2024 SUMMER

UNDERGRADUATE

RESEARCH

SYMPOSIUM

WEDNESDAY, JULY 24

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

Dahnke Ballroom

Welcome to the
Summer Undergraduate Research Symposium and 3MT Competition

Wednesday, July 24, 2024 | 10:00 a.m. - 2:00 p.m.

Dahnke Ballroom, 7th Floor of Duncan Student Center

Schedule

10:00 - 11:00 a.m.	Poster Session 1 (68 Posters)
11:00 - 11:15 a.m.	Break
11:15 a.m. - 12:15 p.m.	Poster Session 2 (68 Posters)
12:15 - 12:30 p.m.	*Buffet Luncheon and Seating for 3MT Competition
12:30 - 2:00 p.m.	2nd Annual 3MT Competition (14 Contestants)

*The luncheon is a ticketed event, requiring check-in at the registration table.

Student Participation

Poster Session	150 Students	136 Posters	23 REU Programs
	6 Colleges	2 Divisions	24 Departments/Centers/Institutes
3MT Competition	26 Preliminary	14 Finalists	11 REU Programs

There are 150 students presenting 136 posters, representing 23 summer REU programs, 6 colleges, 2 divisions, and 24 departments, centers, and institutes at the University of Notre Dame and Saint Mary's College. Fourteen (14) students are competing in the 2nd annual Three Minute Thesis (3MT) Competition, representing 11 summer REU programs (BioREU, CBE SMASH, COS-SURF, ESURE, Naughton Fellowship, NDnano NURF, ND PREP, Physics REU, RAMP, Slatt Fellowship, SROP).

Summer REU Programs

Advanced Wireless Research Experiences (AWaRE), National Science Foundation (NSF) SpectrumX, College of Engineering

Biological Sciences Research Experiences for Undergraduates (BioREU), National Science Foundation (NSF), College of Science

Center for Computer Assisted Synthesis Summer Undergraduate Research Fellowship (C-CAS SURF), National Science Foundation (NSF), Notre Dame Research

Center for Innovative and Strategic Transformation of Alkane Resources (CISTAR Young Scholars), College of Engineering

Center for Research Computing (CRC) Internship, Notre Dame Research

Center for Stem Cells and Regenerative Medicine Summer Undergraduate Research Fellowship, (SCReM-SURF), College of Science

Chemistry-Biochemistry-Biology Interface (CBBI) Program, National Institute of Health (NIH), College of Science

College of Science Summer Undergraduate Research Fellowship (COS-SURF)

CSE Summer Enrichment Program, College of Engineering

Engineering Summer Research Experience (E-SURE), College of Engineering

Glynn Family Honors Program, College of Arts and Letters and College of Science

International Summer Undergraduate Research Experience (iSURE), Notre Dame Global

Mary E. Galvin Science and Engineering Scholars Program, College of Science

Naughton Fellowships, The Graduate School

NDnano Undergraduate Research Fellowship (NURF), Notre Dame Research

ND-PREP, The Graduate School

Research Access and Mentoring Program (RAMP), Institute for Scholarship in the Liberal Arts, College of Arts and Letters

Saint Mary's College Summer Program

Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU, National Science Foundation (NSF), College of Engineering

Summer Education and Engagement for Data Science (SEEDS), Lucy Family Institute for Data & Society, Notre Dame Research

Summer Research Opportunities Program (SROP), The Graduate School

Vincent P. Slatt Fellowship for Undergraduate Research in Energy Systems and Processes (Slatt), Notre Dame Energy, Notre Dame Research

Warren Center for Drug Discovery, William K. Warren Foundation, College of Science

Colleges, Divisions, and Departments/Centers/Institutes

Students conducted summer research in collaboration with REU programs and faculty in 6 colleges, 2 divisions, and 24 departments, centers, and institutes at the University of Notre Dame and Saint Mary's College.

College of Arts and Letters

- Africana Studies
- Anthropology
- Classics
- Institute for Scholarship in the Liberal Arts
- Psychology

College of Engineering

- Aerospace and Mechanical Engineering
- Chemical and Biomolecular Engineering
- Civil and Environmental Engineering and Earth Sciences
- Computer Science and Engineering
- Electrical Engineering

College of Science

- Biological Sciences
- Center for Stem Cells and Regenerative Medicine
- Chemistry and Biochemistry
- Physics and Astronomy
- Warren Center for Drug Discovery

Notre Dame Global

Notre Dame Research

- Center for Computer Assisted Synthesis
- Center for Research Computing
- Lucy Family Institute for Data & Society
- Notre Dame Energy
- NDnano

Mendoza College of Business

- IT, Analytics and Operations
- Management & Organization

Saint Mary's College

- Biology
- Chemistry

The Graduate School

Thank you for attending and supporting undergraduate research!

Poster Session 1

Summer Undergraduate Research Symposium

Wednesday, July 24, 2024

10:00-11:00 a.m. | Dahnke Ballroom

#	Presenter(s)	REU Program
1	Suzanne Aguirre	SROP
2	Angel Alberto Anchondo	Slatt Fellowship
3	Amanda S. Arrufat Román	Slatt Fellowship
4	Joseph Bertram	ESURE Program
5	Taylor Bias	COS-CBBI
6	Sebastian Brock	ESURE Program
7	Aleah Brokemond	ND PREP
8	Julia Bub	Saint Mary's College
9	David Castillo	BioREU
10	Levi Cherek	Slatt Fellowship
11	Anastasía Chibucos	BioREU
12	Olivia Chima-Anyanka	BioREU
13	Kun Yuan Chu	BioREU
14	Mary Collis	Saint Mary's College
15	Adrian Cooney	SROP
16	Emmanuel Correia	Slatt Fellowship
17	Natalie Crowner	CBE SMASH
18	Juan Cruz	SROP
19	Aaron Davis	BioREU
20	Batradz Djikkaity	Slatt Fellowship
21	Emile Dogbe-Gakpetor	SROP
22	Sonia Egenberger	CBE SMASH
23	Darwin Estrella Vicente Caelan Templeton	CSE Summer Enrichment
24	Aidan Finn Sarah Harman	SEEDS
25	Lauren Fuentes-Velazquez	CBE SMASH
26	Susan Joy Gicheha	CRC Internship
27	Carolyn Habel	CISTAR Young Scholars
28	Theo Hatfield	BioREU
29	Corrie Hickson	SROP
30	Raquel Hilton	RAMP
31	Dirichi James-Osondu	SROP
32	Adesola Johnson	BioREU
33	Calvin Josenhans	CRC Internship
34	Hanna Ketsela	SROP
35	Aashin Khatiwada	CISTAR Young Scholars
36	Eoin Killian	Naughton Fellowship
37	Karenna Kung Jordan Letu Vivian Quach Zichu Wang	C-CAS SURF
38	Rafael Labuto	CSE Summer Enrichment
39	Melanie Mae Langgle	SROP
40	Monica Leal Palma Samantha Yu	NDnano NURF
41	Jun Wei Lee	RAMP
42	Anna Leuer	ESURE Program
43	Jack Mangione Leonardo Molina	CSE Summer Enrichment
44	Jonathan Mimnaugh	CSE Summer Enrichment
45	Tanay Nagar	C-CAS SURF
46	Sarah Oliva	Slatt Fellowship
47	Sebastian Pirela	AWaRE
48	Delaney Reynolds	ESURE Program
49	Ben Roper	ESURE Program
50	Mario Ruiz-Yamamoto	CISTAR Young Scholars
51	Ebony Saccento	ND PREP
52	Olivia Sayani	NDnano NURF
53	Reem Shehayib	ESURE Program
54	Jerica Siberón	SROP
55	Anna Skoropad	NDnano NURF
56	Vaibhavi Sunkara	CBE SMASH
57	India Turner	SROP
58	Kiara Vazquez Narvaez	ND PREP
59	Jean Galliano Vega Diaz	CBE SMASH
60	Marcos Villarreal	CBE SMASH
61	Grace Waddell	COS-SURF
62	Oisín Wade	Naughton Fellowship
63	Caleb Wafer	ND PREP
64	Rachel Wallace	CBE SMASH
65	Victor Williams	Slatt Fellowship
66	Carl Xu	AWaRE
67	Swindar Zhou	NDnano NURF
68	Alayne Ziglin	SROP

See back for posters grouped by REU program →

Poster Session 1

Grouped by REU Program

#	Presenter(s)	REU Program
47	Sebastian Pirela	AWaRE
66	Carl Xu	AWaRE
9	David Castillo	BioREU
11	Anastasía Chibucos	BioREU
12	Olivia Chima-Anyanka	BioREU
13	Kun Yuan Chu	BioREU
19	Aaron Davis	BioREU
28	Theo Hatfield	BioREU
32	Adesola Johnson	BioREU
17	Natalie Crowner	CBE SMASH
22	Sonia Egenberger	CBE SMASH
25	Lauren Fuentes-Velazquez	CBE SMASH
56	Vaibhavi Sunkara	CBE SMASH
59	Jean Galliano Vega Diaz	CBE SMASH
60	Marcos Villarreal	CBE SMASH
64	Rachel Wallace	CBE SMASH
37	Karenna Kung	C-CAS SURF
37	Jordan Letu	C-CAS SURF
37	Vivian Quach	C-CAS SURF
37	Zichu Wang	C-CAS SURF
45	Tanay Nagar	C-CAS SURF
27	Carolyn Habel	CISTAR Young Scholars
35	Aashin Khatiwada	CISTAR Young Scholars
50	Mario Ruiz-Yamamoto	CISTAR Young Scholars
5	Taylor Bias	COS-CBBI
61	Grace Waddell	COS-SURF
26	Susan Joy Gicheha	CRC Internship
33	Calvin Josenhans	CRC Internship
23	Darwin Estrella Vicente	CSE Summer Enrichment
23	Caelan Templeton	CSE Summer Enrichment
38	Rafael Labuto	CSE Summer Enrichment
43	Jack Mangione	CSE Summer Enrichment
43	Leonardo Molina	CSE Summer Enrichment
44	Jonathan Mimnaugh	CSE Summer Enrichment
4	Joseph Bertram	ESURE Program
6	Sebastian Brock	ESURE Program
42	Anna Leuer	ESURE Program
48	Delaney Reynolds	ESURE Program
49	Ben Roper	ESURE Program
53	Reem Shehayib	ESURE Program
36	Eoin Killian	Naughton Fellowship
62	Oisín Wade	Naughton Fellowship
7	Aleah Brokemond	ND PREP
51	Ebony Saccento	ND PREP
58	Kiara Vazquez Narvaez	ND PREP
63	Caleb Wafer	ND PREP

#	Presenter(s)	REU Program
40	Monica Leal Palma	NDnano NURF
40	Samantha Yu	NDnano NURF
52	Olivia Sayani	NDnano NURF
55	Anna Skoropad	NDnano NURF
67	Swindar Zhou	NDnano NURF
30	Raquel Hilton	RAMP
41	Jun Wei Lee	RAMP
8	Julia Bub	Saint Mary's College
14	Mary Collis	Saint Mary's College
24	Aidan Finn	SEEDS
24	Sarah Harman	SEEDS
2	Angel Alberto Anchondo	Slatt Fellowship
3	Amanda S. Arrufat Román	Slatt Fellowship
10	Levi Cherek	Slatt Fellowship
16	Emmanuel Correia	Slatt Fellowship
20	Batradz Djikkaity	Slatt Fellowship
46	Sarah Oliva	Slatt Fellowship
65	Victor Williams	Slatt Fellowship
1	Suzanne Aguirre	SROP
15	Adrian Cooney	SROP
18	Juan Cruz	SROP
21	Emile Dogbe-Gakpetor	SROP
29	Corrie Hickson	SROP
31	Dirichi James-Osondu	SROP
34	Hanna Ketsela	SROP
39	Melanie Mae Langgle	SROP
54	Jerica Siberón	SROP
57	India Turner	SROP
68	Alayne Ziglin	SROP

Poster Session 2

Summer Undergraduate Research Symposium

Wednesday, July 24, 2024

11:15-12:15 p.m. | Dahnke Ballroom

#	Presenter(s)	REU Program	#	Presenter(s)	REU Program
1	Zosia Bolde	C-CAS SURF	39	Sara Murray	Slatt Fellowship
2	Nagham Bou Hamdan	ESURE Program	40	Jalynn Murry	COS-Warren Center
3	Bella Cantillo	Slatt Fellowship	41	Jincy Njenga	AWaRE
4	Gabriel Cruz-Ruiz	Slatt Fellowshipg	42	Sbeydi Ponce Duarte	ESURE Program
5	Konrad Czyzewski	COS-SURF	43	Brett Alan Porter	CSE Summer Enrichment
6	Caitlynn Day	BioREU	44	Safa Rahman	ND PREP
7	Jing Ding	iSURE	45	Conner Rauguth Jacob Ackerley	CRC Internship
8	Triet Do	ESURE Program			
9	Austin Dungan	BioREU	46	Oliver Reyes	ND PREP
10	Raghad Elgamal	AWaRE	47	Kamilah Richardson	CBE SMASH
11	Humyra Ferdus Christopher Joseph	CSE Summer Enrichment	48	Inyam Ricketts	Galvin Scholars Program
			49	Nathan Rodriguez	CSE Summer Enrichment
12	Roan Finkle	CRC Internship	50	Roman Sally	CSE Summer Enrichment
13	Steven Frye	ND PREP	51	Joshua Sam	CBE SMASH
14	Lucas Gruber	BioREU	52	Sierra Sanne	SROP
15	Zelalem Haile Vera Casquero García	CSE Summer Enrichment	53	Julia Savino	COS-SURF
			54	Marie Schafer	NDnano NURF
16	Ellie Han	ESURE Program	55	Makenna Schroeder	Saint Mary's College
17	Yiqin He	iSURE	56	Patrick Schwartz	ESURE Program
18	Karyme Hernandez Torrens	CBE SMASH	57	Irvin Aldair Servin Arredondo	NDnano NURF
19	Catherine Hubbard	BioREU	58	Musab Shaikh	BioREU
20	Stephen Hynes	Naughton Fellowship	59	Peyton Shrader	SROP
21	Aliciana Ilias	CBE SMASH	60	Allie Stormer	CBE SMASH
22	Ada Jaramillo	CBE SMASH	61	Sirui Tang	CRC Internship
23	AJ Jones Makuza Mugabo Verite	CSE Summer Enrichment	62	Mrunal Vibhute	CRC Internship
			63	Tianqi Wang	CRC Internship
24	Samuel Kaczor	C-SC&RM SURF	64	Diana Whitfield	SROP
25	Cora Keogh	Naughton Fellowship	65	Bella Wiebelt-Smith	BioREU
26	Georgie Kersman	Saint Mary's College	66	Sequoia Williams	RAMP
27	Giorgi Kharchilava	Slatt Fellowship	67	Jemima Yoon	SROP
28	Elliot Kim	CSE Summer Enrichment	68	Oscar Zavala	CBE SMASH
29	Kathleen Lavelle	BioREU			
30	Mary Ann Martinez Molina	BioREU			
31	Christopher Mc Aleer	Naughton Fellowship			
32	Aoife McLoughlin	Naughton Fellowship			
33	Joshua Moeller	COS-SURF			
34	John Moore	Slatt Fellowship			
35	Kayleigh Moran	Naughton Fellowship			
36	Fernando Moreno	SROP			
37	Arav Mukherjee	AWaRE			
38	Aidan Murray	Slatt Fellowship			

See back for posters grouped by REU program →

Poster Session 2

Grouped by REU Program

#	Presenter(s)	REU Program
10	Raghad Elgamal	AWaRE
37	Arav Mukherjee	AWaRE
41	Jincy Njenga	AWaRE
6	Caitlynn Day	BioREU
9	Austin Dungan	BioREU
14	Lucas Gruber	BioREU
19	Catherine Hubbard	BioREU
29	Kathleen Lavelle	BioREU
30	Mary Ann Martinez Molina	BioREU
58	Musab Shaikh	BioREU
65	Bella Wiebelt-Smith	BioREU
18	Karyme Hernandez Torrens	CBE SMASH
21	Aliciana Ilias	CBE SMASH
22	Ada Jaramillo	CBE SMASH
47	Kamilah Richardson	CBE SMASH
51	Joshua Sam	CBE SMASH
60	Allie Stormer	CBE SMASH
68	Oscar Zavala	CBE SMASH
1	Zosia Bolde	C-CAS SURF
5	Konrad Czyzewski	COS-SURF
33	Joshua Moeller	COS-SURF
53	Julia Savino	COS-SURF
40	Jalynn Murry	COS-Warren Center
12	Roan Finkle	CRC Internship
45	Conner Rauguth	CRC Internship
45	Jacob Ackerley	CRC Internship
61	Sirui Tang	CRC Internship
62	Mrunal Vibhute	CRC Internship
63	Tianqi Wang	CRC Internship
24	Samuel Kaczor	C-SC&RM SURF
11	Humyra Ferdus	CSE Summer Enrichment
11	Christopher Joseph	CSE Summer Enrichment
15	Zelalem Haile	CSE Summer Enrichment
15	Vera Casquero García	CSE Summer Enrichment
23	AJ Jones	CSE Summer Enrichment
23	Makuza Mugabo Verite	CSE Summer Enrichment
28	Elliot Kim	CSE Summer Enrichment
43	Brett Alan Porter	CSE Summer Enrichment
49	Nathan Rodriguez	CSE Summer Enrichment
50	Roman Sally	CSE Summer Enrichment
2	Nagham Bou Hamdan	ESURE Program
8	Triet Do	ESURE Program
16	Ellie Han	ESURE Program
42	Sbeydi Ponce Duarte	ESURE Program
56	Patrick Schwartz	ESURE Program

#	Presenter(s)	REU Program
48	Inyam Ricketts	Galvin Scholars Program
7	Jing Ding	iSURE
17	Yiqin He	iSURE
20	Stephen Hynes	Naughton Fellowship
25	Cora Keogh	Naughton Fellowship
31	Christopher Mc Aleer	Naughton Fellowship
32	Aoife McLoughlin	Naughton Fellowship
35	Kayleigh Moran	Naughton Fellowship
13	Steven Frye	ND PREP
44	Safa Rahman	ND PREP
46	Oliver Reyes	ND PREP
54	Marie Schafer	NDnano NURF
57	Irvin Aldair Servin Arredondo	NDnano NURF
66	Sequoia Williams	RAMP
26	Georgie Kersman	Saint Mary's College
55	Makenna Schroeder	Saint Mary's College
3	Bella Cantillo	Slatt Fellowship
27	Giorgi Kharchilava	Slatt Fellowship
34	John Moore	Slatt Fellowship
38	Aidan Murray	Slatt Fellowship
39	Sara Murray	Slatt Fellowship
4	Gabriel Cruz-Ruiz	Slatt Fellowshipg
36	Fernando Moreno	SROP
52	Sierra Sanne	SROP
59	Peyton Shrader	SROP
64	Diana Whitfield	SROP
67	Jemima Yoon	SROP

2nd Annual
Summer Undergraduate Three Minute Thesis (3MT) Competition

Wednesday, July 24, 2024

12:30-2:00 p.m. | Dahnke Ballroom

There are 14 REU students participating in the 2nd annual Three Minute Thesis (3MT) Competition, representing 11 REU programs. Contestants are listed below alphabetically. Each will explain their research in a language appropriate to a non-specialist audience within three minutes, using one slide. Three awards will be given: First Place and Second Place, determined by a panel of judges, and a People's Choice award, determined by the audience. Winners will receive cash prizes, thanks to the generosity of the Meruelo Family Center for Career Development. Thomas Meyers, Graduate Career Consultant for the College of Arts and Letters, will emcee the event.

3MT Contestant	REU Program
Katie Burns	College of Science Summer Undergraduate Research Fellowship (COS-SURF)
Adrian Cooney	Summer Research Opportunities Program (SROP), The Graduate School
Emmanuel Correia	Vincent P. Slatt Fellowship for Undergraduate Research in Energy Systems and Processes (Slatt), Notre Dame Energy, Notre Dame Research
Sarah Foess	Physics REU, College of Science
Theodore Hatfield	Biological Sciences Research Experiences for Undergraduates (BioREU), National Science Foundation (NSF), College of Science
Brian Joseph	College of Science Summer Undergraduate Research Fellowship (COS-SURF)
Eoin Killian	Naughton Fellowships, The Graduate School
Jun Wei Lee	Research Access and Mentoring Program (RAMP), Institute for Scholarship in the Liberal Arts, College of Arts and Letters
Reem Shehayib	Engineering Summer Research Experience (E-SURE), College of Engineering
Vaibhavi Sunkara	Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU, National Science Foundation (NSF), College of Engineering
Kiara Vazquez Narvaez	ND-PREP, The Graduate School
Grace Waddell	College of Science Summer Undergraduate Research Fellowship (COS-SURF)
Keyang (Swindar) Zhou	NDnano Undergraduate Research Fellowship (NURF), Notre Dame Research
Alayne Ziglin	Summer Research Opportunities Program (SROP), The Graduate School

MERUELO FAMILY CENTER
FOR CAREER DEVELOPMENT

10:00 – 11:00 A.M.
POSTER SESSION 1

ABSTRACTS

The Power of Parental Acceptance: How Perceived Parental Connection Shapes Youth Well-being

Suzanne Aguirre
Summer Research Opportunities Program (SROP)

Mentor, Contributors, Faculty Advisor:
Yunyan Zhao, Graduate Student
Jenny Padilla, Assistant Professor of Psychology
College of Arts and Letters

Abstract

Previous research underscores the importance of parental emotional availability in increasing self-esteem and reducing depressive symptoms among youth. Building on this, my research explores the distinct contributions of perceived maternal and paternal acceptance on adolescent well-being. This study examines the influence of youths' perceptions of maternal and paternal's acceptance on their self-esteem and depressive symptoms. Data was collected from 84 Mexican-origin two-parent families in the Northern Indiana area. Youth were between the ages of 12 and 18. Our findings reveal that both maternal and paternal acceptance are significantly associated with higher self-esteem and reduced depressive symptoms in adolescents, which highlight the critical roles both mothers and fathers play in different facets of adolescent mental health. In Mexican culture, the concept of familismo emphasizes strong family bonds and loyalty, which is particularly relevant here. Understanding these culturally specific dynamics is crucial for informing more effective family-centered interventions for Mexican-origin families. Our research underscores the importance of fostering positive parent-child relationships to mitigate adverse adjustment outcomes in adolescents, thereby promoting healthier and more resilient youth. By leveraging strong emotional connections with mothers and fathers, interventions can effectively support the mental health and development of adolescents. This study lays the foundation for further research into the nuanced impacts of mother- and father-adolescent relationships on youth outcomes, particularly within the context of Mexican-origin families.

Thermophysical Characterization of Concrete and Grout Materials

Angel A. Anchondo
Vincent P. Slatt Fellowship

Mentor, Contributors, Faculty Advisor:
Paul J. McGinn, Professor of Chemical and Biomolecular Engineering
Yahya C. Kurama, Professor of Civil and Environmental Engineering and Earth Sciences
Brad Weldon, Henry J. Massman Collegiate Professor in Civil Engineering
Subhash L. Shinde, Associate Director of ND Energy
College of Engineering
Craig M. Newtson, Interim Department Head and Professor of Civil Engineering
New Mexico State University

Abstract

Modular construction has become more popular as engineering has made progress with advanced technology. Modular construction of reinforced concrete buildings is done by pre-casting concrete structural components away from the building site, transporting them to the site, and placing and connecting them with other concrete components. The connections between the concrete components are often the most critical locations that govern the performance of these structures. This ongoing research is investigating the compatibility between concrete and cementitious grout materials in grouted connections for nuclear modular reinforced concrete building structures. For example, it is important to determine the coefficient of thermal expansion of adjoining concrete and grout materials to understand how the joints behave at high temperatures since dissimilar thermal deformations can cause structural or durability failure.

Materials tests were conducted at the Materials Characterization Facility (MCF) and at the department of Chemical and Biomolecular Engineering at the University of Notre Dame. The Thermo-Gravimetric Analysis and Differentials Scanning Calorimetry (TGA/DSC 3+) tests were conducted to evaluate cement paste and two different pre-packaged commercial grouts. Each material had three phases of weight loss and energy absorbed during high temperature exposure up to 1000° C. The paste and grout materials all had three endothermic phases; the first one being loss of water mass and the other two due to chemical decompositions. Furthermore, dilatometer measurements showed contraction of the cement paste at 600° C, while the grout products expanded with increased temperature. Additional results, including testing of limestone aggregate and cement paste-sand mixtures, will be presented from ongoing tests. Ultimately, this research is investigating ways to make the construction of nuclear reinforced concrete building structures more efficient, without compromising structural or durability performance as compared with conventionally built cast-in-place monolithic structures.

