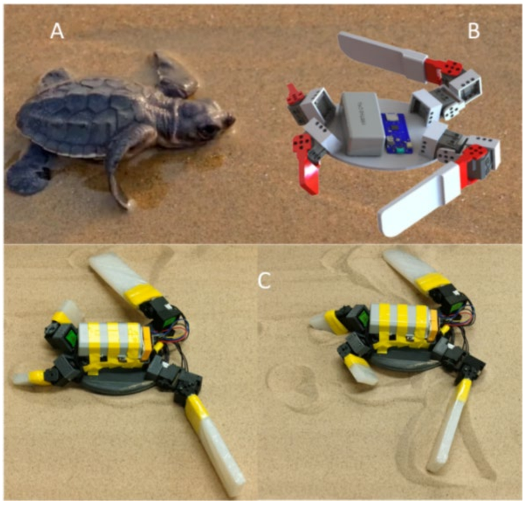
Sea turtle inspired robots provide a unique combination of traits which could prove to make them very effective in a range of roles from delivery or amphibious search and rescue robots to providing an alternative to conducting biological research on live specimens of at-risk creatures. The aim of this project was to investigate the different motion gaits (methods e.g., walking or running for humans) of sea turtles and their effectiveness in different environments through the use of a small turtle robot. Of particular interest was testing various gaits and fin configurations on different surfaces to find which combinations were most effective to allow future designs to be optimised for their given task.The robot consisted of a 3D printed body and 4 fins controlled by 6 servo motors. An IMU was added to enable the robot to travel further in the same direction without veering off course as this improved the repeatability of experiments. The dimensions of the fins were designed to be similar to those of baby sea turtles in terms of relative size compared to body and length of front fins in comparison torear fins. Fins of various stiffness were developed to investigate which performed best in each circumstance.

It was found that the robot was capable of traversing many environments including, sand, pebbles, steps and inclines (hard surface and sand inclines). In particular the “diagonal” gait, consisting of the right front and left rear working in tandem followed by the left front and right rear fins, performed well in all situations. The “all together” gait, consisting of all 4 fins working synchronously, worked well on sand but the symmetry of its motion sometimes lead to it getting stuck more easily on pebbles and particularly on steps. The rigid flippers made the robot traverse more quickly particularly on sand and on steps. However, on pebbles and when approaching obstacles, they sometimes would make contact which would cause substantial rotational or translational motion which could result in the robot being pushed off course, backwards or getting stuck. The more flexible flippers however would simply deform around these obstacles allowing the robot to continue more easily. This shows that there are different environments where the optimal stiffness varies. This explains why real sea turtles are able to vary the stiffness of their fins on command.

It was clear from these findings that the sea turtle robot form has promise and can be utilised for various purposes due to the wide range of operating conditions and adaptability with different gaits being used depending on the task. Future versions can use a combination of the different gaits and even use machine learning and variable stiffness fins to be able to decide which gait and fin stiffnessis optimal for the particular situation it finds itself in.



Mechanical Deformation Induced By Tumor Progression Analyzed In Patient MRIs

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The study of tumor progression as it relates to brain cancer has been an ongoing curiosity. There are several factors that promote tumor growth, including solid (mechanical) stress and tissue stiffness. Estimating the physical stresses that tumors generate in brain cancer patients is one way to further analyze the tumor microenvironment. The compression of brain tissue by tumor mass is understood to be a major cause of the life-threatening symptoms observed in patients diagnosed with brain cancer. Brain tumor solid stress damages surrounding normal brain tissue by compressing blood vessels and neurons, and reducing the number of neurons in the cortex. In this study, our goal was to characterize the deformation of the brain due to a growing tumor. We did this by tracking anatomical landmarks in the brain over multiple longitudinal MRI images. This work could offer insight into how brain tumors exert a mechanical force on the surrounding brain tissue and cause damage leading to the abnormalities and dysfunctions in the brain. Since the tumors grow in such a confined space, being the cranium, they must replace or displace the surrounding tissue being affected. Two classic tumor phenotypes are nodular and infiltrative tumors; modular tumors exert a higher solid stress as they expand and displace surrounding tissue while infiltrative tumors replace healthy brain tissue as they grow. Understanding this type of progression, particularly in the cases of different tumor phenotypes, is essential to advancing our knowledge of brain cancer, and developing effective treatment strategies. This research has the potential to revolutionize our understanding of brain tumors and the role of the mechanical microenvironment in their progression.

Characterizing the Effects of Ethanol in Zebrafish Embryonic Nephron Development

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Fetal alcohol spectrum disorders (FASD) encompass a broad range of effects caused by prenatal alcohol exposure. In the United States, conservative estimates place the incidence of FASD at a rate of 5 in 100 births. Children afflicted with FASD can have symptoms ranging from congenital defects of the heart, eyes, and kidneys, as well as poor development of facial structures such as the nose and mouth. Invisible complications such as learning disabilities, socio-developmental delays and emotional disorders are also highly prevalent. There is no known cure for FASD and in utero detection methods are not available. In terms of urinary tract defects, kidney and renal related maladies remain an underreported and rather uncommon diagnosis within patients with FASD. In order to better understand the renal phenotypes associated with prenatal alcohol exposure, we employed the zebrafish, Danio rerio, a vertebrate species well suited for developmental nephrology and teratological work that has been used extensively to model FASD. We treated zebrafish embryos with ethanol to examine its effects on the formation of renal cell populations. Using whole mount in situ hybridization for renal cell markers, we determined that both tubule and non-tubule populations are greatly perturbed by alcohol exposure. Further, we found that retinoid acid, a vitamin A derived chemical associated with mitigating the effects of ethanol exposure in zebrafish and other animals, was sufficient to partially rescue several renal alterations caused by early ethanol exposure. These studies have revealed several consequences of ethanol exposure, as well as interactions with retinoid acid, that lead to the deregulation of kidney development, thereby contributing novel insights relevant to the broader field of FASD research.