Simulating the Effect of External Electric Fields on the Glass Transition of 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide with Molecular Dynamics

Amanda Sofia Arrufat Roman
Vincent P. Slatt Fellowship

Mentor, Contributors, Faculty Advisor:
Fernando Carmona, PhD Candidate, Department of Chemical and Biomolecular Engineering
Yamil Colón, Assistant Professor of Chemical and Biomolecular Engineering
College of Engineering

Abstract

Ionic liquids (ILs), compounds composed entirely of ions with melting points below 100 °C, exhibit many beneficial properties for industrial processes and are becoming crucial in energy storage technologies. We present the findings from molecular dynamics simulations of the ionic liquid 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide ([Bmim][NTf2]) subjected to varying strengths of external electric fields (EEFs). Our goal is to compute and understand how EEFs influence the glass transition temperature (Tg) of this IL. For this analysis we used LAMMPS, and a recently established method to compute the Tg by graphically determining the break in linear behaviour more accurately. The IL was cooled from 380 to 150 K at a 5 K/ns cooling rate for determining the glass transition temperature and exposed to 12 electric fields of varying strengths, ranging from 0.000 to 0.100 V/Å. Preliminary results indicate that the Tg of [Bmim][NTf2] decreases with EEF, similar to results in the literature. These results are supported by previous analysis of the liquid phase dynamics and structure that reveals that the EEF reduces the activation energy for diffusion, lowering the energetic barrier for molecular movement and, as a result, decreasing the Tg. By enhancing our understanding of the thermodynamic properties of ILs, we move closer to designing improved solvents through the manipulation of their thermodynamic properties.

References:

- Brennecke, J. F.; Maginn, E. J. Ionic Liquids: Innovative Fluids for Chemical Processing. AIChE J. 2001, 47, 2384−2389.
- Carmona, F: et al. Consistent and reproducible computation of the glass transition temperature from molecular dynamics simulations J. Chem. Phys. 161, 014108 (2024)
- Carmona, F.; et al. Molecular Dynamics Simulation of the Influence of External Electric Fields on the Glass Transition Temperature of the Ionic Liquid 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide. The Journal of Physical Chemistry B 2023 127 (20), 4623-4632
- Joseph, K.; Navigating the Pros and Cons: Advantages and Disadvantages of Ionic Liquids. J Polymer Sci. 8:19. (2023)
- Moya, X.; Defay, E.; Mathur, N. D.; et al. Electrocaloric effects in multilayer capacitors for cooling applications. MRS Bull. 2018, 43, 291−294.

Simulating Parallel Graph Algorithms

Joseph Bertram
Engineering Summer Research Experiences (E-SURE)

Mentor, Contributors, Faculty Advisor:
Peter Kogge, Ted H. McCourtney Professor of Computer Science and Engineering
College of Engineering

Abstract

An example of an algorithm for graph processing is subgraph isomorphism, which allows one to extract a subset of graphs from a larger graph based on a pattern given. Such problems inspire the execution of graph algorithms in parallel instead of serial for efficient and faster manner of computation. To harness the power of parallel execution requires an in-depth study on the potential of such an architecture.

This project introduces a simple python package, called the Migrating Thread Simulation Package (MT-SIM), allowing for writing python codes that approximate code written for parallel multithreaded systems. The purpose of introducing such a package is to be later used for emulating graph algorithms running in parallel, keeping track of where computation would occur if it were to be done in parallel machines.

The performance of migrating architecture was evaluated using Dijkstra's single-source shortest path algorithm on both simple small graphs and randomly generated big graphs. The edges that connect vertices were distributed among the nodes of the parallel migrating architecture. Accessing a set of edges requires the machine to hop from one node to another. Preliminary results working with small graphs show a migration takes place when trying to run Dijkstra's algorithm. As is expected, larger graphs show a bunch of more migration happening. This finding shows the potential of exploiting the power of migrating parallel architectures to run graph algorithms in a fashion that is both faster and efficient.

Production, Molecular Characterization, & Crystallization of a Behcet's Disease Related Protein-HLA

Taylor Bias
Chemistry-Biochemistry-Biology Interface (CBBI) Program

Mentor, Contributors, Faculty Advisor:
Eliza Kovriguina, Lab Manager
Gihan Perera, Graduate Student
Brian Baker, Coleman Professor of Life Sciences, Department of Chemistry and Biochemistry
College of Science

Abstract

Behcet's Disease (BD) is an inflammatory disease whose pathology is well known and is prominently influenced by genetics and the immunological response. The strongest genetic predisposition and primary risk factor for BD is Human Leukocyte Antigen (HLA)-B*51, one of many thousands of HLA variants made within human populations. However, the role of HLA-B*51 in the disease is unknown. Understanding the structural and functional features of this protein may help to elucidate the possible HLA-B*51-related pathogenic mechanisms in Behcet's disease. This study shows assembly, purification, and characterization of HLA-B*51 with a peptide ligand, IPYQDLPHL. The HLA-B*51 heavy chain and β2 microglobulin subunit (β2m) were individually expressed as inclusion bodies in E. coli, refolded together with the peptide, and purified chromatographically via FPLC. Using differential scanning fluorimetry, the melting temperature (Tm) of the complex was found to be 61.5°C indicating a stable peptide-HLA complex and high affinity peptide binding. An initial crystallization trial was performed by using a sparce matrix screen from Hampton Research, using hanging drop crystallization. These crystals were harvested for analysis via X-ray crystallography. We anticipate the structure of this complex will indicate key physical aspects that will relate HLA-B*51 to the underlying molecular mechanism of Bechet's Disease.

References:

1. Kedzierska K, Koutsakos M. The ABC of Major Histocompatibility Complexes and T Cell Receptors in Health and Disease. Viral Immunol. **2020**, 33 (3), 160-178.
2. Gur M, Golcuk M, Gul A, Erman B. Molecular dynamics simulations provide molecular insights into the role of HLA-B51 in Behcet's disease pathogenesis. Chem Biol Drug Des. **2020**, 96, 644–658.

Laser-Based Fabrication of Glass to Metal Seals

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Engineering Summer Research Experience (E-SURE)

Mentor and Faculty Advisors
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Abstract

Glass-to-metal seals are a critical component used in technologies that require electrical signals to be transmitted into or out of vacuum-tight or extreme-temperature environments. A typical glass to metal sealing process requires precisely formed metal and glass components, which must then be carefully bonded in a high temperature furnace. These processes require specialty tooling and are time consuming. In this project, we seek to create a quick, flexible glass-to-metal sealing technique by using a laser-based glass forming process. In lieu of the typical chemical or compression bond used in most glass to metal seals, we inject a rod of glass into threaded metal nuts. The penetration of the glass into these threads creates the seal. In this study, we explore two separate methods of creating the hydraulic force necessary for this method. First is using a backing plate underneath the nut, and second is permitting the glass to ball before insertion. The latter is particularly interesting, because it has the additional benefit of working to place seals on larger parts that are not suitable for a backing plate. We parameterize these methods in terms of length and speed of glass insertion, as well as glass temperature and hydraulic force exerted on the threads of the nut. We then explore how these parameters influence the strength of the final seal.

The Evaluation of the Requirement for CXCL5 and CXCR2 and their Autocrine Roles in Promoting Bone Metastasis in Mice

Aleah Brokemond
ND PREP

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Abstract

Bone metastasis is not as well understood as some may think, especially in terms of the molecular processes that cause it and its prevalence worldwide. When cancer starts in one part of the body, such as the lungs or breasts, then spreads to the bones is classified as bone metastasis. Here, we shall investigate these obscure molecular processes of bone metastasis through evaluating the necessity of the stromal chemokines CXCL5 and CXCR2 in promoting the proliferation of cancer cells in bone. Additionally, we will also examine how the autocrine roles of CXCL5 and CXCR2 contribute to promoting cancer cell proliferation within bone. In turn, FVB mice will be undergoing intracardial (IC) injection, and the tibia bones in their left and right hind legs will be collected and cultured with PyMT cells that are ± CXCL5/CXCR2, with CXCL5/CXCR2 being either overexpressed (OE) or knocked down (KD). As for examining the need for stromal CXCL5, IC injections are to be done on CXCL5 WT and KO mice, and their bones were collected and cultured with PyMT cells. Similarly, IC injections will be done on CXCR2 WT and KO mice, and their collected bones are to be cultured with PyMT cells. Over two weeks media is collected every other day for chemokine analysis of CXCL1, 2, 3, 6, 7, 8 by Eve Tech protein array or ELISA. After this, immunohistochemistry (IHC) for the bone samples will be carried out using keratin/Ki67 staining to provide evidence that proliferation is indeed occurring in the bones.

Elucidating the Ototoxicity of Cisplatin and its Alternatives Using Computational Chemistry

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Abstract

The chemotherapy drug, cisplatin, is often administered when treating testicular, ovarian, bladder, lung, cervical, head, and neck carcinomas1. While proving to be 90% effective in fighting cancer, cisplatin induces negative side effects such as ototoxicity (hearing loss), which increases by five times with cisplatin chemotherapy. Even though some preventatives have undergone clinical trials, there is no FDA approved preventative that successfully and safely protects the cochlea from cisplatin-induced hearing impairment1. For hearing loss to be present, apoptosis of cochlear hair cells needs to occur. This is done by oxidative cell stress, which is activated by a surge in production of reactive oxygen species (ROS) such as free radicals. Investigating the pathway towards apoptosis, cisplatin interacts with water, removing a chlorine to form an adduct. This adduct further interacts with hydrogen peroxide to produce water, a hydroxide anion, and a hydroxyl free radical. The intention behind this research is to propose a cisplatin alternative that is unlikely to produce the free radicals, while maintaining its efficacy in cancer treatment. The research is conducted theoretically utilizing computational chemistry techniques such as density functional theory (DFT). The DFT calculations output the energies needed in determining reaction coordinate diagrams of cisplatin and its alternatives. The reaction coordinate diagrams provide the activation energies required to produce ROS. With larger activation energies, the pathway towards ROS production is less likely to occur, therefore less likely to induce the negative side effect of hearing loss.

Characterization of Atypical ABC Transporters in the Fungal Pathogen *Cryptococcus Neoformans*

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Abstract

Cryptococcus neoformans is an opportunistic fungal pathogen responsible for significant mortality, particularly among AIDS patients. This is due, in part, to suboptimal treatments and the development of antifungal resistance. We have previously described the first of 4 atypical ABC transporters in this fungus, *PDR6*, which affects both antifungal resistance and host interactions; the other 3, *PDR2*, *PDR4*, and *PDR7*, are completely uncharacterized. In this study, we want to expand on the cellular function of *PDR6* and begin to study *PDR4* and *PDR7* by tagging them with a fluorescent protein and assessing their localization. Furthermore, phenotypic assays will be conducted to assess antifungal resistance and virulence traits in mutants missing these ABC transporters. Initial findings indicate that *PDR6* plays a dual role in drug resistance and intracellular transport, and *PDR4* is important for virulence in the waxworm invertebrate model. Since these atypical transporters are conserved in other fungal pathogens, understanding their functions in *Cryptococcus* may pave the way for novel therapeutic strategies against fungal infections in general. These insights have the potential to significantly impact public health by reducing the global burden of cryptococcal and fungal infections.

Reactivity of a Three-Coordinate Nickel Carbene Complex with Strained Olefins

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Abstract

Olefin metathesis is an important reaction for carbon-carbon double bond formation widely used in total syntheses, industrial polymerization reactions, and pharmaceutical drug synthesis. Industry-standard “Grubbs-related” olefin metathesis catalysts utilize ruthenium, which is energetically intensive to mine and costly to remove after use. Consequently, vast academic research has been conducted to synthesize carbene catalysts from more abundant and nontoxic metals such as iron and nickel. Unfortunately, iron and nickel have a propensity to undergo a competing cyclopropanation reaction instead of metathesis. However, recent work in the Iluc lab suggests that iron can be used for ring-opening metathesis reactions involving strained norbornadiene derivatives. This work builds upon this conclusion and determines whether nickel will demonstrate this reactivity under similar conditions. The carbene complex, [(dtbpe)Ni=CPh_2] [dtbpe = 1,2-bis(di-*tert*-butylphosphino)ethane], was reacted with an equimolar amount of benzonorbornadiene in C_6D_6 at 60°C to generate a 1:1:1 ratio of [(dtbpe)Ni(BZNBDE)] [BZNBDE = benzonorbornadiene], 1,5-Dihydro-1,5-methano-naphthalene-3,3-diphenyl-cyclopropane, and unreacted starting material. The proposed mechanism is a [2+2] cycloaddition between the carbene and BZNBDE, generating a metallocyclobutane, which goes through a reductive elimination to generate the cyclopropane. The transient Ni(0) species then coordinates to BZNBDE generating [(dtbpe)Ni(BZNBDE)]. [(dtbpe)Ni(BZNBDE)] was confirmed via independent synthesis by reducing [(dtbpe)$NiCl_2$] in the presence of BZNBDE and was structurally characterized by x-ray diffraction.

Exploring the Role of STING Pathway Activation in Niemann-Pick Type C Disease

Anastasía Chibucos
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Abstract

Niemann-Pick Type C (NPC) disease is a rare genetic disorder characterized by the accumulation of lipids, particularly cholesterol, within various tissues due to mutations in the NPC1 or NPC2 genes. These mutations disrupt lysosomal function, impairing autophagy and increasing oxidative stress. The liver and spleen commonly exhibit hepatosplenomegaly from cholesterol buildup, while the brain suffers neuronal loss, demyelination, and neurofibrillary tangles, notably affecting Purkinje cells crucial for motor coordination.

Recent studies by Dr. Nan Yan at UT Southwestern indicate an immune component in NPC disease involving the STING pathway. Unlike the canonical cGAS-STING pathway, NPC-related STING activation depends on cholesterol. Normally, STING is retained in the ER by the Insig-SCAP-SREBP complex and trafficked minimally to the Golgi. In NPC1 mutant cells lacking ER cholesterol, STING is hyperactive and inadequately degraded, triggering chronic interferon pathway activation and neurodegeneration.

This research aims to clarify STING's role in NPC by measuring phosphorylated STING (P-STING) levels in wild-type and I1061T mutant NPC cells in mouse and human models. It also investigates whether NPC1 mutations affect STING-NPC1 interactions using co-immunoprecipitation and Western blotting. Additionally, the study assesses if STING activation alters lysosomal pH via the FIRE-pHLy biosensor in cells overexpressing wild-type and mutant STING. These efforts promise insights into STING's contribution to NPC progression, potentially guiding therapies targeting this pathway.

Western blot analysis revealed elevated STING levels in NPC1 mutant fibroblasts (I1061T) compared to wild-type controls, yet no increase in phosphorylated STING, indicating heightened STING expression without enhanced activation in NPC conditions. These findings underscore STING pathway involvement in NPC pathogenesis, highlighting avenues for therapeutic development.

References:

1. Bingxu Liu et al. ,Human STING is a proton channel.Science381,508-514(2023). DOI:10.1126/science.adf8974
2. Chu, TT., Tu, X., Yang, K. et al. Tonic prime-boost of STING signalling mediates Niemann–Pick disease type C. Nature 596, 570–575 (2021). https://doi.org/10.1038/s41586-021-03762-2
3. Klein AD, Alvarez A, Zanlungo S. The unique case of the Niemann-Pick type C cholesterol storage disorder. Pediatr Endocrinol Rev. 2014 Sep;12 Suppl 1:166-75. PMID: 25345099.
4. Kunkel, T.J., Townsend, A., Sullivan, K.A. et al. The cholesterol transporter NPC1 is essential for epigenetic regulation and maturation of oligodendrocyte lineage cells. Nat Commun 14, 3964 (2023). https://doi.org/10.1038/s41467-023-39733-6

Dorsal Root Ganglion Circuitry: The Crucial Role of Voltage-Gated Calcium Influx in Zebrafish (*Danio rerio*)

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Abstract

The construction of the nervous system requires precise cell navigation. In the somatosensory pathway, dorsal root ganglion (DRG) neurons undergo careful assembly. These cells relay sensory signals from the peripheral to the central nervous system, precisely entering the spinal cord at the dorsal root entry zone (DREZ) before synapsing with spinal neurons. However, more needs to be studied on what factors guide DRGs to this target area. We investigated whether navigation to the DREZ depends on the gene *Cacna2d1a*, which encodes the alpha2/delta1 subunit of N-type voltage-gated calcium channels. Studies have shown calcium signaling to rearrange the growth cone cytoskeleton, regulating how DRGs respond to guidance cues and reach their synaptic partners. To enrich these findings, we explored the role of Cacna2d1a in zebrafish to uncover if calcium influx, specifically through voltage-gated channels, is necessary for DREZ entry. In situ hybridization was first employed to detect Cacna2d1a's mRNA expression spatially. The effect of inhibiting calcium influx via voltage-gated ion channels on DREZ entry was then closely examined through a series of drug treatments using gabapentin, a direct alpha2/delta1 inhibitor. The experiments were performed on developing zebrafish to quantify the difference in the number of tnfα^{+} DRGs between the gabapentin-treated and untreated groups. Tnfα serves as a biomarker indicating successful entry of DRGs into the DREZ. The gabapentin group exhibited a significant decrease in the number of tnfα^{+} DRGs, consistent with observations in *Cacna2d1a* crispants, reinforcing the subunit's role in proper axonal navigation of DRGs.

Investigation of VRK-1 inhibition to Induce Nuclear Blebbing and Cellular Senescence as a Potential Therapeutic for PDAC

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Biology REU Program

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Abstract

Pancreatic ductal adenocarcinoma (PDAC) is a highly aggressive and often lethal form of pancreatic cancer with a 5-year survival rate of 12%. Current therapeutics offer marginal improvements in 5-year survival, highlighting the need for new approaches. This study investigates the potential of inducing cellular senescence in PDAC cells through inhibition of Vaccinia-Related Kinase 1 (VRK1). Previous work in the Vaughan lab has shown that knock down VRK1 reduces BAF phosphorylation, reduces BAF/Lamin A interaction, and leads to nuclear blebbing. Evidence also suggests that nuclear blebbing leads to DNA leakage and activation of the cGAS-STING pathway and cellular senescence. It remains unclear what stage of the cell cycle is inhibited by VRK1 inhibition. It is also unknown the order in which nuclear blebbing, STING activation, and senescence occur. To determine this, we have synchronized NRK2-H2B-mcherry cells using a thymidine and nocodazole block and treated with VRK1-IN-1, a potent VRK1 inhibitor. To determine if VRK1 inhibition affects a certain stage of mitosis, cells will be synchronized and stained for tubulin and Lamin A. We expect that VRK1 inhibition will result in abnormal or delayed telophase. We will also determine when cellular senescence and STING activation occur in response to VRK1 inhibition by synchronizing cells and taking cellular lysates as timepoints following mitosis. We will then blot for phosphorylated IRF3, a marker of STING activation, and p21, a marker of cellular senescence. We expect that VRK1 inhibition will result in STING activation prior to the activation of cellular senescence.

Analysis and Comparison of First Row Transition Metal 2,3,5,6 tetrakis(pyridine-2-yl)pyrazine Complexes and Bis(2,3,5,6-tetra-2-pyridylpyrazine-κ3 N2,N1,N6)ruthenium(II)

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Abstract

Bis(2,3,5,6-tetra-2-pyridylpyrazine-κ3 N2,N1,N6)iron(II) ([Ru(tppz)2]2+) is an inorganic complex with a wide variety of applications including energy conservation, pharmaceuticals, molecular wires, and–especially–photoredox catalysis. However, with the high expense of ruthenium-based compounds, it would be more cost effective to synthesize and employ cheaper, first row transition metals interacting with tppz (2,3,5,6-Tetrakis(2-pyridyl)pyrazine) in these fields instead. In this work, we compare computational results for various metal tppz complexes to experimental results to confirm the validity of the computations performed. We also analyze the similarities between first row transition metal coordination complexes with tppz to [RuTPPZ2]2+ by comparing the molecular orbitals and UV vis data. All of this information provides important preliminary steps that potentially can lead to the identification of a first row transition metal photoredox catalysis candidate.

The Effects of Acculturation on Depression Levels among Mexican-American Adolescents

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Abstract

Previous research has indicated that Latino youth experience higher levels of depression compared to White and Black youth in the US. Recent studies have explored the relationship between acculturation and mental health among Latinos, yet most have focused on Latinos more broadly and within cultural enclaves. Limited information is available on how the process of acculturation specifically impacts Mexican-American adolescents living outside cultural enclaves. This study aims to address this gap by examining the association between acculturation and depressive symptoms among Mexican-American adolescents living in the South Bend area.

Results indicate that while Anglo orientation was not significantly associated with youth's reports of depressive symptoms, higher orientations to Mexican culture was significantly associated with fewer depressive symptoms. Overall, these findings provide a glimpse into the dynamic between cultural values and mental wellbeing and contribute to the ongoing discussion on more adaptive acculturation strategies.

Keywords: Acculturation, Mexican, Adolescents, Depression, Wellbeing

Molecular Dynamics Simulations: High-Performance Computations for Salt-Solvent Systems

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Abstract

This research study dynamics of salts in various solvents through the lens of molecular dynamics (MD) simulations. The primary objective is to illustrate the complex interactions and dissociation mechanisms of salts at the molecular level by constructing detailed free energy landscapes. Utilizing high-performance computing, advanced sampling techniques are employed to meticulously simulate and analyze these systems.

Salts are integral to numerous energy-related applications, including batteries, fuel cells, and solar cells. The behavior of salts in solvents significantly influences the efficiency, stability, and overall performance of these technologies. MD simulations provide critical insights into the microscopic processes governing salt dissolution, ion transport, and molecular interactions, which are essential for optimizing materials and conditions to enhance energy storage.

This study bridges theoretical research and practical applications, offering a comprehensive understanding of salt-solvent interactions. Additionally, the findings contribute to the development of more efficient materials development and innovation, pharmaceutical advancements and the chemical interactions. By comprehending the molecular dynamics of salts in various solvents, this research paves the way for significant advancements in energy technologies. The insights gained not only enhance the performance and efficiency of existing systems but also contribute to the development of innovative solutions for sustainable energy in the future.

Forming Microparticle Adsorptive Membranes to Enable Continuous Solute Removal Processes

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Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

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Abstract

Growing populations, environmental conservation, and industrial prosperity all require the maintenance of a clean water supply. Adsorptive separation processes offer a solution for the efficient removal of dilute contaminants, such as heavy metals and PFAS. However, the inherently unsteady nature of these approaches increases cost and complexity. Therefore, to enable continuous steady operation, the idea of contacting a contaminated water stream and a slurry of adsorptive microparticles countercurrently was proposed. Here, we show that a polymer membrane casting solution containing 4, 6, or 8wt% polysulfone (PSF) and 2wt% poly(styrene)-block-poly(acrylic acid) (PS-PAA) dissolved in 2-pyrrolidone can be formed into spherical adsorptive microparticles using a Non-Solvent Induced Phase Separation (NIPS) technique without sacrificing functionality. To form the microparticles, casting solution microdroplets were pipetted directly into a dilute non-solvent bath. Using a static formation method, microparticles of average diameter of ~1000 μm and maximum binding capacity ~0.60 mmoles of copper bound per gram of adsorptive PS-PAA could be generated. A dynamic formation method results in particles with average diameter of ~650 μm, similar binding capacity, and a higher control of sphericity. These results demonstrate how microparticle size and shape can be manipulated through formulation method without altering the functionality of their adsorptive membrane composition. The results of this study will prompt further investigation into the factors that affect microparticle size and shape in an efficient NIPS formation process. Optimization of the adsorptive microparticle could lead to the creation of adaptable continuous adsorption systems for contaminant removal or resource recovery.

Constraining Frontal Plane Shear Forces Utilizing Modified CAM Joints for Proper Knee-Exoskeleton Functionality

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Abstract

When accounting for most of the older population, we can see a common struggle in lower limb force generation. The torque generated at the joints by muscles tends to deteriorate with age, thus older adults struggle with common activities such as walking, sit-to-stand, crouching, etc. Failure to generate this torque causes this community to have limited movement and rely on caregivers. Another problem arises when looking into the caregivers, they take on awkward positions to help the elderly; thus, overcompensating with other muscle groups such as the lower back, arms, and shoulders, causing a chain reaction of problems that can affect the quality-of-life. This problem can be addressed by introducing wearable robotic devices such as ELVIA (Elastic Locomotion Via Instrumented Apparel).

ELVIA is an exoskeleton device that reduces human knee torque exertion during sit-to-stand transitions. It is used to assist able-bodied wearers by augmenting strength using mechanically passive components, reducing the amount of effort needed to execute sit-to-stand maneuvers. The device's main component is the elastic bands, these are responsible for storing elastic energy and outputting it as kinetic energy to help the host execute movements. These bands are attached to four braces that wrap the thigh and shank on the frontal and posterior planes and keep them in place. Multiple centers of rotation originate at the CAM joints located at the interfaces of the knee, these are the components that permit the device to abduct and adduct on a given pivot point. To avoid dislocation in the joints, three potential solutions were presented. The first proposed solution of the CAM models used Velcro as a contact surface to avoid dislocation of the exoskeleton due to medial/lateral loading, but under high loads and constant movement, the contact surfaces failed. The second potential solution utilized V-Belts, these are a practical a solution to our dislocation problem, constraining shear forces caused by medial/lateral loading and maintaining the device in its pivot point, conserving functionality through the entire range of motion. By attaching a V-Belt to the upper CAM joint and creating a groove in the lower CAM, we allowed multiple centers of rotation and constrained the lateral/medial loads, thus maintaining functionality. Our third potential solution is a compliant mechanism, it uses elastic deformation to rotate about an axis and constrains lateral loading. Additional research is needed to validate our compliant mechanism solution, but it is very likely it will solve our dislocation problem.

References:

1. P D, TJJoap H. Age causes a redistribution of joint torques and powers during gait. J Appl Physiol. 2000;88(5):1804–1811. doi: 10.1152/jappl.2000.88.5.1804
2. S. Hignett, "Work-related back pain in nurses," J. Adv. Nurs., vol. 23, no. 6, pp. 1238–1246, Jun. 1996, doi: 10.1046/j.1365-2648.1996.13423.x.

Pharmacological Inhibition of Fragile-X Neurons Fails to Bolster Endocannabinoid Fragile X-Associated Pathway

Aaron Davis
Biological Sciences Research Experiences for Undergraduates (BioREU)

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Abstract

Fragile X Syndrome (FXS) is the leading heritable cause of intellectual disability and autism, caused by *FMR1* silencing and subsequent loss of FMRP, a postsynaptic transcriptional regulator. Past FXS studies utilizing non-human model systems have had variable, often unsuccessful clinical outcomes, producing inconsistent results due to physiological differences between human and mouse neurons. However, we utilize a novel, human *in-vitro* approach avoiding these pitfalls, acting as a screen for translatability of past animal studies in a human system. Animal models implicate the endocannabinoid (eCB) pathway in FXS pathology. Of particular interest are the enzymes diacylglycerol lipase-alpha (DAGL) and monoacylglycerol lipase (MAGL), which synthesize or hydrolyze the eCB 2-arachidonoylglycerol (2-AG), respectively. Since CB1R is understimulated in FXS, we hypothesized that DO34-inhibition of DAGL would exacerbate and JZL184-inhibition of MAGL would rescue the phenotype, evaluated via phospho-synapsin:synapsin ratio and calcium transient frequency, biomarkers of our pathway. Hallmarks of FXS are decreased inhibition of synapsin (a synaptic vesicle-associated protein) phosphorylation and presynaptic calcium intake. The current study seeks to corroborate Jung and colleagues' FMR1-knockout mouse finding that JZL184-MAGL inhibition rescued impaired 2-AG-mediated plasticity, an impairment analogous to DO34-DAGL inhibition.

Preliminary results from our system fail to bolster current understanding of the eCB-FXS pathway, with DO34-DAGL inhibition having little to no effect on the phospho-synapsin:synapsin ratio. Currently, mouse hippocampal cultures are being treated with DO34 and JZL184 to recreate Jung and colleagues' findings and subsequently evaluate whether our preliminary human data is indicative of a lack of translatability from a mouse model.

References:

Jung, K., Sepers, M., Henstridge, C. M., Lassalle, O., Neuhofer, D., Martin, H., Ginger, M., Frick, A., DiPatrizio, N, V., Mackie, K., Katona, I., Piomelli, D., and Manzoni, O. (2012). Uncoupling of the endocannabinoid signalling complex in a mouse model of fragile X syndrome. *Nature Communications*. **3.**

Composite Nanofibers as Effective Adsorbents for Li^+ Extraction

Batradz Djikkaity
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Abstract

With the majority of natural lithium deposits distributed in bodies of water, the oceans offer an excellent potential source of this finite mineral. This makes the development of lithium-ion sieves (LISs) with high adsorption capacity highly desirable in order to extract lithium from seawater and other brines. In this project, a degree-of-experiment approach was used to fabricate inorganic lithium manganese oxide ($LiMn_2O_4$) nanofibers with spinel structure through a combination of electrospinning and calcination. Spinel hydrous manganese oxide, which has high lithium selectivity, was derived from $LiMn_2O_4$ by Li^+–H^+ exchange, a process often done through acid treatment. To prevent degradation of the spinel structure from acid treatment [1], electrochemical intercalation will be used to facilitate this ion exchange instead. To carry this out, a coating of polyethylene-oxide (PEO) around the LIS will be required, which will also be done through electrospinning. A replicable process to create $LiMn_2O_4$ nanofibers was found through controlling electrospinning and calcination parameters. This allowed nanofibers with a minimized diameter to be fabricated, which maximized their specific surface area and augmented the accessibility of active sites to Li^+ ions. These findings contribute toward a viable method in implementing a future full-scale Li^+ extraction process from seawater, crucial for lithium-ion batteries used in electric vehicles and other electronics.

References:

[1] Chen, Q., Chen, Z., Li, H., & Ni, B. (2024). Advanced lithium ion-sieves for sustainable lithium recovery from brines. *Sustainable Horizons*, *9*, 100093. https://doi.org/10.1016/j.horiz.2024.100093

How The Accuracy of Model Forecast Is Impacted by The Length of Historical Data Impacts

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Abstract

Deciding on what time period to use in preparing forecasts can greatly affect the accuracy of your forecast. This research delves into how the accuracy of a model forecast is impacted by the length of time frame of historical data used. The training data used in this study is the GDP of Ghana from 1960 – 2023. Employing the ARIMA model, forecasts were generated and coded using the R programming language. The study conducted continuous annual forecasts from 2001 through 2023, systematically comparing these forecasts against actual GDP outcomes over varying historical time periods. The mean absolute percentage error was calculated for the different time periods used for the forecast. Findings reveal a notable impact of the historical data length on forecast precision, demonstrating that using extensive historical data can significantly affect the reliability of the forecast. This research contributes to the field of econometrics by providing insights into optimal data selection strategies, thereby enhancing the development of accurate forecasts. These findings are pertinent for individuals and organizations aiming to make informed management decisions based on robust predictive models.

Photonic Quantum Technologies Based on Metal Organic Frameworks

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Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

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Abstract

Metal-organic frameworks (MOFs) are hybrid materials that contain a metal node covalently bonded to organic linkers. MOFs are crystalline structures and porous which allows for a wide range of applications. Some applications include gas separations, drug delivery, catalysis, chemical sensing, and more recently, optical devices. By tuning the node and linker chemistries, MOFs can have optical properties that can be applied to photonic quantum technologies, such as quantum computing, quantum information, and quantum security. Studies have shown that non-centrosymmetric MOFs with non-zero second order susceptibilities are required for photonic quantum technologies. However, synthesis of large MOF crystals is required to analyze experimental optical properties, which presents a significant challenge. [1] Recent work has demonstrated the synthesis of large sized MOFs of MIRO-101, which makes it desirable for using them in photonic quantum technologies**.** In this study, we were able to overcome the synthesis challenges, creating a large single crystal of MIRO-101. Since creating the large size crystals of MIRO-101, looking into characterizing the optical properties of the structure is necessary for application in quantum information technologies. Recently, we have analyzed the optical properties of halogenated MIRO-101 MOF crystals by using nonlinear optical simulations which offers an avenue for tuning the nonlinear optical properties. This is because halogenated structures create an electron withdrawing effect on the linker and we want to determine how and if it influences the optical properties. Future work will focus on synthesizing halogenated MIRO-101 MOF crystals and measuring their optical properties to compare with the simulated values. This work can be useful in proposing and validating a new generation of quantum optics materials.

References:

[1] Garcia-Garfido, Juan M., et al. "Millimeter-Scale $Zn(3\text{-}Ptz)_2$ Metal–Organic Framework Single Crystals: Self-Assembly Mechanism and Growth Kinetics." *ACS Omega*, vol. 6, no. 27, July 2021, pp. 17289–98. *DOI.org (Crossref)*, https://doi.org/10.1021/acsomega.1c01272.

Incorporating Demographic Diversity to Mitigate Social Biases in Offensive Content Detection

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College of Engineering

Abstract

The detection of toxic language online, which encompasses hate speech, abuse, and offensive content — presents a significant challenge in the field of Natural Language Processing. This detection of this content is important due to how offensive content can affect mental health. This task is complicated by the subjective nature of what constitutes toxic language; toxic language is based on annotators' beliefs and identities. Our research seeks to solve these problems by highlighting the biases in current toxic language detection systems and proposing a new model that considers both the majority and minority of annotators' opinions to better address these biases. The primary purpose of this study is to develop a more nuanced understanding of how demographic diversity and annotator disagreement influence toxic language detection. We employed analytical methods, including demographic bar analysis, heatmaps, correlation analysis, clustering using K-Means, and Principal Component Analysis.

Our correlation and clustering analyses reveal that demographic factors significantly influence toxicity perception. For instance, older annotators had higher agreement rates for some situations due to their generational differences. Compared to traditional methods that treat annotator disagreement as noise, our approach emphasizes capturing the diversity of opinions to improve detection accuracy. Intersectional analysis showed that combined demographic factors provide a deeper understanding of labeling patterns, and case studies on controversial topics highlighted the different perspectives among the demographic groups. Our research underscores the necessity of incorporating demographic information and modeling annotator disagreement to develop more inclusive and representative toxic language detection systems.

Increased Exposure to Data Science and Research Methods Enhances Student Confidence and Proficiency

Sarah Harman and Aidan Finn
Summer Education and Engagement for Data Science (SEEDS)

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Anh Thu (Nancy) Le, Postdoctoral Associate, Department of Psychology
Ying (Alison) Cheng, Professor of Psychology and Associate Director, Lucy Family Institute for Data and Society
College of Arts and Letters

Abstract

The 2024 SEEDS program goal is to provide Data Science education to high school students in the South Bend area. The three high school students participating in the SEEDS program come from Upward Bound, a federally-funded program seeking to prepare underserved, high-achieving students for college. SEEDS works to expose students to careers in Data Science, which only one of the three students knew existed as a profession on day one. During the first part of the program, we developed a curriculum for the students covering coding, statistics, and data science. In the second section, we have taught students using this curriculum, allowing them to gain valuable skills in both data science and research.

We gave three surveys (onboarding, midpoint, and endpoint) to the students, measuring their confidence in their: Data Science proficiency, general research ability, and presentation skills. These surveys were designed to track both their confidence and proficiency as they progress through the curriculum. We have also monitored students' performance on weekly coding challenges, practice problems, and live debates to monitor their progress in the above skills.

Students have shown increased confidence in their ability to analyze and solve Data Science problems by over 25% during the first half of the program. They have also demonstrated growth in their ability to tackle complex problems, present data to classmates, and use statistical methods to answer Data Science questions.

Acid-Doped Polybenzimidazole Membranes for Enhanced H_2/CO_2 Separation

Lauren D. Fuentes Velázquez
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

Mentor, Contributors, Faculty Advisor:
Joseph Emery, Graduate Student
Ruilan Guo, Frank M. Freimann Collegiate Professor of Engineering, Department of Chemical and Biomolecular Engineering
College of Engineering

Abstract

The elimination of pre-combustion carbon dioxide (CO_2) is essential to satisfy future demands for hydrogen (H_2) production as an alternative clean fuel. H_2/CO_2 mixtures resulting from syngas processing currently use thermally driven and extremely energy intensive separation methods, such as pressure swing absorption. Using polymer membranes for H_2 purification processes provides a more energy-efficient and cost-effective alternative as they are modular, have a smaller footprint and can separate gas at high temperatures. Commercial *meta*-polybenzimidazole (*m*-PBI), which is the current state of the art polymer membrane for H_2/CO_2 separations, has excellent thermal stability and molecular size-sieving capability. However, *m*-PBI has very low H_2 permeability due to its dense chain packing induced by hydrogen bonding, and efforts to improve H_2/CO_2 separation performance of PBIs have faced selectivity/permeability trade off challenges. In this study, new PBI-based membranes were formulated from blends of *m*-PBI and a highly permeable pentiptycene-containing PBI (PPBI) in systematically varied compositions, which were doped with phosphoric acid (PA) post-fabrication. The added bulky pentiptycene units disrupt chain packing by increasing free configurational volume of the PBI structure improving H_2 permeability, while PA doping regulates free conformational volume via proton transfer or hydrogen bonding for enhanced H_2/CO_2 selectivity. We investigated the gas transport properties of the membranes and are currently testing to demonstrate that at elevated temperatures, the acid doped *m*-PBI and PPBI blends have enhanced H_2/CO_2 separation. These findings will represent a novel approach to further develop polymer-based membranes for H_2 recovery, and a pathway towards achieving cleaner and sustainable energy solutions.

Human Perception of LLM-generated Text Content in Social Media Environments

Susan Gicheha
International Summer Undergraduate Research Experience (iSURE)

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Paul Brenner, Sr. Associate Director, Center for Research Computing; Professor of the Practice
Notre Dame Research

Abstract

The rise of Large Language Models (LLMs) on social media platforms introduces significant opportunities. However, bots on social media could potentially be seen through negative effects such as manipulation threats, biases, privacy concerns, and the spread of propaganda by malicious bots, as seen during the 2014 elections when automated accounts manipulated public opinion. As LLMs become more sophisticated, the differences between human-produced and AI-produced content have become extremely small. This study aimed to assess how successfully humans can identify the true nature of users on social media without the ability to interact, examine patterns in their identification, as well as to understand the effects that LLM-generated text can have on humans by testing the Uncanny Valley theory.

We recruited over 1000 participants and were each randomly assigned two posts, each with five replies, and tasked with identifying which replies were written by bots.

We found that participants only 42% of the time successfully identified the true nature of user posts in social media environments, with a high false negative rate of 49% indicating participants incorrectly identified bots as humans. We also found patterns in how humans identify LLM-generated text content in social media discourse. With regards to the Uncanny Valley, findings suggest that the participants experienced discomfort when reading posts they believed were bot generated. Notably, only 54 participants were 100% accurate in identifying the true nature of posts and also experienced the Uncanny Valley effect.

Development of Polymeric Membrane Materials for High-Performance Gas Separation in Thermally Challenging Environments

Carolyn Habel
CISTAR Young Scholars Program

Mentor, Contributors, Faculty Advisor:
Sandra Weber, PhD Student; Agboola Suleiman, PhD Student
Ruilan Guo, Frank M. Freimann Collegiate Professor of Engineering, Department of Chemical and Biomolecular Engineering
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Abstract

This research aims to develop organosoluble pentiptycene-containing polybenzoxazole (LsPPBO) membrane materials capable of performing gas separations in thermally challenging conditions (>100°C). In the CISTAR shale gas treatment process, hydrogen separation from methane is to be performed between dehydrogenation and oligomerization steps, occurring at temperatures around 600°C and 200°C, respectively. Current industrial gas separation membranes operate efficiently at ambient temperatures, necessitating energy-intensive cooling and heating cycles. To reduce operational costs and energy consumption, thermally stable polymeric membrane materials offering high permeability and selectivity are needed. A key objective of this research is synthesizing high molecular weight LsPPBOs, coupled with the enhancement of their selectivity through acid doping. Acid doping plays a pivotal role in optimizing membrane performance as it facilitates crosslinking of polymer chains via proton transfer and hydrogen bonding. These processes effectively reduce free volume within the membrane, thereby improving selectivity for specific gas pairs crucial in applications such as hydrogen recovery, natural gas purification, and air separation. The organosolubility of pentiptycene-containing polybenzoxazole (LsPPBO) membranes is vital for their fabrication and structural integrity under harsh conditions. By developing membranes capable of superior performance under harsh conditions, this research aims to enhance industrial efficiency and sustainability, paving the way for innovative solutions that impact energy consumption and operational costs in gas separation industries.

Exploring Transcriptional Regulation of ESX-1 Secretion Under Stress and Through Tool Development

Theodore Hatfield
Biological Sciences Research Experiences for Undergraduates (BioREU)

Mentor, Contributors, Faculty Advisor:
Rebecca Prest, Graduate Student
Patricia Champion, Professor of Biological Sciences
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Abstract

Mycobacterium tuberculosis infections are a global health pandemic that causes approximately one-million deaths yearly. Pathogenic mycobacteria infect host phagocytic cells, including macrophages, where they initially reside in the phagosome. Mycobacteria lyse the phagosomal membrane allowing for intracellular replication. This lysis is primarily mediated by the highly regulated ESX-1 secretion system. The complex and associated substrates are conserved across virulent mycobacterium species. Regulation of ESX-1 occurs via three transcription factors, WhiB6, EspM, and EspN, which work at the *whiB6* promoter region. WhiB6 is a transcription factor that promotes the expression of ESX-1 associated genes. EspM directly represses *whiB6* expression. In the absence of EspM, EspN directly activates *whiB6* inducing ESX-1 expression. Our understanding of how these transcription factors regulate ESX-1 is limited. Given EspM and EspN have domains predicted to be responsive to environmental stressors, we hypothesize stress directly impacts EspM and EspN activity. We exposed *M. marinum* mutant strains with different variants of EspM and EspN to dormancy, carbon starvation, and oxidative stress conditions. Beyond these transcription factors, the EspE and EspF ESX-1 associated substrates negatively regulate transcription. However, understanding of the mechanisms by which they do this is limited. To fill these gaps, we are developing tools to further study their role in transcriptional regulation, and produce novel visualization of the non-antigenic EspF protein. In gaining further understanding of the conditions that these regulatory proteins are most responsive to, and by developing new methods to study mycobacterial regulation, our understanding of ESX-1 transcriptional regulation during infection can be improved.

Investigating the Secretion Mechanism of Virulence Proteins produced by Pathogenic Bacteria

Corrie Hickson
Summer Research Opportunities Program (SROP)

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Patricia L. Clark, O'Hara Professor of Chemistry and Biochemistry, Associate Vice President for Research, and Concurrent Professor of Chemical and Biomolecular Engineering
College of Science, Notre Dame Research, College of Engineering

Abstract

Gram-negative bacterial pathogens secrete virulence proteins to the cell surface to mediate many pathogenic functions, including host cell adhesion, invasion, survival in harsh conditions, and evasion of the immune response. The largest family of secreted virulence proteins is autotransporter proteins (AT). The Clark lab has extensively studied pertactin, an AT produced by *Bordetella pertussis*, the causing agent of whooping cough. Like all ATs, pertactin must remain unfolded in the periplasm to be successfully secreted to the cell surface. However, it is largely unknown how ATs can remain unfolded in the periplasm without being degraded by quality control proteases. The Clark lab created truncated pertactin mutants to gain insights into features that allow pertactin to resist degradation in the periplasm and be successfully secreted to the cell surface. Preliminary results revealed that deleting the C-terminus of pertactin impairs extracellular secretion. Interestingly, the expression of the pertactin mutant lacking the C-terminus (P.93ΔPCt) caused growth defects in *E. coli*. Here, using a combination of cell growth and western blot assays, we show that accumulation of P.93ΔPCt in the periplasm potentially activates the bacterial stress response, resulting in significant protein degradation.

Overall, our data suggests that the pertactin C-terminus could serve as a binding site for chaperones to protect unfolded pertactin from degradation in the periplasm. Further investigations are needed to elucidate the connections between pertactin secretion, chaperone binding, and cellular stress response. Clarifying these connections will deepen our understanding of the general AT secretion mechanisms, opening new avenues for the development of novel antibiotics.

The Protective Power of Fatherly Warmth

Raquel Hilton
Research Access and Mentorship Program (RAMP)

Mentor, Contributors, Faculty Advisor:
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Adriana Miranda, Adrian Cooney, Suzanne Aguirre, Denisse Aguilar, Undergraduate Students
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Abstract

Given how gender shapes the structure and organization of the family, gender-typed personality traits can significantly influence the emergence of depression symptoms within the family unit. This consideration is particularly relevant as parents' and youths' personality qualities are closely tied to the dynamics of parent-child relationships, a pivotal aspect of adolescent development in Mexican culture. Expressivity traits, such as empathy, warmth, and nurturing behaviors, may manifest differently in mother-child relationships compared to father-child relationships. Mothers' higher levels of expressivity tend to be more prominent than fathers', and existing research suggests that mothers' personalities may have a stronger impact on the quality of these relationships.

Contrastingly, there is limited evidence linking instrumental traits—such as courage, strength, and competitiveness—to family outcomes. This study aimed to investigate how parental gender-typed personality traits are associated with reduced depression symptoms in Mexican American adolescents, independent of biological sex. Data were collected from 84 Mexican American families in Northern Indiana, including mothers, fathers, and two adolescent-aged siblings (51% girls). Moderation analyses revealed associations between parental personality characteristics and adolescents' depressive symptoms (M=14.225). Notably, fathers' possession of instrumental traits was negatively correlated with depressive symptoms in girls.

Practically, these findings underscore the potential of modifiable expressive traits in parents to mitigate depression symptoms among Mexican American adolescents. Traits such as kindness and sensitivity foster a supportive and emotionally nurturing family environment that buffers against depressive symptoms. Therefore, interventions targeting these traits could enhance overall mental well-being within the family unit, promoting healthier outcomes for all family members.

Emerging Profiles of Resilience and Psychopathology among Women Exposed to Intimate Partner Violence

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Summer Research Opportunities Program (SROP)

Faculty Advisor:
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College of Arts and Letters

Abstract

Intimate partner violence (IPV) is a critical issue that has significant effects on the psychological well-being of women. Social-ecological resilience (i.e., the resources and assets available to women across multiple systems) can play a critical role in mitigating these effects. This study investigates the profiles of resilience and psychopathology among pregnant women exposed to IPV. Participants included 101 pregnant women recruited from Women, Infant, and Children (WIC), Food and Nutrition Service program in a midsize Midwestern city.

Using the Resilience Research Centre Adult Resilience Measure, this study assessed resilience and psychopathology outcomes, depressive symptoms and PTSS, using the Center for Epidemiologic Studies Depression Scale and the Post Traumatic Stress Disorder Checklist for DSM-5 Scale, respectively. Cluster analysis was employed to identify distinct profiles of resilience and psychopathology. Five distinct clusters emerged: (C1) Subclinical Psychopathology and Low Resilience [9.9%], (C2) High Depression and Resilience [12.1%], (C3) Low Psychopathology and High Resilience [59.3%], (C4) Moderate Depression and Resilience [9.9%], (C5) High Psychopathology and Low Resilience [8.8%]. After identifying the clusters, ANOVAs were used to evaluate differences in cluster membership by exposure to adversity (i.e., adverse childhood experiences, intimate partner violence). The findings reveal a statistically significant difference between (C3) Low Psychopathology and High Resilience cluster and (C5) High Psychopathology and Low Resilience cluster in terms of exposure to adverse childhood experiences. However, there was no significant difference among the clusters in terms of intimate partner violence subtype exposure (i.e. psychological aggression, physical assault, etc.).

Investigating the Role of Retinoic Acid on Podocyte Development

Adesola Johnson
Biological Sciences Research Experiences for Undergraduates (BioREU)

Mentor, Contributors, Faculty Advisor:
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Josh Moeller, Undergraduate Student
Rebecca A. Wingert, Elizabeth and Michael Gallagher Associate Professor
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College of Science

Abstract

Chronic Kidney Disease (CKD) is a widespread disorder that affects millions of Americans yearly. The mechanisms underlying CDK are not yet fully understood and treatment options remain limited. The human kidney is a complex organ with multiple functions, including blood filtration, urine production, and maintaining homeostasis in the body. Research using animal models like the mouse and zebrafish has greatly advanced knowledge about the development of nephrons, which are structural and functional units in the kidney comprised of numerous specialized cell types. The retinoic acid (RA) signaling pathway is a highly regulated system for patterning of the nephron as well as other organs in development. The objective of this research is to investigate the role of RA and its potential role in the activation of the early renal progenitor genes, *lhx1a, and pax2a*, in the emergence of the podocyte cell lineage during nephron formation. The role of RA in the activation of these genes remains undefined. In this study, drug treatments using exogenous RA or the RA synthesis inhibitor, DEAB, were conducted on zebrafish embryos, and whole-mount *in situ* hybridization was performed to visualize the transcripts of *lhx1a* and *pax2a.*

Interestingly, RA treatment led to increased *pax2a* expression in the podocyte region. Studies to further explore these results with immunofluorescence are ongoing. Deciphering the effects of RA on early renal progenitor gene expression can provide new insight into the mechanisms of kidney development and regeneration, which may inform pharmaceutical interventions to target kidney disease.

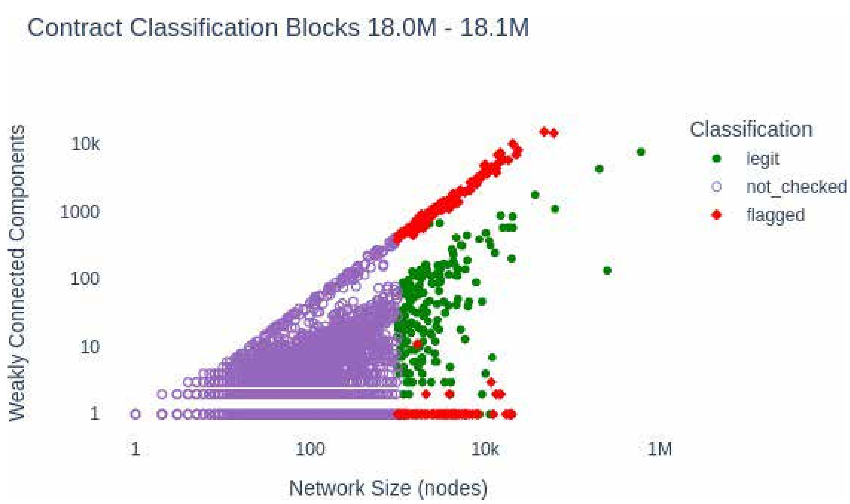
Identifying Cryptocurrency Scams with Analysis of ERC-20 Token Networks

Calvin Josenhans
Center for Research Computing (CRC) Internship

Faculty Advisor:
Andrey Kuehlkamp, Research Assistant Professor, Center for Research Computing
Notre Dame Research

Abstract

Ethereum is currently the second largest blockchain by market capitalization and a popular platform for cryptocurrencies. As it has grown, the high value present and the anonymity afforded by the technology have led Ethereum to become a hotbed for various cybercrimes. This project seeks to understand how these scams may be characterized and develop methods for detecting them. One key feature of Ethereum is the ability to use programmable smart contracts to implement the behavior of other cryptocurrencies on top of the existing infrastructure by implementing the ERC20 token interface. Such contracts can potentially be used to impersonate legitimate tokens and defraud users. By parsing the event logs emitted by these ERC20 contracts over two different periods of 100,000 blocks, we construct token transfer graphs for each of the available ERC20 tokens on the blockchain. By analyzing these graphs, we find a set of characteristics by which suspicious contracts are distinguished from legitimate ones. These observations result in a simple model that can identify scam contracts with 90% accuracy. This shows that the mechanism by which scams function strongly correlates with their transfer graphs, and that these graphs may be used to augment scam-detection mechanisms to make Ethereum a safer place.