Charge-Functionalized Nanofiltration Membranes Exhibit Multi-Valent Ion Rejection

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In recent years, nanofiltration (NF) membranes have been used as means to modulate the flux of target solutes for the purpose of both water filtration and solute recovery. The principal means by which these separations occur is through steric-based rejection, which can be achieved by making the pore size of the NF membrane smaller than the target solute. More recently, work has been done to alter the membrane chemistry, allowing for specific ligands to be attached to the pore wall that afford more specific control over the mass transfer of target solutes. One of the best ways to go about doing this is through targeted electrostatic interactions between the ligand in the pore wall and the solute itself.

The purpose of this study is to explore these electrostatic interactions and expand on their efficacy, efficiency, and consistency. By first adding an azide moiety to the membrane pore-wall chemistry, copper-catalyzed alkyne-azide cycloaddition (CuAAC) "click" chemistry reactions can be performed to attach many alkyne-terminated ligands to the membrane for the purposes of functionalization. Functionalization reactions were monitored in various stages using Fourier-Transform Infrared Spectroscopy (FT-IR), wherein the peak indicating an azide group at ≈2100 cm-1 would quickly disappear over the course of 120 seconds. This would occur because during the reaction the azide moiety would react with the alkyne-terminated ligand to form a triazole. In this study, the alkyne-terminated primary amine propargylamine is utilized to provide a positive charge that will electrostatically repel multivalent cations from undergoing transport through the membrane.

Here we show that by functionalizing the membrane pore wall with pH-dependent charged ligands, consistent high rejection of multivalent cations can be achieved. During rejection experiments using a 1 mM solution of MgCl2, 65% rejection was observed, however, this value decreased as the concentration of the solute increased, likely due to ionic interactions between the Magnesium and Chloride ions. These findings add to the usefulness of NF membranes as a means to perform separations, act as filters for harmful contaminants to otherwise potable water, and improve the recovery rates for valuable trace metals in solution. I anticipate this study to be a starting point for more sophisticated automation of membrane functionalization, as well as ligands that demonstrate pH-independent performance.

Animating Construction Process of Modular Lapped Reinforced Concrete Connections to Accelerate Nuclear Building Project Schedules

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Nuclear power plants are expensive to build with long building construction project duration. Decreasing the on-site construction time of nuclear facilities would significantly reduce the overall project costs. Construction of reinforced concrete (RC) buildings by assembling and connecting large prefabricated modules would allow significant efficiencies in construction. However, state-of-practice connection designs typically used in non-nuclear buildings do not provide the structural strength and stiffness continuity required for nuclear applications. This project, funded by the Nuclear Regulatory Commission, is experimentally and numerically investigating the design, materials, behavior, durability, and construction of lapped connections for safety-related nuclear RC buildings. The novel lapped geometry of the connection provides "face-to-face" (rather than "end-to-end" or "butt") joint interfaces with large surfaces to develop the required continuity of the strength and stiffness of the structure. The lack of straight-line discontinuities across the structure thickness enhances the connection performance. Work conducted as part of the Vincent P. Slatt Fellowship by the Center for Sustainable Energy at Notre Dame developed a visual animation of the proposed construction process for nuclear RC buildings with lapped connections.

Understanding the Interactions Between Non-Equilibrium Plasma and Nanomaterials in a Fluidized Gliding Arc

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Non-equilibrium plasmas have emerged as a way to enhance traditional thermal catalysis methods. They produce a highly reactive environment of radicals, free electrons, and high energy gas molecules that can drive reactions at atmospheric temperature and pressure, as opposed to traditional catalysis methods. Gliding arcs are a relatively new non-equilibrium plasma reactor configuration that produce a plasma with unique, spatially varying properties by flowing gas between diverging, knife-like electrodes. Gliding arcs are very promising for catalysis purposes because of their ability to handle high throughput of gas (the proposed reactor operates at over 10 L/min opposed to other reactors which operate at under 1 L/min). In this work, we designed and fabricated a gliding arc reactor with a sprouted bed to support a chemical catalyst. We defined operating parameters for this gliding arc (flow rate, plasma voltage, plasma power and gas composition) to catalyze reactions in a mixture of methane, argon, and nitrogen gas, as a model chemical system to recycle methane into valuable chemicals at point-of-source refining operations using only electrical power. Some interest has risen in reacting methane with nitrogen (N2), which is readily available in the atmosphere, to produce value-added chemicals such as pyrrole and pyridine. Many studies have put effort into reacting methane and nitrogen in dielectric barrier discharges (DBDs), but gliding arcs may prove to be better suited in achieving the desired reactions.

Graph Embedding in Quantum Computers

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Many graph problems are NP-complete or harder, making the discovery of efficient quantum algorithms for them of significant value. Thus, how such graphs can be “embedded" in an array of qubits in a quantum computer, and how many such qubits will be needed to embed the graph are interesting questions. This poster documents an organized attempt to at least partially answer these questions through experimentation. It reviews the currently known embedding algorithms, and applies them in a controlled fashion to a variety of graphs with specific characteristics. Multiple topologies for qubit couplings are considered, first idealized and then with the presence of faulty qubits. The minorminer, clique, and layout-aware algorithms are used to embed complete, fixed uniform degree, random degree, and power law graphs into the D-Wave Chimera, Pegasus, and Zephyr topologies for various graph sizes and percentage of faulty qubits. Each embedding is evaluated for accuracy, time to completion, the number of qubits used in the embedding, and the size and diameter of the resulting “qubit chains.” Results show that clique embedding is by far the fastest algorithm, but requires the greatest number of qubits and is limited to complete graphs. The layout-aware algorithms yielded the highest percentage of valid embeddings for complex problems. Minorminer, the industry standard embedding algorithm, prevailed in nearly every other case.