Synthesizing Squaraine Dye Ligands for Transition Metal Catalysts

Hanna Ketsela
Summer Research Opportunities Program (SROP)

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Brandon Ashfeld, Professor of Chemistry and Biochemistry
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Abstract

Dianiline squaraine dyes are organic dyes characterized by an electron-deficient cyclobutenedione core and two para-substituted anilines. Such squaraine dyes are regularly employed in biological imaging and ion-sensing, but their use as a synthetic tool is relatively unexplored. The use of these dianiline squaraine motifs as ligands in various metal-catalyzed reactions is a long-standing goal in the Ashfeld lab. Our group recently reported on the use of proline-squaraine ligands in Rh-catalyzed cyclopropanation reactions.

The current study aims to design and synthesize a new class of dianiline squaraine-based dyes as a new class of transition metal ligands to catalyze the regioselective C–H functionalization of *N*-heterocyclic substrates. A significant challenge in the construction of new squaraine ligands is the installation of ligating functionality at specific sites around the squaraine core. Initial attempts to use bromine as a functional handle for transition metal-catalyzed cross couplings proved problematic in assembling the squaraine building block. We hypothesized that the electron-withdrawing nature of bromine deactivates the aniline and prevents the reaction between the bromo-substituted aniline and the semi-squaraine from occurring. Thus, by replacing the bromine substituent on the aniline with an electron donating heteroatom, activation of the aniline drives the resulting semi-squaraine acylation event to produce the desired unsymmetrical squaraine dye. As the project progresses, we will employ this heteroatom substituent as a functional handle to improve the performance attributes of the squaraine-based ligands.

Integration of Ni-Kegging-Polyoxometalate on Zinc Metallic Organic Framework and SBA-15 for Ethylene Oligomerization and Plotting Reactions Using Stochastic Kinetic Simulation

Aashin Khatiwada
CISTAR Young Scholars Program

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Jason Hicks, Tony and Sarah Earley Collegiate Professor of Energy and the Environment and Associate Dean for Graduate and Postdoctoral Affairs
College of Engineering

Abstract

The synthesis of the Ni-Kegging-Polyoxometalate (POM) ($K_5PW_{11}O_{39}{\cdot}Ni^{2+}$) and its characterization was done so in order to determine its purity and to verify that the right molecule was synthesized using Phosphorus Nuclear Magnetic Resonance. After verification of the molecule, the POM was integrated into two different structures in order to create grounds for catalysis: a framework of zinc and pyridine, and SBA-15. SBA-15 was used as it is more resistant to temperature than the zinc and pyridine framework, and in addition it also provides accessibility of nickel as an active site; important for catalysis. Once the POM was integrated into these two different structures, it was characterized, and then reacted with ethylene in order to record how well it performed in catalysis. The synthesis of both the metallic organic framework of zinc and pyridine and the framework of SBA-15 was also done and characterized. Both deterministic and stochastic kinetic models were created with the use of Python. The stochastic model was created using the Gillespie algorithm, modeling the reaction of chemicals with probability. In essence, the deterministic model was created in order to compare the stochastic model, acting as a standard of comparison. The stochastic model was used in order to help investigate and evaluate the parameters of catalysis of the POM.

SAR Studies of Aniline-Based Adjuvants as Potential Suppressors of Colistin Resistance in Bacteria

Eoin Killian
Naughton Fellowship

Mentor, Contributors, Faculty Advisor:
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Abstract

With the exit of major pharmaceutical companies from the development of new antibiotics and the recent global COVID-19 pandemic, the rise of multi-drug resistant (MDR) bacteria has become an increasingly worrying health concern across the globe. According to the CDC's 2019 Antibiotic resistant (AR) Threats Report, multi-drug resistant bacteria cause as many as 35,000 deaths each year in the US alone, resulting from over 2.8 million infections annually.[1] One particular antibiotic, colistin, is often administered as a last-resort drug to fight multi-drug resistant strains of gram-negative bacteria, however, resistance to this drug is building quickly, with reports of ineffective use in clinical settings.

Here we propose the development of molecules, termed antibiotic adjuvants that circumvent bacterial resistance mechanisms in order to potentiate colistin against resistant gram-negative strains of bacteria such as *Acinetobacter baumannii* and *Klebsiella pneumoniae*. Previous research reported the development of similar adjuvant scaffolds based on the structure of IMD-0345,[2] a known IKK-β inhibitor and a potent suppressor of colistin resistance in several gram-negative strains. Of the analogues tested, four lead compounds with similar or superior activity against colistin resistant bacteria were identified.[2] In this research, we continue the development and SAR studies of these adjuvants as potent suppressors of colistin resistance with a particular focus on improving their aqueous solubility, decreasing mammalian toxicity muting their effects on IKK-β.

References:

1. CDC. Antibiotic Resistance Threats in the United States, 2019. Atlanta, GA: U.S. Department of Health and Human Services, *CDC*; **2019.**
2. Nemeth, A.; Basak, A.; Weig, A.; et al. Structure–Function Studies on IMD-0354 Identifies Highly Active Colistin Adjuvants*. ChemMedChem* **2020**, 15 (2), 210-218.

Closing the Gap in Training Materials for Chemical Data Scientists

Karenna Kung, Jordan Letu, Vivian Quach, Zichu Wang
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(C-CAS SURF)

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Xiuxiu Tang, Postdoctoral Researcher, Psychology
Ying (Alison) Cheng, Professor of Psychology
Olaf Weist, Grace-Rupley Professor of Chemistry and Biochemistry
Xiangliang (Lynn) Zhang, Leonard C. Bettex Collegiate Professor of Computer Science
College of Arts and Letters, College of Engineering, College of Science

Abstract

Machine learning (ML) methods allow for novel exploration of the chemical space to advance traditionally lab-based chemical tasks. However, chemists often suffer from difficulties when employing these ML methods, and cannot find training platforms that are suitable to educate themselves on the application of these algorithms. The Cybertraining for Chemical Data Scientists (C2D) project aims to identify and fill these gaps and build a training platform for data chemists.

Initially, we identified potential ML solutions for common chemical problems. Thus, a survey was distributed to members of the NSF Center for Computer Aided Synthesis. Based on these results, we collected and cataloged existing materials for the most common methods. A total of 125 materials across 7 chemical problems (reaction prediction and optimization, molecular property prediction and optimization, retrosynthesis, yield prediction, and information retrieval) were evaluated based on several criteria: their difficulty to students from chemical and computer science backgrounds, respectively; information they conveyed about the chemical problem and ML techniques; code implementation; and discussion of applications of the algorithm.

We observed that most materials either provided insufficient detail to enable independent implementation, or were beyond the level of targeted trainees. To remediate the shortage of chemistry-related materials, we adapted and annotated codebases from existing academic publications into simplified code intended to be run by new programmers. Ultimately, we aim to provide a platform that adapts to the level of the learner by selecting from a diverse range of resources, thereby enabling computational methods to become more accessible to chemists.

Building a Graphical User Interface for Transparency of Drone Flights' Authorization

Rafael Labuto
CSE Summer Enrichment Program

Mentor, Contributors, Faculty Advisor:
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Jane Cleland-Huang, Frank M. Freimann Professor of Computer Science and Department Chair, Computer Science and Engineering
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Abstract

Recent research suggests that by 2035, small Unmanned Aerial Systems' (sUAS) activities will reach up to 65,000 operations per hour, surpassing the current levels of manned air traffic. Due to the substantial differences between sUAS and manned air traffic, the FAA and NASA have introduced the Unmanned Aircraft System Traffic Management (UTM) concept. The UTM is an ecosystem to manage sUAS traffic and allow operations in locations where air traffic services are not provided. Currently, when a drone requests authorization to perform a mission in a controlled UTM air-zone, a team of safety analysts is responsible to determine whether the planned mission is likely to be completed successfully. Nevertheless, the fact that this process is manual represents a loss of efficiency in drone operations, hindering scalability. To tackle this challenge, our team has proposed the development of a Safety-Aware Drone Ecosystem (SADE), with a fully automated SADE Authorization Manager (SAM). Drones communicate their authorization request to the SAM using MQTT (Message Queuing Telemetry Transport), then the SAM is responsible for granting or denying permissions almost instantaneously for both simple and complex flight requests, offering support for remedial actions when permissions are denied, and scaling up to hundreds of thousands of sUAS. Research done with sUAS stakeholders identified "distrust in AI" as an important concern regarding an automated on-entry decision system, therefore, my work builds a Graphical User Interface (GUI) that displays messages exchanged between multiple sUAS and the SAM. In the future this will be extended to provide increased transparency to the decision-making process.

References:

[1] Gohar, Usman, Michael C. Hunter, Agnieszka Marczak-Czajka, Robyn R. Lutz, Myra B. Cohen, and Jane Cleland-Huang. "Towards Engineering Fair and Equitable Software Systems for Managing Low-Altitude Airspace Authorizations." In *Proceedings of the 46th International Conference on Software Engineering: Software Engineering in Society*, pp. 177-188. 2024.

The Ceramic Analysis of Collier Lodge Site (12PR36)

Melanie Langgle
Summer Research Opportunities Program (SROP)

Mentor, Contributors, Faculty Advisor:
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College of Arts and Letters

Abstract

The Collier Lodge Site (12Pr36) is on the southern edge of Porter County in Indiana in the northmost part of the Kankakee Marsh. The archaeological site is uniquely represented by its extensive ceramic assemblage that spans from 1000 BC to historic times. Despite this trove of ceramic data, the chronology of the site and Northwestern Indiana region has been unresolved. This research established a chronology based on the pottery found at Collier Lodge from archaeological excavation from 2003 to 2023. It then utilized comparative sites to determine the appropriate archaeological phase concurrent with the ceramics found. The research uses ceramic analysis to gain insights into the cultural, social, and historical contexts that shaped the Collier Lodge site. Using quantitative and qualitative data, patterns regarding the ceramic's styles and functionalities, trade routes, sources, and site formation processes were established.

This study pinpointed when variations in ceramic assemblages occurred at the Collier Lodge Site and implemented the theory that the variety of wares is credited to the interaction amongst a range of prehistoric indigenous groups found in the heartland of America. These interactions, and occasional co-habitation led to a culmination of cultural practices regarding ceramic manufacture and adaptations of style. Based on the patterns distinguished by the ceramic data collected from Collier Lodge, the site can be detrimental to the perception of the Northwestern Indiana region and surrounding areas.

Nanoparticle-mediated Reprogramming of Cells to Fight Cancer

Mónica Leal Palma, Samantha Yu
NDnano Undergraduate Research Fellowship (NURF)

Mentor, Contributors, Faculty Advisor:
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Meenal Datta, Assistant Professor of Aerospace and Mechanical Engineering
Ryan K. Roeder, Professor of Aerospace and Mechanical Engineering
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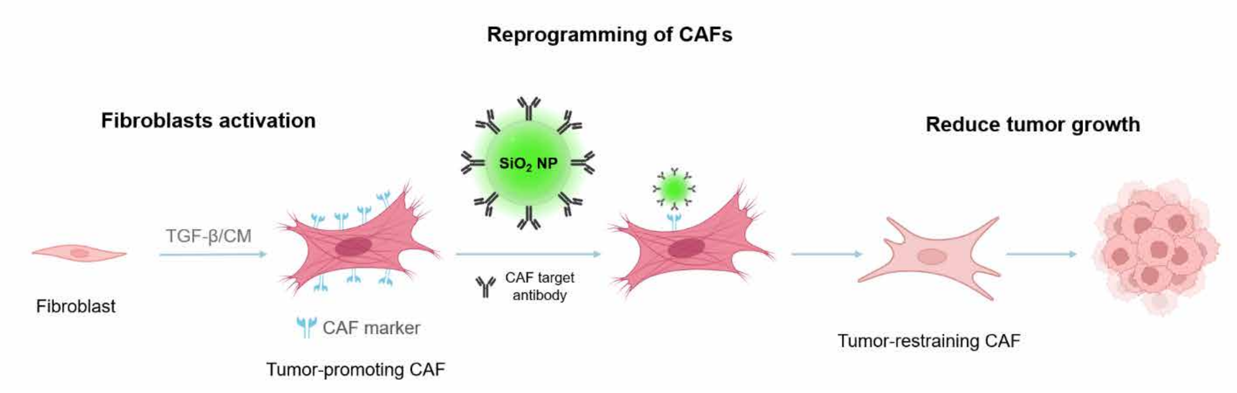
Abstract

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 (FAP) 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, recent evidence has shown that there are certain CAF subtypes which can also exhibit anti-tumor activity. Despite this revelation, these tumor-restraining CAFs remain a source of untapped therapeutic potential. With this in mind, we propose using fluorescent silica nanoparticles (SiO_2 NPs) as a platform for targeting and reprogramming CAFs into an anti-tumor state. Nanoparticle were chosen as the mode of delivery due to enhanced targeting specificity, high payload, protection of delivered biomolecules and imaging capabilities.

Fluorescein isothiocyanate (FITC) and rhodamine isothiocyanate (RITC) SiO_2 NPs were synthesized using a modified Stöber method. RITC/FITC-SiO_2 NPs exhibited unchanged hydrodynamic size of ~125 nm and ~113 nm respectively 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/RITC-SiO_2 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 RITC/FITC-SiO_2 NPs with protein A biobeads. In contrast, NPs without IgG exhibited no agglomeration, as expected, when mixed with protein A biobeads. The SiO_2 NPs demonstrated the capability of loading different fluorophores for various imaging purposes by loading FITC and RITC individually in this study.

NIH3T3 murine fibroblasts were cultured and treated with human recombinant TGF-β and 4T1 murine triple negative breast cancer cell conditioned media (CM). Following TGF-β/CM treatment, RT-qPCR and immunofluorescence staining were used to evaluate the expression of activation markers, functional markers, and markers typically upregulated in different CAF populations. Assays to investigate fibroblast functionality through wound healing and non-selective uptake of NPs by fibroblasts were also performed.



Can Work Civilize? British Political Economy and Indian Indenture

Jun Wei Lee
Research Access and Mentoring Program (RAMP)

Faculty Advisor:
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College of Arts and Letters

Abstract

From the mid-19th century to the early-20th century, the British Empire imported masses of indentured laborers from South India to the Straits Settlements to work on British agricultural settlements. But why did the British Empire undertake this operation when it could have instead used indigenous Malay labor? This research project addresses this question through a survey of recent literature in colonial labor history and utilizes archival material from the British Library and the Kew National Archives to argue that colonial policy was directed by two different approaches: liberal and culturalist. The liberal view saw labor as the great civilizer. Through plantation labor, British policy envisioned that indentured laborers Indians gaining industry and independence; in contrast, the British rationalized their inability to recruit Malay labor as evidence of native indolence. To reform native indolence, the British incentivized Indians to settle in the Straits Settlements after their indenture contracts, hoping to use them as intermediary colonizers. In contrast, the culturalist view reflects the imperial tendency to view colonialism's mission as preserving native custom. This perspective explains why British recruitment efforts shifted towards transplanting entire villages from South India, while accounting for British hesitancy to engage communal forms of Malay labor. Finally, I explain why British recruitment was concentrated in South India. As Sunil Amrith notes, pre-colonial empires connected South and Southeast Asia through the Bay of Bengal. The British appropriated these histories of migratory patterns to justify the naturalness of labor exploitation.

Exploring the Numerical Resolution of the Lagrangian Method for Representing Marine Fog

Anna Leuer
Engineering Summer Research Experience (E-SURE)

Mentor and Faculty Advisor:
Rolf Seh, Graduate Student
David Richter, Associate Professor of Civil and Environmental Engineering and Earth Sciences
College of Engineering

Abstract

Cloud simulation is important because clouds drive radiative processes in the atmosphere, which cool or heat the planet depending on their properties. Clouds also lead to precipitation, which is important for human activities. Cloud modeling can lead to better predictions for weather models and help us understand what is happening to our climate.

The Lagrangian cloud model, when used for marine fog, simulates the particles in fog as clusters of aerosols with similar properties. The model utilizes multiplicities to assign the number of particles to the cluster. This multiplicity is kept constant and the number of clusters is derived from the constant multiplicity. The simulation can be run with different multiplicities and will result in the same overall distribution.

The refined process maintains the number of clusters constant while deriving the multiplicity. Each cluster can have a different multiplicity of particles so that there are varying amounts of particles in each cluster. This flexibility allows researchers to obtain more detailed information about specific aerosol clusters. They can generate a larger number of clusters for detailed examination, and a smaller number of clusters for less focused analysis. There can be multiple types of aerosols and this method allows for these to be accurately represented.

Identifying Drug Users on Social Media

Jack Mangione and Leonardo Molina
CSE Summer Enrichment Program

Mentor, Contributors, Faculty Advisor:
Billy (Tianyi) Ma, Graduate Student
Yanfang (Fanny) Ye, Galassi Family Collegiate Professor in
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Abstract

Lucrative profits have driven the evolution of illicit drug trafficking in recent decades, chiefly on social media platforms, which offer direct-to-consumer mediums for drug trade. The rapidly evolving landscape of social media enables sellers to adapt and avoid algorithmic detection, posing a significant threat to public health and safety. Previous research mainly leverage (Heterogeneous) Graph Neural Networks to tackle this issue that merely integrate the content information, i.e., user profile and posts, into user features and consider the relationships among these user nodes, while ignoring the complex relationships between entities, i.e., users and posts. Moreover, most existing drug trafficking dataset are balanced data which fails to mimic the real-world scenario. In light of this, we propose an imbalance Heterogeneous Graph Neural Network for drug trafficking (iHG-DT) to learn the user representations from both forms of heterogeneity (nodes and edges). To better mimic the complex relationships in real-world application on social media, we build a new imbalanced dataset from Twitter called Twitter-HetDrug that integrates three types of nodes and seven types of relationships. We benchmark our proposed model against (Heterogeneous) Graph Neural Networks on the Twitter-HetDrug and DBLP heterogeneous graph datasets. Our proposed method (iHG-DT) outperforms all baseline methods in F1 macro and accuracy, which demonstrates its superiority in learning from complex semantic heterogeneous relationships.

The Visualization of the HiFuzz Tests

Jonathan Mimnaugh
CSE Summer Enrichment Program

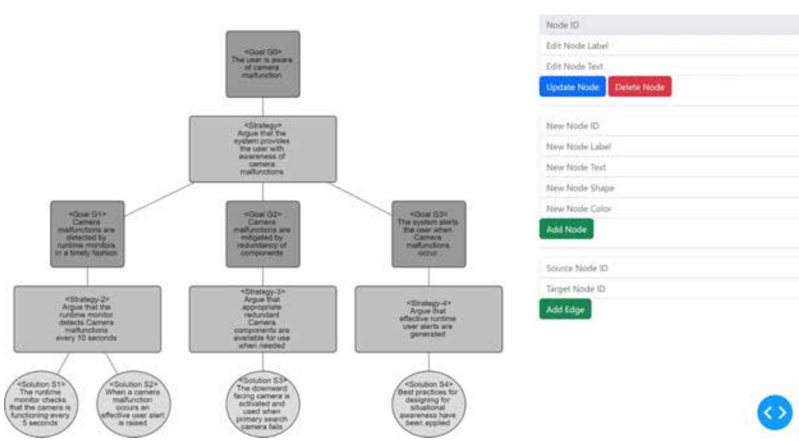
Mentor, Contributors, Faculty Advisor:
Shahbaz Ali Khan, Graduate Student
Jane Cleland-Huang, Frank M. Freimann Professor of Computer Science; Department Chair of Computer Science and Engineering
College of Engineering

Abstract

Small Unmanned Aerial Systems (sUAS) must adhere to strict safety requirements when used in high-stress emergency response situations. However, the increasing use of sUAS raises the risk of major incidents, a good percent of which have been human-made. To tackle this, researchers have been using Fuzz testing to find possible human-prone errors. Fuzz testing is an approach to software testing aimed at identifying system vulnerabilities and defects by injecting random inputs. Human Interaction Fuzzing for small Unmanned Aerial Vehicles (HIFuzz) system [1] is a fuzz testing pipeline developed to identify possible human inputs that could lead to drone mission failures. My project creates safety cases in the form of decision trees to visualize the project's goals, strategies, solutions, HIFuzz test data, and additional information. These safety cases are intended to help understand how to address issues with the HIFuzz system, set goals, and develop solutions. The ultimate goal of HIFuzz is to autonomously generate safety cases by taking in data and producing a complete and detailed safety case with all relevant information. Because the end game of the project is to have the safety cases be created autonomously they will need to be reviewed post-rendering by humans on the loop. Therefore, we created a web-based interactive safety case, featuring the ability to edit text in the nodes, create nodes, delete nodes, and move nodes and the decision tree itself. By implementing my project into the overall HIFuzz project, the human-on-the-loop can visualize the goals and strategies needed to combat issues they will encounter while seeking to improve their overall system.

References:

[1] Chambers, Theodore, Michael Vierhauser, Ankit Agrawal, Michael Murphy, Jason Matthew Brauer, Salil Purandare, Myra B. Cohen, and Jane Cleland-Huang. "HIFuzz: Human Interaction Fuzzing for Small Unmanned Aerial Vehicles." In *Proceedings of the CHI Conference on Human Factors in Computing Systems*, pp. 1-14. 2024.



Exploring Performance of LLMs Fine-tuned on Synthetic Code-switched Text

Tanay Nagar
Center for Computer Assisted Synthesis Summer Undergraduate Research Fellowship (C-CAS SURF)

Mentor, Contributors, Faculty Advisor:
Anna Sokol, Graduate Student
Grigorii Khvatskii, Graduate Student
Nitesh Chawla, Frank M. Freimann Professor of Computer Science and Engineering and Director of Lucy Family Institute for Data and Society
College of Engineering

Abstract

Language models (LMs) exhibit significant performance discrepancies on subjective, translation-variant tasks when prompted in different languages (Zhang et al; 2023) (Li et al; 2024), particularly underperforming in low-resource languages like Hindi, Yoruba, and Swahili. This bias stems from an imbalance in language data utilized during pre-training and training of LMs. Our research investigates whether fine-tuning LMs on synthetic code-switched data—where multiple languages are interspersed within sentences—can mitigate this bias. We explore two primary methods of generating code-switched data: the mt5 pre-trained model (Mondal et al; 2022) and LLM generation techniques, working with the Llama3 language model. Our benchmark for evaluating these methods is the Common-Sense Question-Answering task (Talmor et al; 2019), which provides a robust framework for assessing language model performance across multiple languages. We aim to enhance LM performance in low-resource languages (Hindi) while maintaining their proficiency in high-resource languages such as English.

Advancing Towards a Sustainable Future for the Nuclear Fuel Cycle

Sarah Oliva
Vincent P. Slatt Fellowship

Mentor, Contributors, Faculty Advisor:
Zoe Emory, Graduate Student
Jennifer Szymanowski, Facility Staff Scientist
Peter C. Burns, Henry J. Massman Professor of Civil and Environmental Engineering and Earth Sciences
College of Engineering

Abstract

Uranyl peroxide cage clusters (UPC) have been proposed as a route to more efficient extraction of uranium during spent nuclear fuel reprocessing (Fig. 1). Typically, uranyl peroxide cage clusters are synthesized in a uranyl bearing aqueous solution with an excess of hydrogen peroxide. This study investigates how utilizing non-thermal plasma discharge into an alkaline uranyl bearing aqueous solution could provide sufficient hydrogen peroxide for uranyl peroxide cage clusters to self-assemble in aqueous solution.

Samples were gathered from multiple plasma electrolysis experiments, in a plasma reactor and were interrogated by UV-Vis spectroscopy to determine the concentration of hydrogen peroxide. After consistent results were demonstrated, the solution from the reactor was added to an alkaline uranyl bearing solution. Samples were then taken from the uranyl bearing aqueous solutions and investigated and analyzed by electrospray ionization mass spectroscopy (ESI-MS) to observe the production of uranyl peroxide cage clusters. ESI-MS showed that multiple uranyl peroxide cage clusters had assembled in solution. On-site use of non-thermal plasma discharge has the potential to eliminate the transport of hazardous and costly hydrogen peroxide while providing the means to synthesize UPCs for more efficient fuel reprocessing.

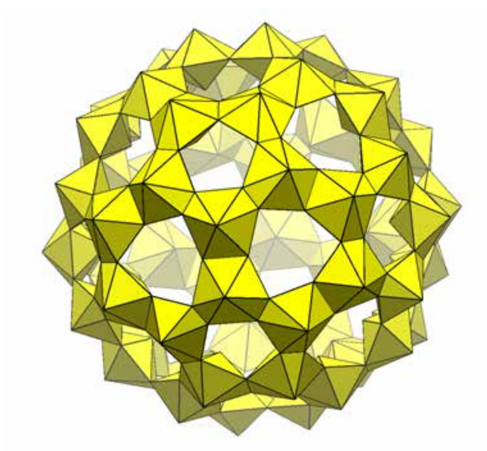


Figure 1. An example uranyl peroxide cage cluster with uranyl polyhedral shown in yellow

Measurement and Analysis of Ultra-Wideband (UWB) Signals

Sebastian Pirela
Advanced Wireless Research Experiences (AWaRE)

Mentor, Contributors, Faculty Advisor:
Omkar Mujumdar, Graduate Student
Bingyan Lu, Graduate Student
Nick Laneman, Professor of Electrical Engineering, Co-Director of Wireless Institute, and Director of SpectrumX,
College of Engineering

Abstract

Motivated by the US National Spectrum Strategy's examination of the 7.125-8.4 GHz band, this project focuses on the precise measurement and analysis of Ultra-Wideband (UWB) signals, a key technology embedded in many modern smartphones for high-accuracy location tracking. UWB operates by emitting short pulses of energy across a broad frequency range, including 3-10 GHz, allowing for exceptional distance measurement precision. A notable example is Apple's AirTag, which leverages UWB to locate items within centimeters. UWB's broad spectrum coverage and low energy pulses present significant measurement challenges due to their faint nature and susceptibility to interference. My research aims to develop a lab-based setup for capturing UWB signals and to incorporate advanced signal processing techniques for enhancing detection and accuracy.

The project involves three key phases: researching and selecting high-precision measurement equipment, designing and implementing a measurement setup, and applying sophisticated algorithms to differentiate UWB signals from noise. This approach will enable the precise characterization of UWB signals, supporting the efficient spectrum management goals of the National Spectrum Strategy. The implications of improved UWB signal measurement extend across various industries. In smart home technology, UWB can facilitate seamless device interaction and automation based on precise location data. In automotive applications, UWB enhances vehicle access and security. Additionally, in healthcare, UWB's accurate real-time tracking can improve asset management and patient care. By advancing the accuracy of UWB signal measurements, this project contributes to the broader objectives of efficient spectrum utilization and technological innovation, ultimately supporting the deployment of next-generation wireless technologies while avoiding harmful interference.

Thermal Emission-based Geometric Mapping of Specular Glass Surfaces

Delaney Reynolds
Engineering Summer Research Experience (E-SURE)

Faculty Advisors:
Robert Landers, Advanced Manufacturing Collegiate Professor of Aerospace and Mechanical Engineering; Edward Kinzel, Associate Professor of Aerospace and Mechanical Engineering
College of Engineering

Abstract

Traditional line scanners used in metrology applications rely on the diffuse reflection of light off the part's surface to determine the object's form. Specular surfaces such as glass cannot be measured by these scanners unless the surface is dusted. To circumvent this time-consuming procedure, we proposed a method to measure the geometry of specular surfaces through the use of thermal emission, as heat absorption is a diffuse process. Our system is implemented by locally heating the surface of a glass object with a CO_2 laser. A thermal camera detects the thermal profile of the area where the laser and part intersect. Height changes across a surface are calculated from the laser's angle of incidence and the vertex of the profiles' horizontal location. The resolution is obtained by measuring an optical flat, which has surface variations on the order of a nanometer. Our measurement algorithm filters the data to remove noise. In experimental studies, variation in variables such as laser power, stage velocity, and filtering methods were explored to determine their impact on the measurement resolution. Our algorithm achieves a 10-micron resolution for both flat and curved surfaces. Dusting a part and using a traditional line scanner is difficult to incorporate into applications where the part is undergoing in-line processing. Our thermal emission-based measurement technique has the potential to pave the way towards an integrated methodology for the measurement of glass, even in processing applications.

Simulating Ice Growth in Mixed-Phase Clouds

Benjamin Roper
Engineering Summer Research Experience (E-SURE)

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

Abstract

The Pi Chamber is an apparatus at Michigan Tech that is used to produce artificial clouds and study their characteristics. Currently an intercomparison study is being conducted to study mixed-phase clouds. Mixed-phase clouds contain both ice particles and liquid droplets. In the test procedure, the Pi Chamber is brought to turbulent equilibrium, then saline aerosol is injected until the average radius and concentration of cloud droplets reaches steady state. At this point, Ice particles are injected into the Pi Chamber. The Ice crystals absorb the moisture from the air and grow from sublimation. The cloud becomes glaciated when the mass fraction of all particles is 90% ice.

The existing simulation is a Lagrangian model that is coupled with a turbulent simulation written in Fortran. The particles and their properties are stored in memory via a linked list, and each calculation runs through the list from start to finish. The liquid particles use the implicit Backwards Euler method to calculate radius and temperature, but the equations for ice particles are too complex and must use the explicit 3rd order Runge-Kutta method. Ice particles can be added in a separate linked list that follows the different equations. MATLAB script that simulated a single particle. After confirming the equations were accurate, the Fortran simulation was modified with the new equations.

Comparison of Nickel-containing Keggin Polyoxometalate on SBA-15 and a Zinc Metal-Organic Framework in Ethylene Oligomerization and Using a Stochastic Kinetic Models to Model Reactions

Mario Ruiz-Yamamoto
CISTAR Young Scholars Program

Mentor, Contributors, Faculty Advisor:
Alba Scotto D'apollonia, Graduate Student; Michael Appoh, Graduate Student
Jason Hicks, Tony and Sarah Earley Collegiate Professor of Energy and the Environment, and Associate Dean for Graduate and Postdoctoral Affairs; William Schneider, Dorini Family Chair of Energy Studies, Department Chair and Professor of Chemical and Biomolecular Engineering
College of Engineering

Abstract

The Ni-Keggin POM ($K_5PW_{11}O_{39}{\cdot}Ni^{2+}$) was synthesized and characterized to determine its purity. It was then incorporated into two different structures to facilitate catalysis. The POM was grafted onto an SBA-15 support to facilitate the accessibility of nickel as an active site for catalysis. For a different catalyst, the POM was encapsulated into a framework of zinc and pyridine. These two catalysts were then characterized and reacted with ethylene to measure their results in catalysis. Different kinetic models were constructed using Python. A deterministic kinetic model was constructed using an ordinary differential equation solver and a stochastic model was constructed using the Gillespie algorithm to model individual molecules. The deterministic kinetic model was used as a basis for understanding differences in changing parameters of the stochastic kinetic model. This stochastic kinetic model was then used to explore different parameters of the Ni-Keggin POM.

Predicting Mosquito-borne Disease Outbreaks: Where Will Chikungunya Strike Next?

Ebony Saccento
ND-PREP

Mentor, Contributors, Faculty Advisor:
Alexander Meyer, Postdoctoral Researcher; Stacy Mowry, Graduate Student
Alex Perkins, Associate Professor of Biological Sciences
College of Science

Abstract

Mosquitoes are considered one of the most dangerous animals because they spread diseases. One of these diseases is chikungunya, a viral illness that can cause chronic pain. Chikungunya outbreaks occur seemingly randomly, and presently no vaccine has been proven effective against chikungunya virus (CHIKV) infection. In this study, we are trying to understand which populations are at risk for CHIKV since it is difficult to predict an outbreak and rely on a vaccine that has not been tested. One component of risk is pre-existing immunity to CHIKV from past outbreaks, and the birth and death rates determine how long immunity lasts after an outbreak. We then approach these scenarios by taking data from populations at risk for CHIKV outbreaks and, with help from a mathematical model, the data we're using are population age structure data; the model simulates CHIKV transmission and population aging; and the thing we're predicting is population immunity (or susceptibility, 1 - immunity) over time. The mathematical model will help us understand the relationship between aging, immunity, and outbreak risk. We expect our results to show that areas with a larger, younger population will have higher susceptibility in an outbreak since these populations will unlikely be immune from the disease since they did not have it before. Future directions include the information to predict where the next outbreak may happen so a vaccine trial can be set up, with hopes of getting a CHIKV vaccine officially approved.

Phage-mimicking Nanoparticles as Broad Spectrum Antibacterials

Olivia Sayani
NDnano Undergraduate Research Fellowship (NURF)

Mentor, Contributors, Faculty Advisor:
Carlie Kudary, Biomedical Technician, Berthiaume Institute for Precision Health
Prakash Nallathamby, Research Assistant Professor, Department of Aerospace and Mechanical Engineering, and Associate Director of Berthiaume Institute for Precision Health
College of Engineering

Abstract

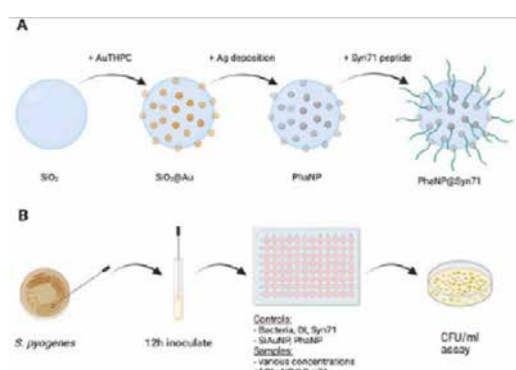
By 2050, antibiotic resistance is expected to affect more people than all types of cancers combined [1]. The rapid emergence and global spread of resistant bacteria, coupled with the low discovery rate of new antibiotics, highlight the urgent need for broad-spectrum antibacterials. Phages have been evolutionarily successful in killing bacteria for millions of years. However, phage synthesis is not scalable and is hyper-specific to single bacterial strains. As an alternative to antibiotics, we have developed phage-mimicking nanoparticles (PhaNPs) that act as broad-spectrum antibacterials by mimicking the protein-turret distribution density on bacteriophages. The antibiotic-free composition of PhaNPs prevents bacteria from developing resistance, and their generally regarded as safe (GRAS) composition helps avoid immunogenic reactions.

Our approach involves synthesizing silica core-shell nanoparticles and capping them with silver-coated gold nanospheres and synthetic antimicrobial peptides. We predict that this will enhance antimicrobial activity. The PhaNPs exhibit pockets of positive charge on the silica core and the amphiphilic surface of the peptide, which attract the PhaNP@peptides to the anionic surface of bacterial membranes. Previous studies have shown that the synthetic peptides syn-71 and syn-20 are effective against both gram-negative and gram-positive species, with a low minimum inhibitory concentration.

Given the structure and zwitterionic charge of the PhaNP@peptides, we hypothesize that these nanoparticles will be effective against ESKAPEE pathogens, which include *Pseudomonas aeruginosa, Acinetobacter baumannii, Staphylococcus aureus, Klebsiella pneumoniae, Streptococcus pyogenes, Corynebacterium striatum, and Enterococcus faecalis*. Additionally, we are testing the hypothesis that PhaNP@peptides will prevent the emergence of resistance in these bacterial species.

References:

[1] *Phage-mimicking antibacterial core–shell nanoparticles. Nanoscale Advances, (2019), 1, 4812–4826. J. Hopf, M. Waters, V. Kalwajtys, K. E. Carothers, R. K. Roeder, J. D. Shrout, S. W. Lee and P. D. Nallathamby*



Building Dynamic Physics-Informed Neural Network with Fast Fourier Transform Analysis

Reem Shehayib
Engineering Summer Research Experience (E-SURE)

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Jayden Vap, Graduate Student
Peter Kogge, Ted H. McCourtney Professor of Computer Science and Engineering
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Abstract

Physics-Informed Neural Networks (PINNs) are data-driven neural networks used in supervised learning models to represent physics equations while maintaining robustness and reliability. Respecting the laws of physics used in a certain problem, PINNs allow incorporating differential equations to study a system's behavior. PINNs are known to work excellently on fitting and seeking easily differentiable and low frequency-solutions; however, they also fall short when learning variations/oscillations, especially unusual and unpredicted ones, e.g. boundary layers or noise. This behavior is related to the notion of overfitting, as a consequence of both a surplus of weights and depth of the network.

This project looked to abate the aforementioned issues by studying an RLC circuit with variations in the low-frequency range and performing a Fast Fourier Transform (FFT) analysis. The designed neural network architecture handles these kinds of variations while considering the frequency domain by utilizing a Fourier Layer neural operator and further addresses overfitting by developing a dynamic PINN. This optimization was inspired by the SuperServe architecture, yet implemented in the learning stage, thus not only making the training comprehensive but also dynamic in the least complex manner while maintaining reliability.

Evaluation of Squarine Dye Based Small Molecules as Possible DYRK1A Inhibitors

Jerica A. Siberón Albertorio
Summer Research Opportunities Program (SROP)

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Gregory Durling, Graduate Student
Brandon Ashfeld, Professor of Chemistry and Biochemistry
College of Science

Abstract

Abnormal expression or activity of human dual-specificity tyrosine phosphorylation – regulated kinase 1A (DYRK1A) is related to congenital and neurodegenerative cognitive disorders such as Alzheimer's, Down syndrome and Tauopathy. Recent studies demonstrated that plant derived compound harmine and N-heterocyclic carbene based substrates are effective competitive inhibitors of DYRK1A thanks to their extended conjugation present in the core scaffold which allows effective binding to the active site. Small molecules have been previously studied as squarine dye-based chemodisimeters, and ortho-substituted dianiline squarine derivatives demonstrate skeletal structure rearrangement upon the addition of nucleophilic phosphine (III). The resulting molecule demonstrates similarities in core scaffold as harmine, with extended conjugation favorable for inhibition to the ATP-binding of DYRK1A. This study aims to further describe the rearrangement properties of the selected squarine dye small molecule scaffold, evaluating interactions with different alkylated phosphine (III) derivatives upon addition. To achieve this, symmetric hydroxy ortho-substituted dianiline squarine was synthetized with phosphine nucleophiles PBu_3, PPh_3, $P(NMe_2)_3$ and $OP(NMe_2)_3$. NMR-spectra of the products demonstrates that rearrangement of the small molecule was successful with PBu_3 and $P(NMe_2)_3$, as these show chemical stability and low steric hindrance characteristics that favor the nucleophilic addition. PPh_3 is a bulky molecule with a poor nucleophilic phosphine ligand and $OP(NMe_2)_3$ is a poor nucleophile because the lone pairs are in resonance along its structure. Further studies could be performed with the addition of other nucleophiles. The rearranged skeletal structures of these molecules present similar characteristics to harmine and could be tested further on for DYRK1A inhibition.

Polymer Crystallization for Automated Materials

Anna Skoropad
NDnano Undergraduate Research Fellowship (NURF)

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Joshua Sam, Undergraduate Student
Gabriel Burks, Assistant Professor of Chemical and Biomolecular Engineering
Yamil Colón, Assistant Professor of Chemical and Biomolecular Engineering
College of Engineering.

Abstract

A lot of research has been done on plastics, and with the rise of machine learning, there has appeared a new opportunity to analyze and study plastic materials. Machine Learning is an exciting chance, which is planned to be used by our group, to further our understanding of polymers. Our primary objective is to contribute to the advancement of sustainable material development and avoid the negative environmental impacts of synthetic polymers.
To study a polymer material, single crystals are needed due to their uniformity and close relation to the material's properties. The team grew single crystals of one of the most used polymers, Polyethylene. Using xylene, it was possible to avoid Van der Waal forces between the polymer chains, regulate the temperatures, and grow evenly distributed single crystals. Self-seeding method was used to grow the crystals and SEM helped identify the crystalline structures of prepared solutions. In order to analyze crystallization of the polymer crystals, a Stokes Trap was used. Under different pressures of the Trap, the crystals change their shapes, and, with the amorphous chains in the fluid, further growth can be induced. Finally, having captured the videos of the changes, a Convolutional Neural Network will help characterize the images. The machine learning process will correlate the properties or procedure of manufacturing with the images of the desired material.

So far, favorable crystallization conditions were found, and the crystals that the team was able to grow have an optimal size for trapping. Further work will be done to learn and modify polymer single crystals, which would help us produce a better product.

Comparing Drug Release Rates for Various Non-Spherical Hydrogels

Vaibhavi Sunkara
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

Faculty Advisor:
Sima Asadi, Clare Boothe Luce Assistant Professor of Chemical Engineering,
Department of Chemical and Biomolecular Engineering
College of Engineering

Abstract

Hydrogels have diverse applications, particularly in drug delivery systems. Transitioning from traditional spherical hydrogels to non-spherical hydrogels offers numerous advantages, including an increased surface area-to-volume ratio, highly targeted drug delivery, and a shorter diffusion path for drugs, thereby enhancing the efficiency of drugs within the body. These non-spherical hydrogels were created by dripping an alginate solution at different angles into a gelation bath. This study aims to analyze the amount of FITC-D, a fluorescent drug that was released into an external solution composed of Phosphate Buffered Saline (PBS) for the various shapes of hydrogels that were synthesized. The experiments provided a more clear understanding on the differences between each of the shapes and how each shape-engineered hydrogel specifically affects drug release rates. The different shapes can target various areas and release drugs at different concentrations into the body, enhancing the accessibility and customization of medication for individual patients. Precise drug delivery minimizes side effects and reduces the need for frequent dosing. As these methods evolve, patients benefit from treatments tailored to their specific needs, resulting in less pain and an improved quality of life. Through personalized medicine, patients can manage their health in a manner that best works for them.

Localization of Neurexin 2 and 3 in Oligodendrocytes and Oligodendrocytes Progenitor Cells

India Turner
Summer Research Opportunities Program (SROP)

Mentor, Contributors, Faculty Advisor:
Veronica Vanoverbeke, Graduate Student
Valeria Perez Negron, Undergraduate Student
Katrina Adams, Gallagher Assistant Professor, Department of Biological Sciences
College of Science

Abstract

Oligodendrocytes (OLs) are glial cells that are important for the proper functioning of the central nervous system because of their ability to form myelin sheaths around neuronal axons, thereby allowing rapid signal conduction. These cells originate from oligodendrocyte progenitor cells (OPCs) present in the ventricular zones of the neural tube during early embryonic development. During early postnatal development, OPCs proliferate, migrate, and differentiate into mature OLs. In addition to generation of OLs, OPCs also perform several additional functions, including synapse pruning and regulation of angiogenesis, as well as receive synaptic input from interneurons. Much less is known regarding what signaling pathways regulate these non-canonical functions of OPCs – both during development and in the adult CNS. Neurexins are proteins of synaptogenesis, which mediate formation at the presynaptic terminal level that allows for communication between neurons within the brain. Neurexins have never been studied in OPCs or OLs. This research sought to determine if Neurexin 2 and 3 are expressed in OPCs and OLs during postnatal development. We found that in P28 mice Neurexin 2 and 3 was expressed on the OLs and OPCs. We then analyzed expression of Neurexin 2 in the adult mouse brain both under healthy and demyelinated conditions. Preliminary results suggest that adult mice's OPCs and OLs expressed Neurexin 2 at similar rates both healthy and demyelinated. The exploration of Neurexin expression in the OL lineage may help to open new avenues of investigation focused on understanding how synaptic proteins regulate glial cell physiology during development and in demyelinating disorders, like Multiple Sclerosis.

Construction of Human Cytomegalovirus UL44 Truncated Genes to Promote an Improved Functional Humoral Response for Vaccine Development

Kiara Vazquez Narvaez
ND PREP

Mentor, Contributors, Faculty Advisor:
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Pilar Pérez-Romero, Associate Research Professor, Department of Biological Sciences
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Abstract

Human cytomegalovirus (HCMV) is a herpesvirus with high global prevalence (60% -100%) that is a major threat for immunocompromised individuals. Besides researchers' efforts, current treatments carry side effects and the selection of resistance mutations, and no clinically approved vaccine exists. Vaccine design should include HCMV antigens capable of eliciting both cellular and humoral protective immunity. A previous study in our group identified the viral phosphoprotein UL44 as an ideal antigen since it is highly conserved, abundant, and elicits a potent immune response. Despite UL44's ability to induce strong humoral and cellular responses, patients' serum antibodies have not demonstrated functional virus neutralization. Based on bioinformatic analysis of UL44, we hypothesize that the native protein may occlude its own neutralizing epitopes which prevents effective neutralization.

To improve the neutralizing antibody response, we will construct two truncated versions of UL44 that lack the C-terminal domain of the protein. The plasmid constructions will be transfected in human cells to express and detect the protein products by Western blot and ELISA. Mice will be immunized with the DNA vaccine formulations to trigger the immune response, and serum samples and spleen cells will be collected. The functionality of the antibody response will be determined by neutralization and ADCC assays, and the T-cell immune response by detecting IFN-γ production upon specific stimulation. We expect to induce an effective neutralizing antibody response with truncated UL44 proteins that expose immunogenic peptides. Our goal is to improve HCMV vaccine development to elicit a protective immune response to all individuals.

Simulated Methane Adsorption in Soft Porous Coordination Polymers

Jean Galliano Vega Díaz
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

Mentor, Contributors, Faculty Advisor:
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Yamil Colón, Assistant Professor of Chemical and Biomolecular Engineering
College of Engineering

Abstract

Soft porous coordination polymers, or SPCPs, are a class of materials characterized by their flexibility and tunable porosity. Similar materials like zeolites and metal-organic frameworks have been used for catalysis, sensing, environmental remediation, etc. Our primary objective is to employ molecular simulations, specifically grand canonical Monte Carlo (GCMC) and molecular dynamics (MD), to assess the adsorption behavior of SPCPs while varying volumes and loadings. We focused on understanding methane adsorption due to its ease of implementation and relevance for energy storage applications. Through LAMMPS simulations and thermodynamic integration, I studied how free energy changes when altering the amount of guest molecules from 0 to 1200 and allowing the volume of the material to fluctuate. With the free energy profiles, we can determine the free energy minimum which corresponds to the structure's equilibrium state. Using the stable states, we can later focus our efforts on the stable phase that is present for each loading. Under different pressures the structure could rearrange itself to turn a closed pore with limited adsorption to an open configuration. Density profiles were also drawn from the simulations to characterize which pores the adsorbate favored and where it was concentrating the methane atoms. By understanding pore-filling mechanisms in response to pressure and structure saturation, we can develop more robust and efficient SPCP-based technologies for carbon capture, gas storage, and separations. My findings underscore the importance of evaluating adsorption isotherms across a range of loadings to capture the full range of adsorption phenomena in SPCPs.

Hydrogels with Convertible Properties Mediated by Heat and Ultraviolet Light

Marcos Villarreal
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

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Connor Schmidt, Graduate Student
Matthew Webber, Keating-Crawford Collegiate Professor of Engineering; Associate Professor of Chemical and Biomolecular Engineering; Acting Faculty Director of Berthiaume Institute for Precision Health
College of Engineering, Notre Dame Research

Abstract

Hydrogels are typically categorized as being either physical and dynamic—able to change their properties over time, or chemical and static—possessing mechanical strength but not allowing for time-dependent change in properties. This research aims to create a host–guest hydrogel using reversible bonds to toggle alternatingly between such dynamic and static states. This envisioned hydrogel relies on a host macrocycle, CB[7], attached to an 8-arm PEG macromer that recognizes a guest ligand attached to another 8-arm PEG macromer. These two components form physical supramolecular crosslinks when mixed, leading to dynamic hydrogel network. A secondary agent can react with the guest ligand, altering its ability to dynamically exchange its binding with CB[7]. This reaction is reversible, with heat driving the reaction to make the bonds more static, and UV light returning these bonds to their original dynamic state. These changes in bonding are then manifest in the bulk material properties of the hydrogel, where its dynamic state offers shear-thinning injectability and its static state offers stable mechanical properties. Currently, we have successfully synthesized all small molecule host and guest ligands. Subsequent work will demonstrate production of dynamic physical hydrogel incorporating these components, followed by rheological testing. Future investigation will focus on utilizing biomarkers or disease-relevant signals to trigger these changes in mechanical properties. With more precise control of material properties, we can better improve the use of hydrogels for drug delivery, biomaterials, and 3D printing applications.

cyfip2 Controls the Precise Deployment of Distinct Actin Structures During Axon Invasion

Grace Waddell
College of Science Summer Undergraduate Research Fellowship (COS-SURF)
Glynn Family Honors Program

Mentor, Contributors, Faculty Advisor:
Henry Bates and Kaitlin McGowan, former Notre Dame Undergraduate Students
Dana F. DeSantis, former Notre Dame Postdoctoral Fellow
Kurt C. Marsden, Associate Professor, Department of Biological Sciences,
North Carolina State University
Cody J. Smith, Elizabeth and Michael Gallagher Associate Professor,
Department of Biological Sciences
College of Science

Abstract

The cellular organization of the nervous system during development is critical to neurons' abilities to communicate information. While we know that a precise spatiotemporal system is necessary for neurons to organize and connect, we do not fully understand these processes at a genetic or molecular level. Using transgenic lines of zebrafish (*Danio rerio*), we performed a large-scale CRISPR-Cas9 screen to identify genetic mechanisms that modulate how the dorsal root ganglion (DRG) sensory neurons connect with the spinal cord during development. In this screen, we found *cyfip2* is required for DRG neurons to connect with the spinal cord. Using CRISPR-Cas9 knockdown and an established mutant line, we found that while *cyfip2* functions in axon invasion into the spinal cord, the formation of the DRG neurons is independent of *cyfip2*. *cyfip2* RNA and protein are localized to the DRG neurons during the estimated timepoints of axonal entry into the spinal cord, further suggesting that *cyfip2* is involved in this process. Using timelapse imaging of growth cones as they invade the spinal cord, we found *cyfip2* functions in the DRG growth cone to deploy the correct actin structures as they navigate and then invade. In an investigation of other genes that may work with *cyfip2*, it was found that *fmr1* has similar roles in the axon invasion process when perturbed via a CRISPR-Cas9 knockdown or in a stable mutant line. Overall, these findings implicate previously unknown genes in this neurodevelopmental process, which could be critical in understanding neurodevelopmental disorders involving sensory processing difficulties.