Land and Cultural Loss: Touristic Development and Neoliberal Reforms in the Yucatán Peninsula

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In 1968, representatives from the Bank of Mexico, Antonio Enríquez Savignac and Ernesto Fernández, traveled to the Yucatán Peninsula and decided to build a modern city, now known as Cancun, with no regard for the area's history. Unfortunately, this resulted in poor campesinos experiencing land dispossession due to touristic development, which was exacerbated by neoliberal policies funded by the Mexican government and foreign investors. In 1994, the Mexican economy collapsed, also known as the 'Tequila Crisis,' due to the sudden devaluation of the peso. As a result, the International Monetary Fund and President Bill Clinton designed a $50 billion bail-out fund with the agreement that Mexico implement neoliberal reforms. These policies encouraged tariff-free trade, foreign investments, trade deregulation, and privatization of land. Moreover, communal lands or ejidos were also privatized and sold to giant corporations who continued to dispossess and exploit the labor of campesinos. Despite the Mexican government's argument that neoliberal policies and touristic development promote economic growth and healthy competition, poor campesinos experience detrimental social effects such as wealth disparities, falling wages, job insecurity, and extreme violence. Tourist destinations such as Cancun and surrounding areas have a higher cost of living, which forces poor campesinos to borrow money from Mexican and foreign banks that inflate interest rates, making it impossible for people to pay off their debt with their meager wages. In my research, I analyze how campesinos in the Yucatán Peninsula have progressively lost their communal lands to large corporations for touristic development due to neoliberal policies that entail loans, debt, and land ownership. The land dispossession of Indigenous people in the Yucatán Peninsula also signifies a loss of culture, political autonomy, financial independence, community, and the right to a dignified home.

Constructing Heterogeneous Systems with Migrating Threads

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Heterogeneity is clearly increasing, especially as “accelerators” burrow deeper and deeper into different parts of an architecture. What is new, however, is a rapid change in not only the number of such heterogeneous cores, but in their characteristics, such as ISA or memory architecture. This project is focused on the problem of how to construct efficient programs that combine multiple heterogeneous concurrent threads. We focus on addressing the issues created by the need today for large software stacks when programming heterogeneous systems. We propose the use of a migrating thread architecture as a “glue” to alleviate this issue. To test our proposal, we conducted an experiment utilizing a heterogenous platform where all threads share the same memory to solve a common machine learning problem that mirrors the kind of computation for which a migrating thread architecture could be useful. The platform used is an NVIDIA Jetson TX1 which contains an NVIDIA Tegra system on a chip that integrates an ARM64 CPU and a Maxwell GPU. The problems tested are a series of sparse support vector machine classification problems that utilize multi-threaded stochastic gradient descent for optimization. We focus on an implementation of the Hogwild++ algorithm in which the GPU, running CUDA, performs local cluster model vector updates while the CPU performs periodic cross-cluster synchronization. We provide an analysis of the existing architectural and software limitations of CUDA that provide obstacles to efficient SGD and arrive at several architectural “lessons learned” which should help guide the future development of such systems.

Analyzing a Hands-On Project-Based Data Science Course Impact on Students' Own Attitudes and Engagement Within the Field

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Due to the growing collection of data in nearly every industry, there is an increasing demand in the labor market for individuals with data science skills. There is also a recognition that understanding data is part of citizen education to the general public. However, exposure to data science concepts and skills is still limited before people reach secondary education, and is particularly limited to underrepresented minority (URM) students. In addition, the complex nature of the field often leads to feelings of self-doubt and apprehension among high school students.

Therefore, through the SEEDS program the first part of our research involves creating and delivering a 3-week curriculum for high school URM students. We first engaged in trainings and curriculum development prior to the arrival of the high school students participating. Our curriculum encompasses various subjects such as data science, statistics, coding, privacy, and ethics, aiming to introduce students to these important fields. It is specifically designed to equip them with both soft and hard skills through educational development, goal setting, journals, and dedicated project work time. To ensure organization and progress, we created a comprehensive program calendar that outlines the daily schedules and our desired outcomes. The students are also actively engaged in the acquisition and analysis of a dataset, employing the scientific method as a guiding framework. They are diligently working towards completing their project, which will culminate in the creation of an ePortfolio.

The second part of our research involves investigating how the three-week project-based program can influence high school students' attitudes – self-efficacy, awareness, aspirations, and interests – and engagement towards data science, and how the current curriculum can be improved.

The research design involved a pre-course, mid-course, and post-course survey administered to a sample of high school students enrolled in the TRiO Program at the University of Notre Dame. The survey was adapted from validated scales to measure attitudes and engagement towards data science (Ober et al., 2023; Whitney et al., 2019).

We hypothesize that implementing hands-on, project-based approaches in curricula can enhance students' positive attitudes and engagement. By providing opportunities for students to actively engage with data science tools and methods, educators can help them develop the skills, confidence, and motivation necessary for successful careers in this rapidly evolving domain.

Throughout the program, we actively observed and assessed our own abilities as facilitators and mentors. We sought feedback from students regarding their learning experiences and adjusted our teaching strategies accordingly. By reflecting on our own strengths and areas for growth, we aim to continually enhance our effectiveness as educators, ensuring that we provide the best possible learning environment for our students. The results from the survey in addition to the hands-on, project-based data science course reflections will highlight findings on students' self-efficacy beliefs. These findings will have significant implications for data science education in South Bend, and how the SEEDS Program will proceed in the future.