Efficient Removal of Textile Dyes from Synthesis Wastewater Using Algal Biomass: A Study on Methylene Blue, Methyl Orange, and Rhodamine B

Oisín Wade
Naughton Fellowship

Mentor, Contributors, Faculty Advisor:
Siwei Gu, Postdoctoral Researcher
Kyle Doudrick, Associate Professor of Civil and Environmental Engineering and Earth Sciences
College of Engineering

Abstract

In the textile industry, a significant portion of the dye used during fabric coloring remains in the wastewater, posing a serious environmental threat. The removal of these dyes from wastewater is critical due to their harmful impacts, which include increased biochemical and chemical oxygen demand, impaired photosynthesis, inhibited plant growth, and bioaccumulation that can lead to toxicity, mutagenicity, and carcinogenicity.

Various techniques exist to address these pollutants, such as adsorption, ion exchange, membrane filtration, and coagulation-flocculation. However, there is a growing need for sustainable and environmentally friendly methods that align with green chemistry principles.

This study focuses on the removal of three textile dyes: methylene blue, methyl orange, and Rhodamine B using three types of macroalgal biomass. The research being conducted investigates parameters such as kinetics, isotherms, thermodynamics, pH effects, and the influence of competing ions on the adsorption process to simulate the real industrial treatment plant. Algae-derived biosorbents offer a promising solution due to their cell wall matrices, which contain a variety of functional groups capable of adsorbing different pollutants. Specifically, dried algae biomass, including wakame kelp and bladderwrack, shows potential as renewable and eco-friendly water treatment tools. These preliminary investigations aim to characterize the effectiveness of these biosorbents in dye removal from wastewater, providing an innovative approach to addressing pollution in the textile industry.

Reducing Mosquito-Related Disease Transmission through Understanding its Interrelated Visual and Olfactory Sensory Systems

Caleb Wafer
ND-PREP

Mentor, Contributors, Faculty Advisor:
Alexis Waldschmidt, Graduate Student
Kimberly Waldschmidt, Undergraduate Student
Joseph E. O'Tousa, Emeritus Professor, Department of Biological Sciences
College of Science

Abstract

The *Aedes aegypti* mosquito is the primary vector for the diseases dengue, chikungunya, and yellow fever which each year are responsible for over fifty million infections and over five thousand deaths world-wide. *Aedes* uses multiple sensory systems, notably olfaction and vision, to drive these behaviors resulting in the identification and biting of human hosts. We used gene editing to create *Aedes* genetic strains that lack specific components of the visual system. The goal of this research project is to investigate the role of these identified genes in the mosquito's olfactory system. We hypothesize that these identified genes also play a role in olfaction such that genetic strains lacking these components will perform more poorly in host seeking behaviors than the strains in which only one of these sensory systems is targeted.

We will use multiple approaches to test this hypothesis. First, we will mine tissue-specific mosquito RNAseq data to determine which of the genes identified as being active in vision are also expressed in the mosquito antennae, the major tissue containing olfactory receptors. Next we will use immunological reagents to pinpoint the antennal cells expressing these genes. Then we will use receptor mapping analysis, as pioneered by other labs, to show that mutant cells do not respond to specific odorants. Finally, we will conduct behavioral assays with normal and mutant strains to see how visual and olfactory information combine to enhance the mosquito's host seeking behavior.

Thus this research aims to identify shared cellular components of vision and olfaction. We hope to identify new and better targets for reducing mosquito host seeking and biting behaviors. In this way the work may ultimately lead to more efficient means of reducing the burden of mosquito transmitted diseases.

Synthesis and Characterization of Copolymer Interlayers for Lithium-Sulfur Batteries

Rachel Wallace
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

Mentor, Contributors, Faculty Advisor:
Piyush Deshpande, Graduate Student
Jennifer Schaefer, Sheehan Family Collegiate Professor,
Department of Chemical and Biomolecular Engineering
College of Engineering

Abstract

In the pursuit of meeting rising energy demands and supporting the transition from fossil fuels to renewable energy sources, batteries are necessary for electric vehicles and grid energy storage. Given that sulfur is an earth-abundant element and environmentally benign, lithium-sulfur batteries (LSBs), in particular, present desirable qualities for future manufacturing and sustainable energy prospects. Additionally, solid-state electrolytes (SSE) are advantageous due to their reduced volatility in comparison to liquid electrolytes. However, via a phenomenon known as the “polysulfide shuttle effect,” whereby active material from the sulfur cathode migrates through the electrolyte and passivates the lithium anode, LSBs exhibit issues with longevity. Copolymer interlayers between the sulfur cathode and SSE within the LSB are proposed to mitigate the polysulfide shuttle effect.[1] Here we examine PEGMA-TFEMA-GMA-STSFI (PTGS) as an interlayer since it is hypothesized to be effective in blocking polysulfides based on the electrostatic repulsion effect and polarity of its monomers. Its capacity to block polysulfides was tested by sandwiching the interlayer at varying amounts of contact time between polymer films with and without polysulfides to induce polysulfide movement with a concentration gradient. The amount of polysulfides allowed through the interlayer was measured using Raman spectroscopy and elemental analysis. The interlayer’s mechanical properties were optimized by decreasing the crosslink density of the copolymer by diluting the crosslinker, hexamethylenediamine. Once PTGS is determined to be mechanically durable, its ability to block polysulfide shuttling will be quantitatively compared to that of PEGDA, which was tested and confirmed to have little to no capacity of blocking the polysulfide sulfide effect.

References:

[1] Inhibition of Polysulfide Shuttles in Li-S Batteries: Modified Separators and Solid-State Electrolytes. Li, Shulion, et al. 2021.

Ink-Jet Printing of CeO_2 Thin Film Targets

Victor Williams
Vincent P. Slatt Fellowship

Mentor, Contributors, Faculty Advisor:
Noah Cabanas, Graduate Student
Ani Aprahamian, The Frank M. Freimann Professor of Physics, and
Concurrent Professor of Chemistry and Biochemistry
Khachatur Manukyan, Associate Research Professor, Department of Physics and Astronomy
College of Science

Abstract

Thin film targets are an essential component for many nuclear measurements and experiments and are challenging to produce. Ink-jet printing coupled with solution combustion synthesis is a novel development with high material efficiency that reduces costs and accomplishes the production of thin films with materials that are otherwise difficult to handle. The printer deposits picoliter-sized droplets of combustible solutions composed of metal nitrates and fuel onto aluminum substrates, which then are heat-treated for combustion synthesis to turn the deposited solutions into thin films of metal oxides. This experiment used cerium nitrate (oxidized) solutions with acetylacetone (fuel) dissolved in a solvent to create thin cerium oxide films. These thin films, with thicknesses of 10 to 100 nanometers, can be used as targets for nuclear measurements and surrogates for actinides in nuclear fuel irradiation studies. This presentation will show a parametric study (heating conditions, droplet deposition step size, solvent type, concentration of solution) to investigate the effects on the uniformity and thickness of thin films

The National Nuclear Security Administration (NNSA) of the United States Department of Energy (DOE) provided financial support for the work through Grant # DE-NA0004093.

Democratizing Radio Wave Exploration: Enhancing Accessibility through Compatibility and Visualization

Carl Xu
Advanced Wireless Research Experiences (AWaRE)

Mentor, Contributors, Faculty Advisor:
Randy Herban, Software Engineer, Wireless Institute
Christopher Wahl, Xiangbo Meng, and Zhiyu Shen, Graduate Students
Bertrand Hochwald, Freimann Professor of Electrical Engineering and Co-Director of Wireless Institute
College of Engineering

Abstract

The RadioHound project aims to democratize access to radio spectrum data by creating a small, affordable device capable of collecting and analyzing radio signals through the RadioHound website. By making this technology accessible to the general public, RadioHound seeks to foster a greater understanding and appreciation of the invisible radio wave landscape that surrounds us daily.

As part of this mission, my role focused on developing the necessary software to ensure compatibility across different operating systems, specifically Linux and Windows. This cross-platform functionality is crucial for broad user adoption, as it enables a wider audience to use the device, regardless of their preferred operating system. By taking Linux-only code and adapting it for Windows compatibility, I contributed to making the RadioHound device more versatile and user-friendly, aligning with our goal of widespread accessibility.

In addition to developing cross-platform code, I helped develop an additional heatmap feature for the detection of radio waves from these small devices. By visually representing this data, the heatmap makes it easier for users to interpret and understand the information. This feature not only enhances the functionality of the RadioHound website but also empowers users to engage with radio wave data in a more intuitive and meaningful way.

Both the development of cross-platform code and the implementation of the heatmap feature support RadioHound's mission by ensuring the device is easy to use and accessible to the layman. These advancements enable more people to participate in the exploration and understanding of the radio wave environment, thereby fulfilling RadioHound's vision of making radio wave data accessible to all.

Developing Electrochemical Aptamer Biosensors in 3D Cell Culture for High-Throughput Drug Testing

Keyang (Swindar) Zhou
NDnano Undergraduate Research Fellowship (NURF)

Mentor, Contributors, Faculty Advisor:
Grayson Huldin and Yinke Jiang, Graduate Students (Fu Lab)
Hyunsu Jeon, Graduate Student (Wang Lab)
Kaiyu Fu, Assistant Professor of Chemistry and Biochemistry
Yichun Wang, Assistant Professor of Chemical and Biomolecular Engineering
College of Science, College of Engineering

Abstract

High-throughput *In vitro* drug testing has become essential for drug discovery and screening of pharmaceutical applications. Traditional 2D cell cultures often fail to replicate the complex cell-cell and cell-extracellular matrix (ECM) interactions found in animal models and human tissues, leading to unreliable drug testing results. In contrast, 3D cell cultures such as organoids provide a more physiologically relevant environment by using biocompatible hydrogels to create customizable Inverted Colloidal Crystal (ICC) scaffolds with uniform and size-controlled organoids, better mimicking tissue-like microenvironments with high yield, versatility, and reproducibility.

However, the geometric miniature and structural complexity of 3D cell cultures pose challenges for obtaining accurate data and spatial information on cellular activities in real-time manner. To address this, we have developed Electrochemical Aptamer Biosensors (EABs) that can be integrated into 3D cell cultures for continuous biomarker monitoring. Micromanipulator is used to hold the needle-shaped EABs for cell insertion. These sensors detect cellular responses by measuring current signals generated from conformational changes in aptamers that bind to specific targets, offering real-time cellular response data with good spatial and temporal resolutions.

To further advance data analysis pipeline, we are developing an automatic data analysis tool with to compute current signals, which features a user-friendly Graphical User Interface (GUI) to filter results, adjust analysis ranges, overlay curves, and generate 3D data displays, providing comprehensive insights into cellular activities.

Our innovative approach not only bridges the gap between traditional 2D cell cultures and the complexity of living tissues but also establishes a powerful platform for high-throughput drug testing with higher precision and reliability. This advancement holds significant potential for improving the accuracy and effectiveness of preclinical drug testing, ultimately contributing to better therapeutic outcomes.

References:

1. Fedi, A., Vitale, C., Giannoni, P., Caluori, G., & Marrella, A. (2022). Biosensors to Monitor Cell Activity in 3D Hydrogel-Based Tissue Models. Sensors (Basel, Switzerland), 22(4), 1517. https://doi.org/10.3390/s22041517

How You Like Them Apples: An Interpretation of Sexual Symbolism in the Priapeia

Alayne Ziglin
Summer Research Opportunities Program (SROP)

Faculty Advisor:
Luca Grillo, Department Chair and Professor of Classics, Department of Classics
College of Arts and Letters

Abstract

This paper analyzes the semantics of apple symbolism in the *Priapeia* by examining double entendres regarding Priapus' twofold godly domain. I argue that the use of apples throughout the corpus contains a sexually charged secondary interpretation in addition to its primary, surface level meaning. The paper identifies three distinct categories concerning the use of the apples in the *Priapeia:* namely, offerings, stolen goods, and products of trees. Within these categories, I have found that different instances of apples contain separate sexually charged meanings, but all of them share an erotic connotation. Some common themes in the interpretation of apple symbolism from the paper include association with a sexually submissive partner or receipt of sexual gratification.

I also discuss how the proposed symbolism of apples interacts with other symbolic objects in the *Priapeia* such as verses and gardens and how these symbolic interpretations contribute to the overall understanding of Priapus. Additionally, the paper examines the use of words with sexual connotations in conjunction with apples to further explore the possible erotic interpretations of apple symbolism. These research insights provide a framework for future interpretations of the *Priapeia* and for examining the relationship between apples and erotic symbolism.

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

ABSTRACTS

Examination of the Effect of the Configuration of Ruthenium on the Selectivity of Asymmetric Hydrogen Transfer

Zosia Bolde
Center for Computer Assisted Synthesis Summer Undergraduate Research Fellowship
(C-CAS SURF)

Mentor, Contributors, Faculty Advisor:
Laura Andreola, Postdoctoral Research Associate
Jacquelin Zak and Elizabeth Reinbold, Graduate Students
Paul Helquist, Professor of Chemistry and Biochemistry
Olaf Wiest, Grace-Rupley Professor of Chemistry and Biochemistry
College of Science

Abstract

Electronic structure calculations of ruthenium catalyzed reactions can provide guidance in determining the stereoselectivity of transition state systems. Noyori introduced chiral ruthenium complexes for asymmetric transfer hydrogenation reactions[1]. Ligands have been worked on to increase the selectivity of this reaction. Work in the Wiest-Helquist group is being done to design novel ligands with phosphine and amine linkage to ruthenium. Prior work by Hall et al. studied the configuration of the metal in these reactions[2]. This study examines the effect of the configuration of the metal on the proposed catalyst. This comparison assumes the ruthenium catalysts interconvert between stereochemistries when in solution, which has some supporting evidence[2] and will be studied further.

Transition states were first optimized in Gaussian, then conformer searches ran through CREST[3] to determine the lowest-energy geometry. This was performed for each variant of the structural isomers. Two transition states were found with high predicted selectivity, determined by comparison of predicted ΔΔGs of each conformer against all other conformers found. The ΔΔEs of the two structural isomers with the highest selectivity were compared, and both were predicted to favor pro R stereochemistry, one by 3.76 kcal/mol and one by 1.47 kcal/mol.
The results of this study will be compared to another isomer with opposite ruthenium stereochemistry, with the goal of determining if the structures compete in solution together. Competition is determined by ΔΔG comparison, and if those numbers are roughly within 2.0 kcal/mol of each other, the structures will be considered competing.

References:

(1) Ryoji Noyori, S. H. Asymmetric Transfer Hydrogenation Catalyzed by Chiral Ruthenium Complexes. Accounts of Chemical Research 1997, 30 (2), 5. DOI: 10.1021/ar9502341.

(2) Hall, A. M. R.; Berry, D. B. G.; Crossley, J. N.; Codina, A.; Clegg, I.; Lowe, J. P.; Buchard, A.; Hintermair, U. Does the Configuration at the Metal Matter in Noyori–Ikariya Type Asymmetric Transfer Hydrogenation Catalysts? ACS Catalysis 2021, 11 (21), 13649-13659. DOI: 10.1021/acscatal.1c03636.

(3) CREST — A program for the exploration of low-energy molecular chemical space, Pracht, P.; Grimme, S.; Bannwarth, C.; Bohle, F.; Ehlert, S.; Feldmann, G.; Gorges, J.; Müller, M.; Neudecker, T.; Plett, C.; Spicher, S.; Steinbach, P.; Wesołowski, P.A.; Zeller, F.; J. Chem. Phys., 2024, 160, 114110. DOI: 10.1063/5.019759

Soft Modular Sea Star Robot Offers Versatile Locomotion on Land and in Water

Nagham Bou Hamdan
Engineering Summer Research Experience (E-SURE)

Mentor, Contributors, Faculty Advisor:
Abu Nayem Md. Asraf Siddiquee, PhD Student
Yasemin Ozkan-Aydin, Assistant Professor of Electrical Engineering
College of Engineering

Abstract

Researchers have drawn inspiration from nature for developing different task-oriented soft robots capable for exploration in various mediums. Building a soft robot with an onboard power supply system that can be deployed in different environments to accomplish specific tasks is critical. This project presents a modular, untethered, soft electric-powered sea star robot that uses five identical shape memory alloy-based limbs to locomote on both ground and underwater. The objective of this project is to investigate the locomotion dynamics of sea stars by building a soft modular robot. Soft silicone material (Ecoflex00-30) was used to fabricate the limb structure and a Nitinol spring with 0.8 mm diameter was incorporated inside it in order to expand and contract. A polyester plastic based Kirigami skin was attached to the bottom surface of the limbs to achieve higher friction and facilitate motion in the desired direction. An Arduino Nano circuit design was created to control the motion. By supplying current to the Nitinol wire for heating and then prohibiting current supply for cooling, a motion is created. Several experiments were conducted on various Nitinol shapes and different actuator designs to know which one had the most precise and flexible motion.

Designing the sea star robot is still in progress and the final modular design will be creating a soft sea star robot that can move even if it lost some of its limbs. This robot can be beneficial for multi-environment monitoring and underwater exploration given its ability to move on land and in water.

3D Printed Model of Buckling Restrained Brace Frame

Isabella Cantillo
Kurama Laboratory

Faculty Advisor:
Yahya C. Kurama, Professor of Civil and Environmental Engineering and Earth Sciences
College of Engineering

Abstract

The buckling restrained brace (BRB) was first created in 1987 in Japan. A buckling restrained brace frame is a building system made of concrete and steel. There is a steel core bar running through the center of the brace that allows tension. Mortar and a layer of concrete encase the steel core to handle any compression within the system. Torsion is expected, and typical in these systems, because of the amount of stress they undergo. This research regards the creation and analysis of a repairable, pre-cast buckling restrained brace. The brace being repairable would be beneficial after these structures experience any seismic activity by reducing the amount of labor needed to fix the brace. Precasting these braces would lower transportation and material costs during the construction process. This research's overall impact would save the seismic design industry a lot of money, time, and labor.

The 3D printed model of the buckling restrained brace was created solely for visual purposes. The creation of this model could be significant to any educational outreach program interested in spreading awareness about seismic engineering, or information on how the buckling restrained brace operates within a structure. Although the structure does not function like a real-life structure would, it represents the way the buckling restrained brace system is built into the structure. Each brace sits at a 45-degree angle; an angle that falls within the range of ideal measurements. Its dimensions were also influenced by dimensions of similar structures and therefore has a 1:50 scale compared to a life-size structure; the bigger scale structure does not actually exist.

Low-temperature Thermal Treatment of PFAS-containing Plants after Phytoremediation

Gabriel Cruz-Ruiz
Vincent P. Slatt Fellowship

Mentor, Contributors, Faculty Advisor:
Kyle Doudrick, Associate Professor of Civil and Environmental Engineering and Earth Sciences
College of Engineering

Abstract

Per- and polyfluoroalkyl substances (PFAS) are considered a rising threat in our society as a major contaminant in soils. This in itself poses a risk for the health of individuals and severely affects our ecosystem. To fight this imminent threat an inexpensive method of remediation known as phytoremediation is being employed. This method is known for being noninvasive and safe practice to avoid further contamination the environment. In our research we utilized "Leucanthemum vulgare lam." due to its reputation of being a heavy metal hyperaccumulator in USDA zones 4-9. On the other hand, managing this contaminated vegetation requires careful disposal to minimize the risk of re-entering the environment.

In this research, we are treating vegetative waste after phytoremediation using additives such as Ca(OH)2 to mineralize PFAS and effectively removing it from the environment. In our research we utilized "Leucanthemum vulgare lam." due to its reputation of being a heavy metal hyperaccumulator in USDA zones 4-9. On the other hand, managing contaminated vegetation will require careful disposal to minimize the risk of the contaminant re-entering the environment. A common method employed in waste management, is to create landfills however, this can leach into aquifers. We can remedy this using an alternative method, incineration. Elevated temperatures have the benefit of break the bonds in the PFAS and converting it into less damaging compounds. Additives such as Ca(OH)2 are being employed to assist mineralization thus efficiently securing the soils from PFAS.

The Relationship between PGAM5 Expression and the Cell Cycle

Konrad R. Czyzewski
College of Science Summer Undergraduate Research Fellowship (COS-SURF)

Mentor, Contributors, Faculty Advisor:
Matthew Fink and Michael Douglas, Graduate Students
Zachary Schafer, Coleman Foundation Associate Professor of Cancer Biology,
Department of Biological Sciences
College of Science

Abstract

Cancer cells often experience altered mitochondrial metabolism due to loss of integrin-mediated attachment to the extracellular matrix (ECM). The mitochondrial phosphatase PGAM5,, has recently been identified as part of a proteinaceous complex that initiates mitophagy, which can eliminate tumor cells during ECM-detachment. However, how ECM-detached cancer cells circumvent mitophagy remains poorly understood. As PGAM5 regulates viability in this context, we have investigated its role in cells not undergoing mitophagy. Our data reported differences when targeting different stages of the cell cycle.

We found that certain cancer cell lines have an innate ability to reduce PGAM5 expression when cultured under ECM-detachment conditions. This reduction is primarily due to transcriptional changes, rather than increased protein turnover. Given that ECM-detachment also impairs proliferation, we investigated PGAM5 expression after treatment with various cell cycle inhibitors. Indeed, our data suggest that PGAM5 expression is linked to proliferation, as arresting cells in G1 with multiple inhibitors results in decreased PGAM5 levels. This supports the conclusion that loss of PGAM5 aids in the survival of ECM-detached cells, offering insights into the intersection between altered mitochondrial function and modulation of cell death pathways in cancer. Relatedly, we then sought to determine whether arresting the cell cycle at other stages results in alterations in PGAM5 expression. We obtained data that suggest using nocodazole, which arrests cells in the G2/M phase. However, these results of the G2/M phase are preliminary and under active investigation.

References:

Hawk, M.A., Gorsuch, C.L., Fagan, P. et al. RIPK1-mediated induction of mitophagy compromises the viability of extracellular-matrix-detached cells. Nat Cell Biol 20, 272–284 (2018). https://doi.org/10.1038/s41556-018-0034-2

Bioaccumulation of PFAS within Wetland Plants

Caitlynn Day
Biological Sciences Research Experiences for Undergraduates (BioREU)

Mentor, Contributors, Faculty Advisor:
Sarah Kleppinger, Laboratory Manager; Alison Zachritz, Graduate Student;
Daniele De Almeida Miranda, Research Assistant Professor
Gary Lamberti, Emeritus Professor, Department of Biological Sciences
College of Science

Abstract

PFAS are a family of nearly 15,000 man-made compounds that are extremely strong and slow to degrade, ubiquitous, and pose severe health risks to both environmental and human health. These compounds are used in the production of several everyday products such as nonstick cookware, firefighting foams, and food packaging. PFAS have leeched into the environment via air and water waste from production facilities, and can be found in freshwater, air, soil, and biota. Because of their longevity, PFAS are able to accumulate within biota and levels magnify as they travel through the food web (biomagnification). A possible solution to remove PFAS compounds from freshwater is phytoremediation - removing a pollutant from an environment via plant root uptake and bioaccumulation.This study will focus on the bioaccumulation of PFAS within wetland plants, how different PFAS compounds (e.g. differing chain length, functional group) travel within a plant, and whether native or invasive plants tend to more readily accumulate PFAS. Several wetland sites at Lake Michigan and Lake Erie will be sampled for water, sediment, and plant life (native *Typha Latifolia* and invasive *Typha Angustifolia*). They will be analyzed using LC-MS to determine PFAS levels and a bioaccumulation factor will be calculated for the plant samples. By gaining a better understanding of how these compounds accumulate within plant life, future efficient phytoremediation methods may be developed to combat PFAS.

Can LLMs Budget Wisely?

Jing Ding
International Summer Undergraduate Research Experience (iSURE)

Mentor, Contributors, Faculty Advisor:
Qingkai Zeng, Zhenyu Wu, and Hy Dang, Graduate Students
Meng Jiang, Associate Professor of Computer Science and Engineering
College of Engineering

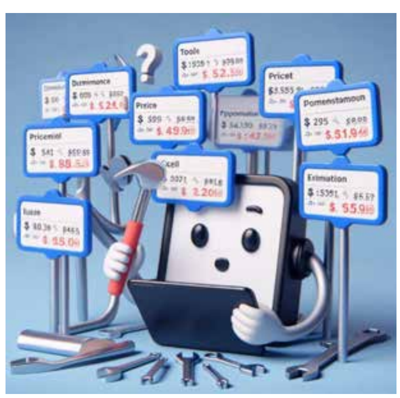
Abstract

Large Language Models (LLMs) are super-smart tools capable of performing various tasks. Recently, they've become even smarter and can now use other tools to solve problems. However, a question that hasn't been explored much is that they never consider the costs of these tools when solving problems. So, can LLMs transition from "being extravagant" to "budgeting wisely"?

In our study, we're looking at this very question. It's a new area, so there's not much work done on it before. We're trying to figure out if LLMs can plan to use the tools well while keeping these costs in mind. When an LLM gets a problem to solve, it has some tools it can use. It needs to find the right answer, but also figure out the best way to use the tools, thinking about how effective they are and what they cost. Our initial efforts are focused on establishing a benchmark based on a mathematical dataset, which includes the fixed costs of some calculators.

Early results show that LLMs can "budget wisely". They can balance a tool's effectiveness with its cost. However, more work is needed to refine this approach and address real-world situations, such as fluctuating tool costs or different problem types.