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Design of Peptide-Based Macrocycles for Discovery of Novel Glucose Binders

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Mentor:
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The rising prevalence of diabetes and high blood glucose present a serious risk worldwide, proving the need for further research into more effective methods to regulate glucose levels. The molecular recognition of glucose through responsive biomaterials has proven highly valuable in increasing the efficiency of diabetic treatments like insulin. Nonetheless, the development of glucose sensors capable of identifying glucose in an aqueous solution remains a significant challenge due to the high solubility of glucose and its chemical similarity to water. Taking these characteristics into consideration, dynamic-covalent recognition and macrocyclic receptor designs have been proposed for the effective and selective binding of glucose. This study aims to use combinatorial libraries of dynamically interacting molecules to screen and optimize for glucose binding. Taking inspiration from glucose-binding proteins in nature, peptide-based libraries were synthesized and characterized by mass spectroscopy and nuclear magnetic resonance (NMR) spectroscopy. The modification of these peptides with different prosthetic groups was also carried out in order to expand the structural diversity of the combinatorial library. Ongoing efforts are underway to screen and characterize these compounds for glucose recognition and binding, toward their eventual applications in blood sugar monitoring and insulin delivery.

Knockdown of Cathepsin B Protein in Mammalian Epithelial Cells Affect Cell Proliferation during ECM-detachment

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When cells detach from the extracellular matrix (ECM), they undergo anoikis, a caspase protein dependent cell death that metastasizing cancer cells are resistant to. Studies have shown that the overexpression of cathepsin B is correlated with metastasis. During ECM-detachment, the lysosomes are observed to be permeabilized and proteases including cathepsin B, are released into the cytosol. Cathepsin B has shown to have a dual role in both the lysosome and cytosol, regardless of pH levels. Cathepsin B's ability to maintain its protease activity across different pH levels makes it an ideal candidate for use in various cell death pathways. This study aimed to assess the effect of cathepsin B on ECM-detached cell viability. Therefore, we performed a western blot to validate the cathepsin B knockdown. Caspase activity was measured using a caspase glo assay to determine the potency of the cathepsin B inhibitor and two cathepsin B short hairpin knockdowns during ECM-detachment. Sytox Green assays were used to analyze cell viability. The Sytox Green assay utilizes a fluorescent dye that only binds with nucleic acids from compromised membranes, allowing for an accurate measurement of dead cells in a population. Caspase activity displayed increases in both cathepsin B short hairpin knockdowns compared to the cathepsin B inhibitor during ECM-detachment.We observed that cells treated with cathepsin B demonstrated a decrease in cell viability when compared to untreated controls via Sytox Green assays.We are currently working on conducting a western blot to measure the abundance of other proteases including cathepsin D and cathepsin L in order to determine if these cathepsin proteins are attempting to compensate for cathepsin B activity.

The Effects of Oxidation and Reduction on a Platinum-Tin Alloy on Silica and Models of Physical Properties

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Mentors:
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A platinum-tin catalyst was made by adding chloroplatinic acid hexahydrate and stannous (II) chloride to an HCl solution, which was then used to put platinum-tin nanoparticles on a silica support via incipient wetness impregnation. The catalyst was reduced with H2 to pretreat it. This was done to have a high surface density of active sites. The catalyst was put in a plasma reactor with quartz wool. A titanium electrode coated in Kapton was inserted to direct current. The reaction was done at -20C to prevent thermal pathways and was analyzed in how it gets reduced in H2 and oxidized in air. Looking at a lissajous plot for both reactions, it shows that the burning voltage was higher in H2. The capacitance on the dielectric was much smaller in air conditions compared to H2 conditions, possibly suggesting that the H2 was more reactive. Additionally, other tests including X-ray crystallography, physisorption, chemisorption, Raman spectroscopy, and thermogravimetric analysis were run on the catalyst to provide insight on its properties. Finally, structural models were used to gain additional insight on how the catalyst might operate. References show that the crystal structure of the nanoparticle is hexagonal close packed. Surface plane Bravais Miller Indices are [0,1,-1,2] and converting that to Miller Indices gives [1,2,2]. With this information as well as Python and the Atomic Simulation Environment module, a model of the surface of the platinum-tin nanoparticle was constructed, which was then used in density functional theory calculations on the vibrational frequency and energy of the nanoparticle employing the Vienna Ab-Initio Software Package.

NSF Engineering Research Center
Center for Innovative and Strategic Transformation of Alkane Resources

Characterization of Tributyl Phosphate Radicals by Electron Spin Resonance

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Tributyl phosphate (TBP) is a vital component in nuclear waste separation processes. These processes use TBP dissolved in an alkane solution to extract uranium and plutonium from an aqueous acidic solution of dissolved fuel. Therefore, it is important to understand the radiolytic degradation pathways of TBP, since it absorbs high doses of ionizing radiation during the separation process. We have studied TBP-derived radicals using room-temperature spin-trapped electron paramagnetic resonance (EPR) and low-temperature EPR.

The spin-trapped method allows for the identification of short-lived TBP radicals as spin-trap adducts. A spin trap, N-tert-butyl-α-phenylnitrone (PBN), was dissolved in TBP at various concentrations (2 mM, 10 mM, and 40 mM). To estimate the radiation-chemical yield (G-value) of TBP radicals, we measured the EPR kinetics in situ upon X-ray irradiation of TBP solutions with PBN. Fricke dosimetry was performed to estimate a dose rate using iron (II) sulfate heptahydrate in sulfuric acid with thiocyanide, and the dose rate was calculated to be 211 mGy/s. After PBN was dissolved in TBP and saturated with argon, the solution was placed in BLAUBRAND® disposable micropipettes and sealed with hot glue to ensure no oxygen could penetrate the solution and reduce the signal. Using a Spellman DF3 high-voltage power supply (50 kV, 30 mA) and Thales THX X-rays, the solutions were irradiated. EPR spectra were measured using Bruker EMXplus spectrometer in X-band with ER4119HS standard resonator. This experiment produced spin adducts with α(N) = 13.6 G and α(H) = 1.8 G, which corresponds to alkyl TBP radicals. Signals from H-trapped adducts were noticeably lacking from the spectra, indicating PBN traps mainly alkyl radicals from TBP. The corresponding G-value for the formation of TBP-derived radicals was 2.18 mol/J at room temperature.

For low-temperature EPR experiments, TBP was degassed using a Freeze-Pump-Thaw method, sealed under vacuum, and frozen in liquid nitrogen. The frozen samples were then irradiated with ca. 15 ns 8 MeV electron pulses from an electron linear accelerator. After irradiating, the samples were placed in a Dewar flask filled with liquid nitrogen, and the EPR spectra were acquired at 77K. The resulting spectra were initially thought to be a combination of four different alkyl radicals derived from TBP during irradiation at different carbon atoms (C1-C4) in the alkyl chain (R1-R4). After careful spectrum processing, the simulated spectrum was fitted as a combination of R1 (10%), R3 (52%), and R4 (37%).

The last attempted experiment was to examine the radicals produced by TBP when it was mixed with n-dodecane, as the PUREX process uses a TBP in kerosene solution to extract uranium and plutonium from spent nuclear fuel. Though samples were degassed and sealed under vacuum, the low-temperature EPR experiment showed an accumulation of additional n-dodecane radicals together with TBP radicals. We also noticed that the EPR pattern and intensity change with and without the addition of TBP. We plan to continue our work on this experiment to quantitatively compare the yield of TBP radicals in solvent and without spectra.

Cortical Thickness Patterns in Developing Fetal Brains with Spinal Bifida

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The human brain is well-known for its highly folded cerebral cortex that develops during gestation. Prior work has established that cortical thickness is linked to foldedness in adult brains and across primates [1][2]. The cortex is found to be thinnest at sulci—the bottom cusps of brain folds—and increases on a spectrum as the curvature of a region approaches that of gyri—the tops of the brain's ridges. It is thought that neurodevelopmental disorders such as autism spectrum disorder and attention-deficit hyperactivity disorder result in differences in cortical thickness. Spina bifida is another severe disorder, wherein the neural tube fails to fully develop, and is associated with abnormal brain development [3]. It is of research interest to quantify how spina bifida affects cortical thickness variations, and in turn reflect on the impact of abnormal cortical morphology. In this study, we calculate cortical thickness of in utero fetal brains, allowing for comparison between developing neurotypical fetal brains and those with spina bifida pathology in their cortical thickness variations. In this work, we utilized MRI 3 tissue-class segmentation data for N=25 subjects (7 neurotypical, 18 pathological diagnosed with spina bifida) of gestational ages 23, 25 and 27 weeks from the publicly-available FeTA 2.2 dataset [4]. Using Python, we separated white and gray matter segmentations, with subcortical structures removed. We manually performed interior filling of each segmentation in ITK-SNAP to create closed surfaces that would facilitate 3D reconstructions. Thereafter, we manually demarcated the longitudinal fissure boundaries each with a segmentation mask. We used these masks in Python to split each white and gray matter segmentation into individual left and right hemisphere segmentations. We reconstructed 3D surfaces for each hemisphere for both the white matter and the gray matter using the AFNI neuroimaging toolbox. For post-processing, we applied 20-40 iterations of Laplacian smoothing and 15-30 iterations of mesh refinement by subdivision alongside mesh repairs to each subject brain in Meshlab. We calculated the cortical thickness at each vertex as the closest linear distance between the white matter and gray matter surface [1], and then calculated the distribution across each hemisphere. Our cortical thickness calculations might help us distinguish brains with spina bifida, facilitating identification and an understanding of how such brains vary morphologically from neurotypical brains, as well as their differences between hemispheres. In future work, we will analyze the remaining data from the FeTA 2.2 dataset to make more generalized conclusions.

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Lagrangian Cloud Model Validation and the Effects of Aerosol Count

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Understanding how clouds form and being able to model their behavior is critical to weather prediction. The Lagrangian cloud model (LCM) is an emerging computational tool for studying clouds, and while it has many advantages, it has not been fully verified. The main advantage of the LCM is its ability to resolve aerosols and related microphysical processes.

The first few simulations we ran were compared against an intercomparison study of other, non Lagrangian, Large Eddy Simulations. This was to serve as a first order evaluation of the model's performance against well established methods. We discovered that while several things did match as expected, there were also many things that did not match up. Of particular interest was the amount of liquid water (ql), which was almost 2 orders of magnitude too low. Looking into the lack of liquid water uncovered two things, both with regards to the aerosols used by the simulation. First, the aerosols used in previous simulations consisted purely of ocean salts. While this makes some sense, as these are simulations of the Marine Atmospheric Boundary Layer (MABL), it is not in line with measured aerosol types and distributions which also include man made pollutants. Second, the concentration of aerosols was much lower than expected with the high cases having approximately 750 aerosols per cubic centimeter. In actuality, less than 1000/cm3 is low and counts above 100,000 are high.

In order to address these discoveries, a series of simulation cases were run with the new aerosol distribution and various amounts of aerosols: pristine (7/cm3), low (75/cm3), medium (7500/cm3), and high (750,000/cm3). The pristine and low simulations performed as expected with the low case having more ql than the pristine. The medium simulation did not complete but looked to follow the expected trend having more ql than the low case. Both the medium and high cases ran into extreme stability problems we are currently attempting to solve. Once the model is properly verified, it will allow us to better understand the dynamics of cloud formation within the MABL and give us another tool to compare other simulations against.