In short, our study highlights the potential for teaching LLMs to "think more like real humans". As LLMs continue to improve, understanding how they make resource decisions will be crucial for their effective use in real-world applications.



Developing Benchmarking System for Quantum Computer

Triet Do
Engineering Summer Research Experience (E-SURE)

Mentor, Contributors, Faculty Advisor:
Ulrik de Muelenaere, PhD Student
Peter Kogge, Professor of Computer Science and Engineering
College of Engineering

Abstract

The first computer was developed during World War II, and about 20 years later, the personal computer was invented to perform a wide range of functions. Quantum computers emerged in the 1990s, but, currently, the most advanced ones are almost as large as a room and only solve specific problems they were designed for. Several factors contribute to the slow development of quantum computers. One reason is that the underlying mathematics and technology are highly complex, making adaptation difficult. Another reason is the lack of a unified approach within the scientific community. Quantum computing community is still exploring various technologies, such as hydrogen atoms and photons. Even within the same technology, variations in qubit numbers, topologies, and compilation algorithms exist. Consequently, claims about the superiority of one system over another are hard to substantiate, and there is no standard benchmarking system for quantum computers. Scientists typically build machines and publish papers about them, requiring multiple papers to compare different quantum computers. We develop a software to extract data from these papers and organize it for convenient evaluation by the scientific community. Our software not only consolidates data from different platforms but also suggests the necessary data for a comprehensive report. We use embedding graph algorithms on SQL database to create connections. This development aims to improve the quantum computing development process by providing a more standardized benchmarking system.

The Role of *frataxin* in Heart and Liver Development in Zebrafish

Austin Dungan
Biological Sciences Research Experiences for Undergraduates (BioREU)

Mentor, Contributors, Faculty Advisor:
Wesley Ercanbrack, Graduate Student
Rebecca A. Wingert, Elizabeth and Michael Gallagher Associate Professor,
Department of Biological Sciences
College of Science

Abstract

Decreased expression of the protein encoded by the *frataxin* gene (*FXN*) results in the condition known as Friedreich's Ataxia (FRDA). FRDA is a rare genetic disease that affects many tissues throughout the body, most notably the heart and central nervous system, leading to the progressive decline of balance and coordinated muscle movement. Because the FXN protein plays important roles in metabolism, it is believed that FRDA's main phenotypes, cardiomyopathy and loss of motor control, are a result of overabundant reactive oxygen species. Our research aims to further understand the roles of FXN during the development of the heart and liver using the zebrafish, as their *fxn* gene is highly conserved with humans.

To create a loss of function zebrafish model, we used an antisense morpholino oligonucleotide to knockdown *fxn.* Through a series of whole mount *in situ* hybridization studies, we examined heart and liver development. In parallel, we used o-dianisidine to examine vasculature and assess blood flow, as well as live imaging to quantify heart rates. Interestingly, *fxn* deficient embryos had significantly more blood pooling around the heart, a lower heart rate, abnormal heart looping, and their hearts were larger compared to wild-type controls.

These findings suggest that *fxn* has essential roles in early cardiovascular system ontogeny. Ongoing studies with Oil Red O and BODIPY to stain lipids will assess liver and digestive tract formation. Taken together, this model has high potential to reveal additional new insights about how *fxn* affects the morphogenesis and function of critical organs.

Wireless Signal Measurement Approach For 6G Spectrum Allocation

Raghad Elgamal
Advanced Wireless Research Experiences (AWaRE)

Mentor, Contributors, Faculty Advisor:
Omkar Mujumdar, Graduate Student; Bingyan Lu, Graduate Student
Nick Laneman, Professor of Electrical Engineering, Co-Director of Wireless Institute, and Director of SpectrumX
College of Engineering

Abstract

Many applications like mobile cellular systems, weather forecasting, and military systems require additional spectrum to operate and enhance their performance. Effectively utilizing the radio spectrum is a significant challenge that needs to be addressed. An important step in making better use of spectrum is determining if there are any bands or allocations that can be repurposed or shared.

This research studies and analyzes the 7.125-8.4 GHz band, focusing on potential allocations that can be shared or repurposed to enable the implementation of 6G technology on mobile devices. 6G provides improved reliability, faster speeds, and broader network coverage, ensuring users can access cellular data seamlessly wherever they are located.

To determine if the band can be shared or repurposed, wireless signals within this band need to be measured to understand the degree to which the allocations are being utilized over time and geographic areas. In this work, we present an approach for taking measurements that consider various parameters, including antenna direction, time of day, different days, different bands, temperature, humidity, and location. As a case study, we conducted initial measurements and experiments to assess the bandwidth utilization at several locations within the University of Notre Dame campus. Our initial findings indicate that the 7.125-8.4 GHz band is not utilized within the university boundaries, which suggests this band can be repurposed for implementing 6G wireless communications in similar areas. We recommend reviewing the FCC Universal Licensing System and NTIA Government Master File to conduct additional experiments near the facilities that have assignments in the band.

A Professional Approach to Data Privacy: Fully Homomorphic Encryption and Threshold FHE in Client-Server Survey Tools

Humyra Ferdus and Christopher Joseph
CSE Summer Enrichment Program

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Abstract

In the age of rapid quantum computing development, quantum computers pose a serious threat to traditional encryption methods such as the Rivest-Shamir-Adleman (RSA) cryptosystem. Fully Homomorphic Encryption (FHE) emerges as an ideal candidate for Post-Quantum Cryptography, as no quantum algorithm has yet been devised to break it. Moreover, FHE allows entities to perform computations on data without the need to decrypt it. Threshold FHE(2) further enhances FHE by distributing the decryption key among multiple parties, ensuring that no single entity can decrypt the data alone, thereby decentralizing data security. To showcase the value of adopting FHE as a standard in industries such as healthcare and government, we developed a client-server survey protocol based on FHE. Each user receives a partial key to encrypt their responses in our protocol. These individual encrypted responses are sent to a central server, which aggregates the responses and analyzes them while preserving individual client privacy. For instance, the server can determine that 50% of participants voted "yes" without identifying individual votes. We utilized the OpenFHE library and employed the Brakerski/Fan-Vercauteren (BFV) scheme, which supports finite field arithmetic for our implementation. This work emphasizes the importance of FHE in building modern cryptosystems that are safe from attacks from quantum-capable adversaries.

References:

1. Kun, J. (2024, May 4). Fully Homomorphic Encryption Overview. Math ∩ Programming. https://www.jeremykun.com/2024/05/04/fhe-overview/
2. Boura, C., Giacomelli, I., Iliashenko, I., & Savas, E. (2022). OpenFHE: Open-Source Fully Homomorphic Encryption Library. Cryptology ePrint Archive, Paper 2022/1625. https://eprint.iacr.org/2022/1625.pdf

Social Media Dayparting

Roan Finkle
Center for Research Computing Summer Internship

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Valentina Kuskova, Associate Director, Lucy Family Institute for Data & Society
Jarek Nabrzyski, Faculty Director, Center for Research Computing; Concurrent Professor of Computer Science and Engineering
College of Engineering, Notre Dame Research

Abstract

Dayparting in television broadcasting involves optimizing programs and advertisements to air during specific time slots to target audiences effectively. This project aims to adapt this methodology for social media posting, focusing on optimizing the content of the posts rather than demographic targeting. Our research leverages natural language processing and web scraping to analyze and model the characteristics of social media posts and assess their performance.

We propose a product for social media managers at media companies that addresses the need for increased ad views, leading to higher revenue. Our solution includes deploying a Data Envelopment Analysis-based output efficiency model, which identifies the best-performing categorized posts and the key elements driving their success. This approach improves upon traditional regression models, which have limitations in this context.

Our dataset consists of metrics from a major city's large newspaper's Facebook posts, including links to their promoted articles. By recommending the optimal weekday and hour time slots for posting based on topic and sentiment, our model helps generate more web traffic, thereby increasing the newspaper's ad revenue.

We want to thank researchers Vamsi Kanuri and Shrihari Shidhar who have published the original idea; we are working on refining the model and validating its effectiveness.

References:

Kamuri, K. V., Chen, Y., Sridhar, S. (2018), “Scheduling Content on Social Media: Theory, Evidence, and Application,” *American Marketing Association Journal of Marketing*, 82(6):89-108

Investigating the Role of The Coxsackie and Adenovirus Receptor in Neuronal Development and Down Syndrome Pathology

Steven Frye
ND PREP

Mentor, Contributors, and Faculty Advisor
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Christopher Patzke, John M. and Mary Jo Boler Assistant Professor, Department of Biological Sciences
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Abstract

The Coxsackie and Adenovirus Receptor (CAR), a type I transmembrane protein, plays critical roles in cell adhesion within cardiac and neural tissues. Encoded by the CXADR gene, located on chromosome 21, CAR might be implicated in Down Syndrome (DS) pathology. This study aims to investigate how CAR overexpression affects neuronal characteristics and contributes to DS phenotypes. We hypothesize that overexpression of CAR in neurons will mimic the neuronal abnormalities observed in DS-patient derived neurons.

Our approach involves generating CAR overexpression and knockout models using induced pluripotent stem cells (iPSCs) and differentiating them into neurons. We will analyze neuronal characteristics, including neurite growth, cluster formation, soma size, and morphology, using advanced imaging techniques like confocal microscopy. Additionally, we hope to gain insight into CAR's role in DS pathology, potentially revealing novel aspects of its function.

Preliminary data show a significant increase in CAR expression in DS iPSC models and altered morphologies in CAR knockout HeLa cells, supporting the hypothesis. We expect to observe neuronal phenotypes similar to those seen in DS models, including altered cluster formation and neurite growth. This research could provide new insights into the molecular mechanisms underlying DS, potentially identifying new therapeutic targets for treating DS symptoms. Future work will explore other chromosome 21 genes interacting with CAR and the long-term effects of CAR modulation on neuronal function and behavior, contributing to a more comprehensive understanding of DS pathology.

Evaluation of RimJ Mediated N-terminal Acetylation and its Impact on Mycobacterial Virulence

Lucas Gruber
Biological Sciences Research Experiences for Undergraduates (BioREU)

Mentor, Contributors, Faculty Advisor:
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Patricia Champion, Professor of Biological Sciences
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Abstract

N-terminal acetylation, a post-translational protein modification conserved from bacteria to higher organisms, remains understudied in mycobacteria. RimJ—a N-acetyltransferase (NAT)—catalyzes N-terminal acetylation of immune stimulating peptides and ribosomal protein 5S in *E. coli*. RimJ is highly conserved between *Mycobacterium tuberculosis* and *M. marinum*—two related pathogenic mycobacterial species. Our lab previously discovered both RimJ and MMAR_1341 acetylate EspF (secreted protein virulence factor essential during macrophage infection) and RfbD and 1668 (proteins involved in lipid biosynthesis). We hypothesize these NATs cumulatively acetylate EspF, RfbD, and 1668 to promote mycobacterial virulence. To identify RimJ's role and its interaction with MMAR_1341, we used genetic and biochemical approaches.

To investigate RimJ's role in EspF acetylation, we generated a mutation (Y180A) in a conserved catalytic region of RimJ and expressed/purified it in *E. coli*. DTNB assays showed RimJ_Y180A still acetylated EspF, indicating the mutation didn't disrupt catalytic activity. DTNB assay of RimJ with the RfbD and 1668 peptides confirm N-terminal acetylation occurs. To assess RimJ's impact on virulence, we infected waxworms with genetically deleted strains of rimJ and its complement strain. These infections showed no decrease in pathogenicity, denying RimJ's direct involvement in mycobacterial virulence. The bacterial-two hybrid system revealed intermediate interaction between RimJ and MMAR_1341. Phenotypic equivalency between *M. marinum* and *M. tuberculosis* were evaluated by purifying rimJ from the *M. tuberculosis Erdman* genome and repeating the previous experiments.

This study contributes to an underdeveloped body of knowledge around N-terminal acetylation in the mycobacterial species and its interaction with key virulent processes.

Iris Presentation Attack Detection

Vera Casquero, Zelalem Haiel
CSE Summer Enrichment Program

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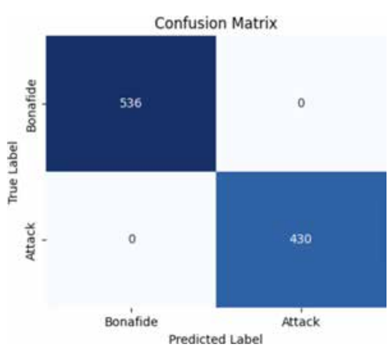
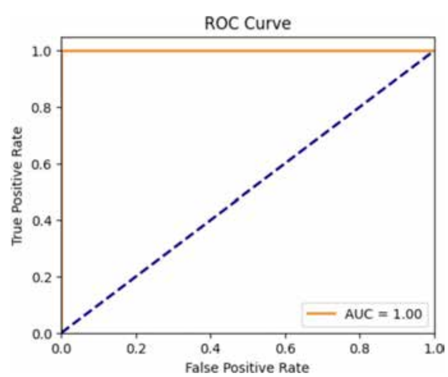
Abstract

Biometric security systems are increasingly used for authentication. Iris recognition is one of the most secure biometric methods due to the uniqueness of the iris patterns. However, it remains vulnerable to attacks such as printouts, digital images, contact lenses, and post-mortem irises. Presentation Attack Detection (PAD) is crucial for enhancing biometric security by identifying such attacks, ensuring user convenience, and safeguarding against unauthorized access. To explore the vulnerabilities of iris recognition systems to replay attacks, we curated a dataset comprising 2651 bonafide (genuine) iris images sourced from the ND3D dataset. The printed replicas of these bonafide iris images were collected using the IriTech sensor. We split this generated dataset into three subsets: train, test, and validation, and trained a ResNet-18 model for iris PAD. The model achieved perfect detection performance on the test data, with accuracy, precision, recall, and F1 scores all at 100%, along with an area under the ROC curve of 100%. The model also recorded a BPCER (Bona Fide Presentation Classification Error Rate) of 0.00% and an APCER (Attack Presentation Classification Error Rate) of 0.00%. These results suggest that the simplicity of the dataset contributed to the model's high performance.





Graph Partitioning in Neutral Atom Quantum Systems

Ellie Han
Engineering Summer Research Experience (E-SURE)

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Peter Kogge, Ted H. McCourtney Professor of Computer Science and Engineering
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Abstract

Neutral atom quantum computing leverages field-programmable qubit arrays of atoms controlled by precise lasers to excite them into Rydberg states. In their current state, these Rydberg atom systems can be used to solve optimization problems. As quantum computing advances through the era of Noisy Intermediate Scale Quantum (NISQ), benchmarking quantum algorithms for optimization problems becomes increasingly useful, particularly for hybrid quantum-classical computing. The graph partitioning problem involves dividing a graph of vertices into even sets while minimizing the number of edges that cross in between. This is ideal to benchmark because of its NP-complete classification as well as its novelty in current quantum benchmarking literature. We use a quantum algorithm to take a graph problem rewritten into a QUBO problem and embed it into the hardware to be partitioned. On a larger scheme, we employ a multi-level algorithm to take a large graph and coarsen it sequentially until it suits the atom array size. The most coarsened subgraph is partitioned using our quantum solver. The graph is sequentially uncoarsened and the partition is refined at each step using a classical algorithm until we obtain the original graph. This study provides valuable insight into the capabilities of emerging technology and directs future research towards solving a broader range of practical optimization problems.

Human Value with LLM

Yiqin He
International Summer Undergraduate Research Experience (iSURE)

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Abstract

This project aims to enhance the accuracy of annotating human values in diverse input documents using a multi-stage process involving large language models (LLMs). Given the inherent challenges and limitations in LLM accuracy for human value judgments, the project introduces a robust framework to improve reliability. Initially, documents are sourced from various media, such as journals, articles, blogs, and videos, and the text is extracted and sanitized to remove unnecessary information.

The core annotation process utilizes an LLM to identify human values within overlapping groups of sentences. To address the accuracy limitations of LLMs, an additional model is trained to verify and refine these annotations. This enhanced classifier ensures more reliable identification of human value keywords and keyphrases.

The final output includes accurately annotated human value keywords and phrases from the input text. This project leverages advanced natural language processing techniques to systematically and reliably identify human values across diverse documents, providing valuable insights into human-centric content in various media.

Assembling Macrophage Spheroids through the Optimization of Hanging Drop Technique

Karyme Hernández Torrens
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

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Meenal Datta, Assistant Professor, Aerospace and Mechanical Engineering
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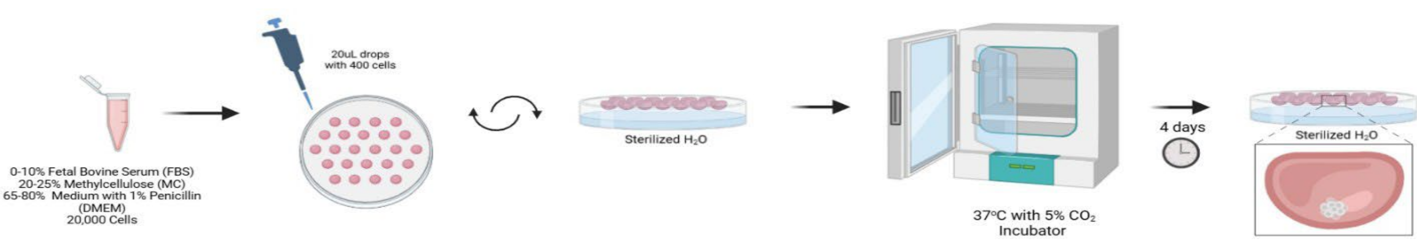
Abstract

As cells of the innate immune system, macrophages possess critical and diverse roles within the body: maintaining homeostasis, orchestrating wound healing, systemic inflammation, among others [1-2]. However, macrophages can be recruited by tumors as tumor associated macrophages (TAMs) and promote tumor angiogenesis, drug resistance, and metastasis [2]. As a result, for various cancer types a high population of TAMs around tumors generally entails adverse prognosis for patients [3]. Emerging strategies for tumor treatment suggest manipulating TAM activation through selective targeting [4] and a path towards refining these strategies can be developed through studying a physiologically relevant 3-D organization of macrophages [5]. Our project focused on using the hanging drop method to make spheroids of RAW264.7 murine macrophages in a facile, convenient, and cost-effective way. These drops were created by making a 1mL solution composed of media, cells, and methylcellulose. The purpose of this research is to optimize the conditions by modifying the additives in hanging drop media, quantity of cells per drop, and drop size. Currently, the best conditions found utilize 20uL drops of 400 cells where the media is composed of a range of 0-1% fetal bovine serum and a 20-25% methylcellulose concentration. Furthermore, the same method was used to generate glioblastoma-macrophage co-culture spheroids for downstream immunomechanical characterization of growth-induced residual stresses. These results show that the optimization of macrophage spheroid growth can be achieved through the hanging drop and therefore provide further understanding on macrophage behavior in the tumor microenvironment and other diseases.

References:

1. DiPietro LA. Wound healing: the role of the macrophage and other immune cells. Shock. 1995 Oct;4(4):233-40. PMID: 8564549.
2. Wynn T., Chawla A. & Pollard J. Macrophage biology in development, homeostasis and disease. Nature 496, 445–455 (2013). https://doi.org/10.1038/nature12034
3. Laviron M, Boissonnas A. Ontogeny of Tumor-Associated Macrophages. Front Immunol. 2019 Jul 31;10:1799. doi: 10.3389/fimmu.2019.01799. PMID: 31417566; PMCID: PMC6684758.
4. Pan Y, Yu Y, Wang X and Zhang T (2020) Tumor-Associated Macrophages in Tumor Immunity. Front. Immunol. 11:583084. doi: 10.3389/fimmu.2020.583084
5. Burchett A., Siri S., Li J., Lu X., Datta M. Novel 3-D macrophage spheroid model reveals reciprocal regulation of immunomechanical stress and mechano-immunological response. bioRxiv (2024.02.14.580327; doi: https://doi.org/10.1101/2024.02.14.580327



Enterococcal Strains’ Adaptations to Host Immune Response and Fibrinolytic Activity

Catherine (May May) Hubbard
Biological Sciences Research Experiences for Undergraduates (BioREU)

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Abstract

Catheter-**a**ssociated **u**rinary **t**ract **i**nfections (CAUTIs) are the most common hospital-acquired infection accounting for 40% of nosocomial infections worldwide. The causative gram-positive bacteria, *Enterococcus faecalis*, represents 11%-30% of CAUTIs. Previous research on *E. faecalis* CAUTIs have used the oral isolate strain, OG1RF. Currently, there is limited research on *E. faecalis* V583, a strain isolated from a patient with urosepsis. Characterization of this strain will help understand *E. faecalis* CAUTIs as V583 has a specific niche for the bladder environment.

The ability for *E. faecalis* to colonize the bladder is dependent on the deposition of fibrinogen (Fg), a healing protein that is recruited to the catheterized bladder and is used as a nutritional source for biofilm formation. Additionally, the *E. faecalis* secreted proteases, specifically SprE, have been shown to degrade C3, plasminogen, and plasmin, which are critical components in immune evasion and the breakdown of Fg. The overall objective of this study is to investigate the differential immune responses and fibrinolytic activity between OG1RF and V583. Here, we showed that V583 is less susceptible to killing by neutrophils and macrophages when compared to OG1RF. Additionally, we have found that V583 has a decreased expression of sprE in urine conditions compared to OG1RF; however, similar protease degradation activity was observed in these two strains.These results suggest that V583 poses a serious global health threat due to its ability to evade the host immune response and dysregulate the fibrinolytic cascade during CAUTIs, warranting further studies and treatment options for these infections.

Verification Solutions for Radiative Transfer in Spherical Geometry

Stephen Hynes
Naughton Fellowship

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Abstract

Radiative transfer, the transfer of energy via photons, is a physical phenomenon relevant to fields as diverse as inertial confinement fusion, modelling global warming, low cost medical imaging, and hypersonic flight, among others. Radiative transfer is governed by the transfer equation, which typically has analytical solutions only for simple cases. Thus, numerical methods must be used for more complex problems that are of practical interest. In order to verify that the production codes used by researchers in the fields alluded to above give accurate results, a smaller more specialised program called a verification solution code must be developed. Beginning with a Python verification solution code that can solve radiative transfer problems in slab geometry, we further develop the code so that it can solve radiative transfer problems in spherical geometry, which is of interest because it is more conducive to verifying three dimensional codes. The accuracy of this new functionality is verified using Su and Olson's analytical benchmark for non-equilibrium radiative transfer [1]. Having tested and verified the functionality, it is then used to generate solutions to a new problem in spherical geometry, namely that of radiative transfer in a medium with a constant specific heat capacity. This problem is of interest because it is more physically realistic than Su and Olson's, but it is also more difficult to solve due to its nonlinearity and greater numerical stiffness. It is hoped that this new functionality will prove useful in verifying larger multipurpose production codes that are used in many fields.

References: 1.Su, B. & Olson, G. L. An analytical benchmark for non-equilibrium radiative transfer in an isotropically scattering medium. *Annals of Nuclear Energy* **24**, 1035–1055 (1997).

Biomimetic 3D Hydrogel Based Modeling Advances in Neuroblastoma Research: The Inverted Colloidal Crystal Scaffold Approach

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Abstract

Neuroblastoma poses a significant challenge in cancer research due to its aggressive nature and prevalence in infants. This cancer arises from immature nerve cells and presents complex genetic characteristics. Nonetheless, traditional 2D cell cultures and animal models have struggled to replicate their tumor biology and therapeutic responses accurately due to their inability to mimic the human body closely. To address this challenge, we developed an Inverted Colloidal Crystal (ICC) Scaffold, utilizing hydrogels and colloidal crystal templating to construct 3D spheroid structures that closely mimic *in vivo* tumor conditions. This work focuses on the formation of neuroblastoma spheroids within the ICC Scaffold to further understand the growth and formation of tumors within the human body. Here, we first assembled alginate microgels into a uniform structure, embedding them into an agarose-based matrix. This structure adopts a hexagonal crystalline packing (HCP) pattern maintaining uniform pore sizes and interconnected pathways, crucial for facilitating optimal transport of suspension cells, drugs, waste, and nutrients. Next, we seeded suspended neuroblastoma cells into the ICC Scaffold, allowing for the natural formation of spheroid within each uniform pore. Utilizing a 96-well plate to conduct the observation of thousands of neuroblastoma spheroids per well, we were able to obtain images (>200μm in diameter) of spheroids and assess their viability using the two photon confocal microscope. Due to the scaffold's intricate internal design, *in vitro* high-throughput high-content screening can be utilized to closely mimic tissue and disease, enhancing biological relevance of results and improving drug discovery outcomes.