A Mobile App for Guided Human-Computer Interaction Fuzz Testing of Small Uncrewed Aerial Systems

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Small Unmanned Aerial Systems (sUAS), such as drones, must meet diligent safety requirements when used in emergency response scenarios. This requires careful design and testing of the hardware, software, communication networks, and human-interaction points in a system as failure in any of these areas can lead to serious accidents. We are therefore creating a mobile application to aid in human-interaction testing. Our goal is to guide humans through the testing process in order to identify potential failures that can occur when humans provide wrong inputs to the system. In our mobile application, users will be provided a set of instructions with live prompts on when to perform various tasks while testing the drones. Example tasks include switching flight modes, pressing the killswitch on the motors, and changing the position of the throttle – all during the flight. Tests are executed first in simulation and ultimately with physical drones following a rigorous safety analysis and mitigation process. The success of the mission will be assessed in two ways, first by directly monitoring the drone to determine if it completed the planned flight without incident, and second by eliciting feedback from the operator via a form in our mobile app. Our application will serve as a useful digital communication tool between the drones and the user. Through the process of making this application, our team has learned about human-computer interaction, wireframing, prototyping, new programming languages, and MQTT messaging networks. We first began by learning React Native and JavaScript and creating an example app to hone in on our new skills. We then made Figma wireframes for our app. We then tried to connect them to Anima, an app that turns the wireframes to react code and then connects them to MQTT. We ended up not using Anima because it only worked with web development, not app development. We decided to utilize the Figma prototypes as a reference for design choices and hard code the app ourselves using Visual Studio Code and Expo Go. To create the app, we used the programming skills we learned at the beginning of summer, such as JavaScript and React Native. We created multiple screens and connected all of them with MQTT (a messaging network system) to a backend mission planner which monitors the flight and generates task prompts at appropriate time. Our mobile app subscribes to MQTT and is notified when a task should be performed. The app will show the user the tasks they need to complete in real time. The user utilizes existing interfaces, such as the drone’s Radio Controller or Graphical User Interface (GUI) to perform the task. By the end of the summer we plan to execute experiments with physical sUAS using the mobile app.

Micro-Organoids Generation by a Gel Droplet Platform for Cancer Drug Screening

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Several alternatives have been applied for modeling disease progression. In the context of cancer progression modeling, spheroids provide a more physiologically relevant tumor microenvironment by incorporating cell-cell interactions, extracellular matrix (ECM), oxygen/nutrient gradients, and hypoxic regions which better reflect the complexity of solid tumors. They also can exhibit increased drug resistance compared to 2D cultures which allow a better prediction of the efficacy of anticancer agents. However, the spheroids' production is limited due to their reproducibility and time consumption.

To tackle this issue we proposed the production of microgels using an elliptical pipette for cell encapsulation by droplet emulsion for high-throughput drug screening. The controlled cell microenvironment created by the uniform microdroplets enhances the reproducibility of the micro-organoids. The microdroplets are uniformly created in < 5 minutes for a single channel. This can be applied to a larger scale to use multi-channel systems at an efficient rate. Furthermore, the uniformly distributed size of the microdroplets can control the size of the tissue constructs to increase their reproducibility.

Uniform microdroplets ranging from 280 to 360 μm were generated using an elliptical pipette with norbornene-modified hyaluronic acid (NorHA) polymer. Prostate (LNCaP) and ovarian (RFP-OVCAR5) cancer cells were seeded on an Aggrewell for generating spheroids of sizes lower than 200 μm to avoid hypoxia. The spheroids were encapsulated using the polymer solution and combinations of DTT and MMP-sensitive crosslinker to allow for ECM degradability and increase the rate of the cell proliferation. Viability assays were performed after day 1. The amount of viable cells was ~83%. WST-1 proliferation assays were carried out by estimating the mitochondrial activity of the cells exhibiting an increase in the cell count from 24 hours to 48 hours after the spheroid encapsulation.

These accomplished results demonstrate the successful creation of a platform for high-throughput drug screening and can be applied to various cell-lines and tumor microenvironments.

PGAM5, a Regulator of Cancer Cell Survival

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The phosphoglycerate mutase protein PGAM5 has been found to be a regulator of cancer cell viability. Recently, the protein was implicated in the regulation of antioxidant activity within cancer cells. A recently published paper described that within extracellular-matrix attached cells, PGAM5 forms a ternary complex and tethers with NRF2 (a master regulator of antioxidants) and KEAP1 (a regulator of NRF2) proteins, both of which regulate antioxidant activity within the cell. Furthermore, a new study finds that within extracellular-matrix detached cells PGAM5 has been found to take on a somewhat different function likely due to an altered structure, and the loss of the protein diminishes ROS levels within the cells. Our study sought to characterize the various functions of PGAM5 in attachment and detachment settings within cancer cell lines. To begin, a knockdown of the PGAM5 gene was introduced in triple negative breast (231s) and cervical cancer (HELAs) cells using a lentiviral vector, and successful knockdown was confirmed through Western blotting. Soft agar colony assays (ECM-detached) were performed using different cancer cells and results showed that the loss of PGAM5 in BSO-treated cancer cells did not have a significant effect on colony formation. Colony formation assays (ECM-attached), are also being performed with different cancer cells, and we predict that the loss of PGAM5 in BSO-treated cancer cells will lead to a decrease in colony formation. Multiple trials of qRT-PCR and Western blot analysis were performed in order to quantify the mRNA and protein levels of NQO1 (a NRF2 target) and GCLC (another NRF2 target involved in glutathione synthesis) in both attachment and detachment conditions within the cancer cells that lacked PGAM5. These results showed that in attachment conditions, the mRNA and protein levels of the genes increased significantly in cancer cells that lacked the PGAM5 protein compared to cancer cells that did not contain the PGAM5 knockdown. However, in detachment conditions, the mRNA and protein levels of the genes did not significantly increase in PGAM5-lacking cancer cells when compared to PGAM5-containing cancer cells. Finally, PGAM5 was probed through Western blot in different cancer cell lines both in attachment and detachment conditions and it was found that in detachment conditions, there is likely a structural modification to the PGAM5 protein due to the appearance of a doublet band not seen in attachment conditions. Taken together, these results suggest that the loss of PGAM5 renders cancer cells in attachment conditions more sensitive to antioxidant inhibitors due to an increased dependency on antioxidant gene/protein expression seen by the increase in antioxidant genes/proteins. Furthermore, in detachment conditions, the loss of PGAM5 does not necessarily affect the response of cancer cells to antioxidant inhibitors (the lack of increase in antioxidant genes/proteins supports this), and this is likely because PGAM5 has a function unrelated to regulating antioxidant activity through the NRF2/KEAP1 complex. Through the results of this study, greater understanding of PGAM5 and its role in attachment versus detachment settings within cancer cells was reached.

Machine Learning Methods for Spectrum Occupancy

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Cellular networks are critical to 21st-century life. We rely on these networks for a range of essential services that we can access from our mobile devices. Mapping out cellular network coverage is an essential part of designing cellular networks, but generating these maps is a time-consuming process. Physics-based simulation models can be used to estimate coverage maps, but these are computationally expensive to generate and often do not capture the variability found in the real world. This research project examines the use of deep learning models in computing urban cellular coverage maps. The model is a 2D convolutional neural network with encoder-decoder architecture, similar to what is often used in image segmentation tasks. The training dataset consists of input tensors that map out buildings and transmitter locations. The dataset's targets are coverage maps for a given transmitter location. These target maps were determined using simple ray-tracing mechanisms. Once trained these deep learning models can be very accurate for samples in the training data, the main problem is to see if a model's predictions generalize to other scenarios. This project investigates how well the trained models generalize across different cities that were not in the training dataset. The model's generalization ability will be evaluated by first partitioning the available cities into a training set and testing set. The model will be trained to minimize an MSE loss function on the training cities. The model's generalization about will be evaluated using the Intersection-over-Union metric on samples in the testing dataset. The outcomes of this assessment protocol will be used to assess how well the trained model generalizes to different urban landscapes.

Amia Calva Show Extensive Chewing to Reposition Prey before Swallowing

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Food transport, how an organism manipulates prey items and moves them to the stomach during feeding, is crucial to animals' survival. This is especially true in fishes, as the large majority of predatory fishes swallow their prey whole. This causes challenges when the prey item is large, and many fishes will even consume prey larger than the predator. So how exactly do fishes transport these large food items to the stomach once they are consumed? How are predators able to consume food items without a mobile tongue or shearing teeth to break down the prey into smaller pieces? Answers to these questions lie in food transport, but the mechanisms involved are poorly understood. Sparse studies have examined chewing/repositioning behaviors, prey transport, and swallowing in carp, tilapia, catfish, and stingrays, with variable conclusions across taxa. This study examines the kinematics of food processing in Amia calva, a generalist predator in the Holostean clade, basal to teleosts in the fish phylogeny - a part of the tree that is missing from the existing literature. We digitized XROMM datasets, created animations, analyzed 15 chews across 2 separate trials in R, and compared the data to other behaviors and across species. Preliminary analysis shows extensive prey repositioning over a series of chews before a swallow. Furthermore, comparison with strikes shows lower but still surprisingly high bone rotations during most chew cycles. Further analyses will quantify the relationship between bone and prey motion, giving us a better understanding of the kinematics of processing in fishes.

The Effect Of Repeated Experimental Design Parameters on the Alignment Between Top-Down Attentional Control and Volitional Control

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Visual attention has been shown to be significantly impacted by top-down information. Recently, the previous assumption that top-down attentional control is directly aligned with volitional control has been proven false by assessing participants' feeling of agency during a spatial cueing task with 3 different cue validity conditions (Gibson et al., 2023). Gibson et al. (2023) found that there were individual differences in the participants' ratings in agency (differing amounts of alignment) across multiple cue validity conditions (25%, 70%, & 100% valid), thus proving that the previous assumption wrong. To investigate what increases the alignment between top-down attentional control and volitional control, Gibson et al. (2023), ran a follow-up experiment to assess the extent to which selecting a parameter of the experiment affects the alignment. They tested this by allowing participants to select which spatial cue was used. The results showed that the ability to select a parameter of the experiment significantly increased the alignment between the two types of attentional control across participants. An interesting effect was observed, in which a portion of the participants selected the same spatial cue over and over again. This phenomena led Gibson et al. (2023) to running an additional follow up experiment, where they prevented the participants from selecting the same spatial cue twice in a row. The results from this third experiment showed a reduction in alignment between the attentional controls across participants. These results imply that the repetition of experimental parameters in a spatial cueing task have an effect on the alignment between top-down attentional control and volitional control. However, the extent to which repetition affects the alignment between top-down attentional control and volitional control has not been directly studied. We are planning to run a series of four experiments to test this. The four experiments will also utilize a spatial cueing task that contain three cue-validity conditions that were used in the previously mentioned experiments conducted by Gibson et al. (2023). The four experiments will differ in the amount the target in a current trial reappears in the same location as the target in the previous trial. Experiment 1 will have 0% repeated target locations, experiment 2 will have 25% repeated target locations, experiment 3 will have 50% repeated target locations, and experiment 4 will have 75% repeated target locations. We hypothesize that the results of the experiment will show that the effect of repetition of target location will have an additive effect and not a main effect to the alignment between top-down attentional control and volitional control. Meaning that the rate that agency ratings increase as cue validity increases is expected to remain constant across the proposed experiments, but the overall agency scores would increase as the percentage of repeated target location trials increases.

A Novel Graphical User Interface for Rapid Deployment of Multi-Drone Missions for Emergency Response

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Drone Response is designed to support the rapid deployment of multiple small Unmanned Aerial Systems (sUAS) for emergency response missions. There are many factors to consider when deploying multiple drones on diverse missions, especially for rapid response situations across a wide variety of environments. The operator must quickly assess the emergency situation, formulate a conceptual plan of action, and define the mission in a way that is understandable to the drones, so that they can conduct the mission autonomously.

In emergency response situations, it is important for users of any technical background to be able to quickly plan missions for the rapid deployment of drones. The previous approach to planning drone missions involved a complex multi-step process that relied on predefined mission workflows. This limited the operator's flexibility in defining task sequences and did not support dynamically adjusting mission requirements, making deployment inefficient to plan and update. The previous GUI also lacked support for customizing missions, such as the ability to specify when cameras are on or off, or the option to assign a drone to be the coordinator of a mission.

This project focuses on redesigning the current method of creating drone missions to enable more intuitive user interactions. We began roughly sketching ideas on a whiteboard and brainstorming a variety of ways to implement the current uses in more straightforward processes while maintaining necessary functionality. This allowed us to plan the updated concept of creating drone regions and routes that can be toggled on and off in the map view, and updated by dragging specific features and drones onto each. For example, if a drone needs to be deployed in a particular region, it can simply be placed in the area, which also displays the corresponding behaviors that can be edited directly on its map view. The drone can additionally be dropped in other regions and routes to rapidly assign or change the sequence of tasks it must follow, thus eliminating the previous multi-step method. The new strategy enables all mission planning to efficiently occur on one screen, with a toolbar displaying icons for all available behaviors at the top and currently active drones displaying real time information on the side.

Through this process, Figma was used to assist in visualizing each of the ideas and sharing the complete redesign goals. By consistently receiving input from others and confirming user understanding of each aspect of the design, each piece of the interface from the icons to the overall interaction methods has been reimagined for optimal use. The current stage of the process involves implementing the design using Angular and continuing to note potential improvements as the interface is updated. Future plans involve conducting user studies with fire fighters and other potential users using wireframes, then progressing to simulations and ultimately real-world deployments.

High-Frequency Response of Thermoelectrically Coupled Nanoantennas

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This work investigates the frequency response of dipole and spiral thermoelectrically coupled nanoantennas (TECNAs) in vacuum. In a TECNA, a resonant antenna excited by long-wave infrared radiation (LWIR) heats the hot junction of a nanoscale thermocouple (NTC). The resulting signal measured at the cold junction of the NTC is a voltage corresponding to the intensity of the optical excitation. The antenna nature allows for TECNAs to be designed to detect infrared radiation of a narrow range of wavelengths and polarizations. In this work, dipole TECNA thermopiles, multiple NTCs connected in series, have been designed to measure linearly polarized light, and spiral TECNAs have been designed to measure circularly polarized light of a specific handedness. An acousto-optic modulator (AOM) is used instead of a mechanical chopper, allowing the optical input signal to be modulated up to 100 kHz. In vacuum, heat loss due to air decreases, resulting in an increased thermal time constant. Therefore, in vacuum, responsivity improves, and device response cutoff frequency decreases. For dipole TECNA thermopiles, responsivity improves significantly in vacuum (by 3x-5x), and measured cutoff frequencies in vacuum (20-35 kHz) are consistently lower than those at atmospheric pressures (35-45 kHz). For singular spiral TECNAs excited by circularly polarized light of matching handedness, responsivity improves significantly in vacuum (by ~2.8x), and measured cutoff frequencies in vacuum (~16 kHz) are consistently lower than those at atmospheric pressures (~38 kHz). The measured extinction ratio in vacuum (~4.5x) is lower than in atmosphere (~8x) but is still large enough that spiral TECNAs can differentiate between right-handed and left-handed circularly polarized light. Future work is needed to characterize TECNA frequency response in vacuum at frequencies higher than 100 kHz.

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Mechanobiological Interactions of Macrophages and Cancer Cells in Glioblastoma Models

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Glioblastoma (GBM) is a brain cancer that builds an immunosuppressive tumor microenvironment and is resistant to immunotherapy. Solid stress – a mechanical force originating and transmitted from cells and extracellular matrix – is thought to contribute to reduced efficacy of anti-cancer therapy. Macrophages are the dominant infiltrating immune cell in GBM tumors, and can comprise nearly half of the tumor bulk. However, macrophage response to solid stress in GBM is largely unknown. In order to explore the interaction between mechanics and macrophages in the glioblastoma tumor microenvironment (i.e., determine their phenotype and function), we compressed murine (Raw 264.7) and human (THP-1) macrophage cell lines in 2-D monocultures. We analyzed changes to macrophage immunity via flow cytometry, western blot, and RT-qPCR. Moreover, we created 3-D spheroids co-cultures of macrophages and glioblastoma tumor cells (U87) using droplet spheroid formation in agarose gels, followed by staining and phagocytosis assay to explore if and how macrophages interact with and/or kill cancer cells. In the future, in vivo studies will provide further insight about the mechanisms underlying macrophage fate and function with the ultimate the goal of reprogramming the GBM microenvironment and developing new therapeutic strategies for clinical trials.

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