Modeling Lymphatic Vessel Formation Using Microfluidic Chips with Static and Oscillatory Flow

Ada Jaramillo
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

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Donny Hanjaya-Putra, Assistant Professor of Aerospace and Mechanical Engineering
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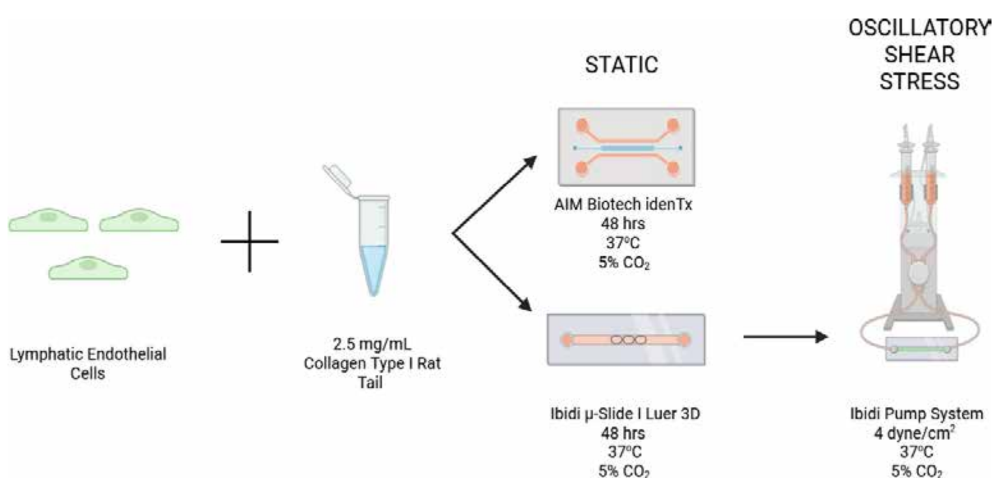
Abstract

Lymphatic diseases such as lymphedema and lymphoma affect millions globally, causing significant morbidity. The lymphatic system, a crucial component of the circulatory system, sustains fluid balance and immune function. This study aims to model lymphatic vessel formation using microfluidic chips to understand the dynamics of lymphatic endothelial cells (LECs) and their interaction with collagen and interstitial flow. Two different types of microfluidic chips (AIM Biotech idenTx and Ibidi µ-Slide I Luer 3D) were used to simulate lymphatic vessel formation. LECs were introduced into a collagen matrix within the AIM chip and cultured in a controlled environment with continuous nutrient supply to support growth. This initial stage facilitated the formation of new lymphatic vessels. In the second stage, the Ibidi chip was connected to a pump system that simulated oscillatory flow, replicating the natural movement of lymph. This setup allowed us to observe the vessels' response to mechanical shear stress. We found that the lymphatic cells within our model can respond to physical changes in their environment. Specifically, the application of shear stress induced by the oscillatory flow led to highlight the vessels' potential for growth under mechanical stimulation. This research contributes to the field of tissue engineering by exploring methods to manipulate lymphatic vessel growth and function *in vitro*, with potential implications for significant medical breakthroughs. Understanding these mechanisms can advance the diagnosis and treatment of lymphatic diseases, offering hope for innovative treatments.



Secure Software-Bench

AJ Jones, Makuza Mugabo Verite
CSE Summer Enrichment Program

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Abstract

A code generation model generates code by taking a prompt from a code comment, existing code, or a combination of both. AI-assisted code generation tools, such as GitHub Copilot, are increasingly being adopted by developers. Despite having the capability to generate functional source code, these models output vulnerable code. These models learn from patterns present in their training datasets. Consequently, if these datasets contain flaws or poor coding practices and vulnerabilities, these issues could be replicated in the code generated by the models. Our project aims to benchmark models with real-world vulnerabilities to see their capabilities to fix them. This investigation is crucial because as AI code generation becomes more prevalent in automating mundane tasks within firms, it is essential to ensure that the generated code is not only functional but also secure and free of vulnerabilities. While AI can create functional code, we aim to determine whether large language models (LLMs) can produce secure code and rectify vulnerable code in real-world software engineering challenges.

To achieve our goal this summer, we worked on collecting real-world vulnerable data. To collect data on real-world vulnerabilities, we iterated through an open-source database of Common Vulnerabilities and Exposures (CVE) from GitHub, spanning from 2017 to 2024. We used GitHub REST APIs, followed by manual and automated filtering of unnecessary data from the collected datasets. We then found merged pull requests where the vulnerability was fixed to craft the prompt. We also focused on learning about prompt engineering, OpenAI APIs, and open-source models hosted on HuggingFace. This involved crafting prompts based on merged pull requests and creating an effective environment for testing these prompts with various LLMs. By being able to fix vulnerabilities in real-world software, our project helps prevent potential vulnerabilities from being exploited with malicious intent by hackers.

Exploring the Role of Cannabinoid Signaling During Renal Multiciliated Cell Development in Zebrafish

Samuel Kaczor
Center for Stem Cells and Regenerative Medicine Summer Undergraduate Research Fellowship, (SCReM-SURF)

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Rebecca A. Wingert, Elizabeth and Michael Gallagher Associate Professor,
Department of Biological Sciences
College of Science

Abstract

Endocannabinoid signaling plays an important role in both the central and peripheral nervous systems. Throughout the body, cannabinoid receptors populate a number of tissues as well. It is known that endocannabinoids bind to these G-protein coupled receptors but the specific role of the receptors is yet to be determined, specifically in the kidneys. A previous chemical screen suggested that cannabinoid signaling can affect development of multiciliated cells (MCCs) within zebrafish kidneys, particularly in regard to the CB1 receptor. To interrogate the role of CB1, we performed drug treatments with AM-281, a CB1 antagonist, followed by whole-mount *in situ* hybridization (WISH) at 24 somite stage (ss) and 28 ss to study mature and progenitor MCC populations. Treatment with AM-281 resulted in no significant difference in the number of mature MCCs when compared to wild-type embryos (WTs). Similarly, treatment with AM-281 resulted in no significant difference in the number of MCC progenitors when compared to WTs. These results suggest that CB1 activity is not required to form renal mature and progenitor MCC populations. Future experiments can be done with morpholino and/or CRISPR-Cas9 knockdown of CB1 to determine if complete removal of receptor function provides the same results. Additionally, these experiments can be repeated at different stages of development to see if this trend remains consistent before or after the time period we treated. Furthering our understanding of MCCs and the signaling mechanisms governing their development may provide direction towards new treatments for ciliopathy diseases in humans.

Optimizing Bio-Inspired Robotic Locomotion Using Geometric Mechanics and Motion Capture Analysis

Cora Keogh
Naughton Fellowship

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College of Engineering

Abstract

This research project studies the locomotion of snakes using a bio-inspired serpenoid robot as a vessel. Studying snake locomotion can lead to significant advancements in robotics, particularly in developing robots capable of navigating complex and dangerous environments, such as inspecting hazardous areas. Mimicking the versatile and adaptive movements of snakes, we aim to enhance robotic agility and efficiency.

Based on prior work, we utilize a Motion by Shape Change simulator grounded in Geometric Mechanics to simulate how snakes move. This advanced algorithm allows us to simulate gaits before we test them using our physical robot which we designed and fabricated. Our planar snake robot has one degree of freedom, and consists of 10 motors and a centralized controller that provides precise control over the robot's movements. Additionally, a power sensor is integrated to measure gait efficiency experimentally. Motion capture technology is employed to meticulously analyze the robot's performance. This system provides high-fidelity data to refine our simulations and optimize gaits. Our comprehensive optimisation process is conducted based on the Centre of Mass Displacement and Efficiency metrics. We aim to create a pipeline to obtain, simulate, and test snake gaits systematically.

Preliminary results indicate that certain gaits significantly enhance the robot's mobility and efficiency, demonstrating the viability of using purely geometric mechanics for gait optimization. This research highlights the potential of bio-inspired robotics and geometric mechanics in advancing robotic locomotion.

The Expression of NCAM in Inner Ear Neurons in Developing Chick Embryos

Georgette Kersman
Neuhoff Summer Research Program
Saint Mary's College

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Abstract

The inner ear is a sensory organ of the body whose function is to detect sounds and motion. Unfortunately, many people are faced with inner ear problems including hearing loss or motion sickness. Thus, determining which proteins are present during normal development can be crucial to understanding and solving these disorders. An integral part of a functioning ear are neuronal projections which relay sensory information such as sounds or changes in motion from the hair cells to the brain for interpretation. Cell adhesion molecules are important for neuronal projections to navigate their way to their targets in the sensory organs. NCAM is a member of the cell adhesion molecule family, but little is known about its presence during neuronal pathfinding during inner ear development. In order to characterize the expression of NCAM, immunohistochemistry was utilized to visualize its presence, or absence in comparison to Myosin 7a, a well-known marker for neurons and sensory cells. Results show that NCAM was detected starting at embryonic day 2 and continuing into embryonic day 7 in chicken, during the process of neuronal pathfinding. Its presence was found in the region of the cochleovestibular ganglion and specialized vestibular regions, including along the epithelium in the region of sensory cells, hair cells. The data collected suggests that NCAM is present during inner ear neuron development in chick embryos. This is beneficial for future studies as NCAM can be used as a marker for neuronal pathfinding in inner ear development of chick embryos.

Dissociative Electron Attachment to Diethyl Carbonate

Giorgi Kharchilava
Vincent P. Slatt Fellowship

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Sylwia Ptasinska, Professor of Physics and Astronomy and Notre Dame Radiation Laboratory
Ian Carmichael, Professor of Chemistry and Biochemistry and Director of Notre Dame Radiation Laboratory
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Abstract

Dissociative electron attachment (DEA) is a resonant process by which a low-energy electron attaches to a molecule, causing excitation into a temporary negative-ion state, and inducing molecular fragmentation into neutral and anionic species. Low energy electrons are produced from ionizing radiation in the atmosphere and in many industrial products such as Lithium Ion Batteries (LIBs)[1]. Diethyl carbonate (DEC) is a symmetric linear carbonate commonly used in the LIB anode and as a fuel additive. DEC has high polarity, low toxicity, is biodegradable, and is associated with high oxygen content and decreased particulate emissions in fuels[2]. DEC is used to synthesize polycarbonates, and as a solvent in pharmaceuticals, fertilizers, pesticides, and dyes. DEC is listed as a volatile organic compound (VOC) and potential photo-pollutant[3]. Because of DEC's wide industrial use, a DEA study can establish the safety of DEC and larger polycarbonate chains. Furthermore, the degradation of DEC and various other carbonates is a chief cause of LIB degradation; our DEA study of DEC serves to illuminate decay pathways in the LIB anode. Furthermore, our study expands the database on DEA to the carbonate functional group. Our analyses of ion yields found 4 anionic fragments: O^-, CH_2CHO^-, $HCOO^-$, and $C_2H_5CO_3^-$. The polyatomic anions are stabilized by charge delocalization activated by dissociation of the carbonate. Making use of the B3LYP functional and the aug-cc-pVTZ basis set, we provide a density functional theory analysis of fragment anions and molecules to determine plausible fragmentation channels associated with each anion.

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[1] F. Wang, F. Varenne, D. Ortiz, V. Pinzio, M. Mostafavi, and S. L. Caër, "Degradation of an ethylene carbonate/diethyl carbonate mixture by using ionizing
radiation," Chem. Phys. Chem. 18, 2799–2806 (2017)
[2] Dunn, B. C., & Guenneau, C. (2002). Production of diethyl carbonate from ethanol and carbon monoxide over a heterogenous catalyst. *Energy Fuels, 16,* 177-181. https://doi.org/10.1021/ef0101816
[3] Katrib, Y., & Deiber, G. (2002). Atmospheric Loss Processes of Dimethyl and Diethyl Carbonate., *Journal of Atmospheric Chemistry, 43*, 151-174. https://doi.org/10.1023/A:1020605807298

Multi-sUAS Collision Avoidance System

Elliot Kim
CSE Summer Enrichment Program

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Abstract

Unmanned Aerial Systems (UAS) have broad applications in sectors such as search and rescue, surveillance, and package delivery, driving the need for advanced automation to enhance efficiency. With the proliferation of drones, collision avoidance becomes crucial to prevent property damage, injuries, or fatalities. Building on previous research [1], which identified critical dynamic factors like geolocation uncertainty, wind profiles, and stopping distances, this project advances the methodology for calculating minimum safety distances between drones. By implementing vectorized safety distance equations, the research applies buffers directionally—adjusting for geolocation and wind in all directions, and for stopping distances in the drone's travel direction. This refinement results in smaller, yet effective safety boundaries, increasing the number of drones that can safely operate in confined spaces. Additionally, a Pygame-based simulation has been developed to visualize drone safety barrier interactions, offering valuable insights into potential collision scenarios during multi-drone missions. This tool enhances strategic planning and real-time safety evaluations.

References:

[1] Pedro Antonio Alarcon Granadeno, Arturo Miguel Russell Bernal, Md Nafee Al Islam, Jane Cleland-Huang. *An Environmentally Complex Requirement for Safe Separation Distance between UAVs.* Requirements Engineering Conference 2024.

Exploring the Role of *irx5b* in Multiciliated Cell Development during Zebrafish Nephrogenesis

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Biological Sciences Research Experiences for Undergraduates (BioREU)

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Abstract

It is estimated that 700 million people worldwide suffer from chronic kidney disease, including 37 million Americans[1,2]. *Danio rerio* (zebrafish) provides a useful animal model to study the kidney as they are 70% genetically homologous with humans and possess similar nephron structures, which are renal functional units. Nephrons are comprised of a glomerulus and segmented tubule that perform blood filtration, secretion, and absorption to excrete wastes and regulate fluid homeostasis[3]. In humans, blood pressure drives fluid flow in the kidney while in zebrafish, fluid flow is also governed by multiciliated cells (MCCs). MCCs are vital in many systems and their dysfunction leads to conditions ranging from infertility to hearing loss. As such, understanding MCC development has many applications.

Iroquois transcription factor *irx2a* plays an important role in promoting MCC formation in nephrons. Here, we performed loss of function studies to explore the function of related family member *irx5b*. *irx5b* knockdown resulted in a reduction of renal MCC number, pericardial edema, hydrocephaly, and delayed renal clearance. Interestingly, *irx5b/irx2a* double knockdown caused a further reduction of renal MCC number compared to independent knockdown of either gene. Taken together, these preliminary data suggest that *Iroquois irx5b* plays a critical role in zebrafish MCC development during nephrogenesis, where it works alongside *irx2a* to specify MCC fate. Future studies including mutant *irx5* -/- analysis, gene expression studies, and immunofluorescence to look at MCC structure in *irx5b* deficient embryos will help to delineate the exact role *irx5b* plays in multiciliogenesis during zebrafish kidney ontogeny.

References:

[1] Francis, A., Harhay, M.N., Ong, A.C.M. et al. (2024). Chronic kidney disease and the global public health agenda: an international consensus. Nat Rev Nephrol 20, 473–485. Retrieved July 12, 2024, from https://doi.org/10.1038/s41581-024-00820-6

[2]Kidney Disease Statistics for the United States - NIDDK. (2023, May). National Institute of Diabetes and Digestive and Kidney Diseases. Retrieved July 12, 2024, from https://www.niddk.nih.gov/health-information/health-statistics/kidney-disease

[3]Preuss H. G. (1993). Basics of renal anatomy and physiology. Clinics in laboratory medicine, 13(1), 1–11. Retrieved July 12, 2024, from https://pubmed.ncbi.nlm.nih.gov/8462252/

Targeting Ferroptosis to Improve Red Blood Cell Storage

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Abstract

Ferroptosis is an iron-dependent type of cell death caused by excessive lipid-peroxidation in membranes. Previous studies suggest that ferroptosis affects red blood cell (RBC) storage, with higher glutathione peroxidase 4 (GPX4) expression levels correlating with improved RBC preservation in blood banks.[1] Our preliminary findings show that RBCs are highly sensitive to ferroptosis induced by GPX4 inhibitors, raising the question of whether blocking ferroptosis benefits RBC storage. To address this, we apply a novel approach to detect ferroptosis of RBCs via the reducing reagent resistant (3R) transferrin receptor 1 (TfR1) dimer in extracellular vesicles. Through the storage of red blood cells under conditions that mimic storage practices typically used in clinical settings, various ferroptosis inhibitors at different dosages were utilized. Mouse RBCs were stored with various ferroptosis inhibitors, including deferoxamine (DFO), liproxstatin-1 (Lip-1), and ferrostatin-1 (Fer-1), and the cell integrity was monitored during a 21-day storage period. The impact on RBC integrity was assessed through cell lysis evaluation and western blot analysis for the presence of TfR1 3R dimer. The data indicates that all ferroptosis inhibitors show protection against storage-induced RBC lysis, with DFO providing the best protection. The preservation of cell integrity and reduction of ferroptosis were evidenced by the significantly lower OD405 values and the absence of TfR1 3R dimer. By identifying the potential positive effects of ferroptosis inhibitors in prolonged red blood cell viability, our research aims to contribute to the optimization of blood storage conditions, ultimately improving the safety and efficacy of stored blood for transfusions.

References:

1. Stolwijk, J. M., Stefely, J. A., Veling, M. T., van't Erve, T. J., Wagner, B. A., Raife, T. J., & Buettner, G. R. (2021). Red blood cells contain enzymatically active GPx4 whose abundance anticorrelates with hemolysis during blood bank storage. Redox biology, 46, 102073.

Social Media Bot Deployment Policies: Theoretical and Practical Implications

Christopher Mc Aleer
Naughton Fellowship

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Catrell Conley, Cormac Kennedy
Paul Brenner, Sr. Associate Director, Center for Research Computing; Professor of the Practice
Notre Dame Research

Abstract

The emergence of Large Language Models (LLMs) holds significant promise for transforming social media platforms. However, this advancement also introduces substantial security concerns, as it may facilitate malicious actors in exploiting online users. We aim to evaluate the strength of security protocols on prominent social media platforms in mitigating the deployment of LLM bots. We examined the bot and AI-generated content policies of seven popular social media platforms: X, Instagram, Facebook, Threads, TikTok, Mastodon, and Reddit. Using Selenium, we developed a web bot to test enforcement mechanisms regarding these policies. Emulating the actions of a malicious actor, we manually created user accounts, automated the login process, scripted posts, and leveraged the OpenAI API to generate a simple "test" post. The experiment was conducted with human-in-the-loop to observe the content generated by the LLM-bot. We successfully accessed each social media account and made a single "test" post. Our findings indicate significant vulnerabilities within the current enforcement mechanisms of these platforms. Despite having explicit policies against bot activity, all platforms failed to detect and prevent the operation of our LLM bots. This finding reveals a critical gap in the security measures employed by these social media platforms, underscoring the potential for malicious actors to exploit these weaknesses to disseminate misinformation, commit fraud, or manipulate public opinion. Thus, it is both recommended and necessary that policies and technical measures are made to be aligned to defend users on these platforms from being manipulated.

Multi-Omic Analysis of Gliomas

Aoife McLoughlin
Naughton Fellowship

Maksym Zarodniuk, Graduate Student
Meenal Data, Assistant Professor, Aerospace and Mechanical Engineering
College of Engineering

Abstract

(Not available at this time)

Ethanol Exposure Effects Regulators of Renal Patterning in Zebrafish

Joshua Moeller
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Abstract

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 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 poorly understood aspect of FASD. To gain new insights about how prenatal alcohol exposure fundamentally affects kidney ontogeny, 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 spatiotemporal expression patterns of transcription factors associated with renal progenitor patterning. Using whole mount *in-situ* hybridization for specific kidney lineage markers, we determined that both renal tubule, non-tubule, precursory populations, and regulators of nephron patterning are greatly perturbed by alcohol exposure. Moving forward, this model can be used to further ascertain how renal gene regulatory networks are affected in FASD, which can be used to explore therapeutic options.

Modeling Diafiltration Cascades for Use in Lithium-Ion Battery Recycling

John Moore
Vincent P. Slatt Fellowship

Mentor, Contributors, Faculty Advisor:
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William Phillip, Rooney Family Collegiate Chair of Engineering and Professor of Chemical and Biomolecular Engineering
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Abstract

Current Lithium-Ion Battery recycling processes like hydrometallurgy utilize harsh organic solvents and energy-intensive steps to separate and recover precious cathode materials like lithium and cobalt due to their cost. This project investigates the replacement of this step with a cascade of membrane modules, which would cut down on the energy needs and environmental impact of the process.

Membrane nanofiltration (NF) technology is an application of commercial membranes that allows for more specific control over solute rejection properties by allowing for the fractionation of similarly sized (but differently charged) ions, by exploiting their valence-dependent rejection properties.

Diafiltration involves the countercurrent connection of membrane “modules” to each other, such that the effluent streams of module one become the influent streams of the subsequent/previous module, depending on whether the stream is retentate or permeate. (Figure 1). Monovalent lithium is concentrated in the permeate, while divalent cobalt is concentrated in the retentate.

A model was developed and experimentally verified for these diafiltration cascades, which gave insight into their recovery and purity capabilities with relevant solute concentration ratios. This analysis was done by varying intrinsic model parameters like the membrane rejection, feed and diafiltrate volumes, and concentration. Key insights from the model include the tradeoff between purity and recovery, as well as the diminishing advantage of staging.

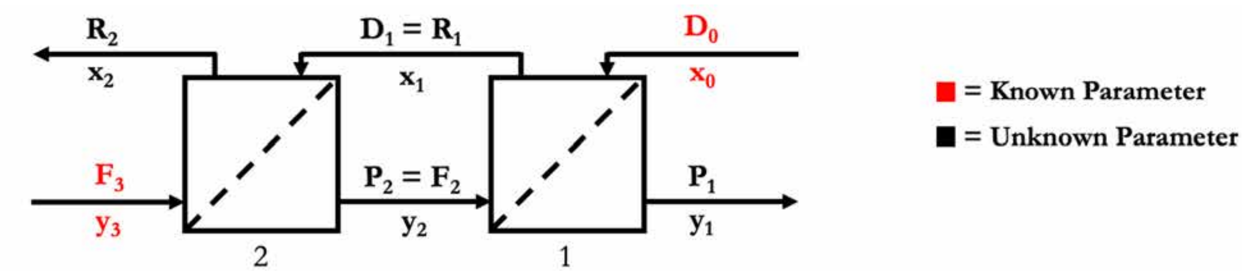

Figure 1. Graphical representation of a two-stage diafiltration cascade. R represents a retentate flow, D a diafiltrate flow, F a feed flow, and P a permeate flow, while x and y represent molar concentrations of solute.

Small Molecule Disrupters of Hsp90/Aha1 Interaction to Prevent Tau Aggregation

Kayleigh Moran
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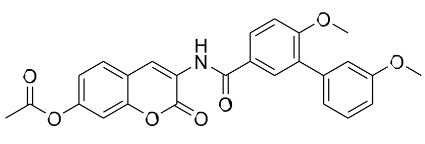
Brian Blagg, Charles Huisking Professor of Chemistry and Biochemistry and Director of Warren Center for Drug Discovery and Development
College of Science

Abstract

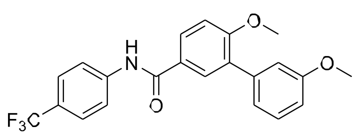
Current estimates suggest that 6.9 million Americans aged 65 and over are living with Alzheimer's Disease (AD), and this number is predicted to triple by 2060. Improperly folded microtubule-associated protein tau (MAPT, tau) is believed to be the main cause of a class of neurodegenerative tauopathies. Furthermore, larger tau aggregates called neurofibrillary tangles drive neurodegeneration. Oligomeric tau can seed to healthy cells and spread the disease. Therefore, MAPT is seen as a promising target for preventative medicines against AD.

The 90 kiloDalton heat shock protein (Hsp90) is a ubiquitous, ATP-dependent molecular chaperone with various roles in the maintenance of cellular proteostasis, yet it relies upon various co-chaperones to facilitate the maturation of client substrates, such as MAPT. The ATPase homologue 1 (Aha1) is one such co-chaperone that enhances Hsp90's inherently low ATPase activity and regulates its allosteric timing. In fact, it has been previously demonstrated that the disruption Hsp90-Aha1 protein-protein interactions (PPIs) with small molecules can block tau fibril formation without compromising Hsp90's other chaperone activities.

The coumarin containing KU-177 (**Figure 1**,**Top**) is a small molecule inhibitor which has been previously developed by the Blagg lab. This inhibitor disrupts the interaction between Hsp90 and Aha1, which inhibited tau aggregation. However, KU-177 exhibited poor physiochemical properties which would not make it a suitable drug candidate. We are currently performing Structure Activity Relationship (SAR) studies and optimization on our lead compound, ND-AHA-8 (**Figure 1, Bottom**). Upon the preparation of derivatives with improved properties, their biological evaluation of these compounds will then follow.



KU-177



ND-AHA-8

Figure 1: Structure of KU-177 and ND-AHA-8.

Bio-Inspired Multi-Robot Systems for Collective Object Transport

Fernando Moreno
Summer Research Opportunities Program (SROP)

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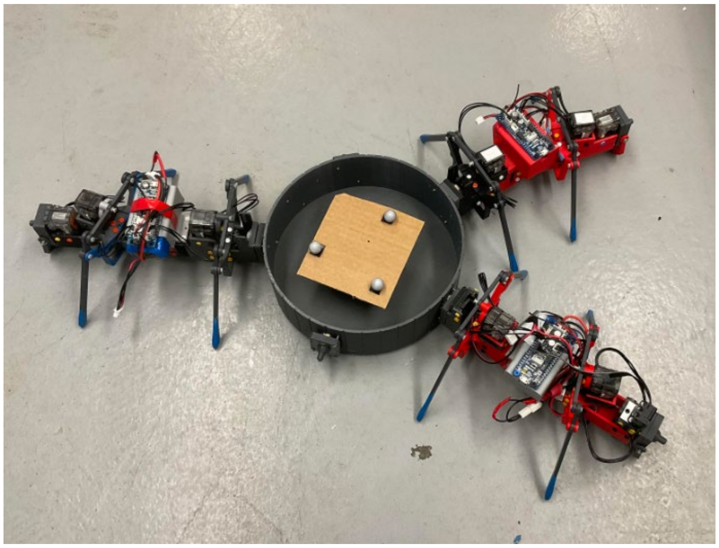
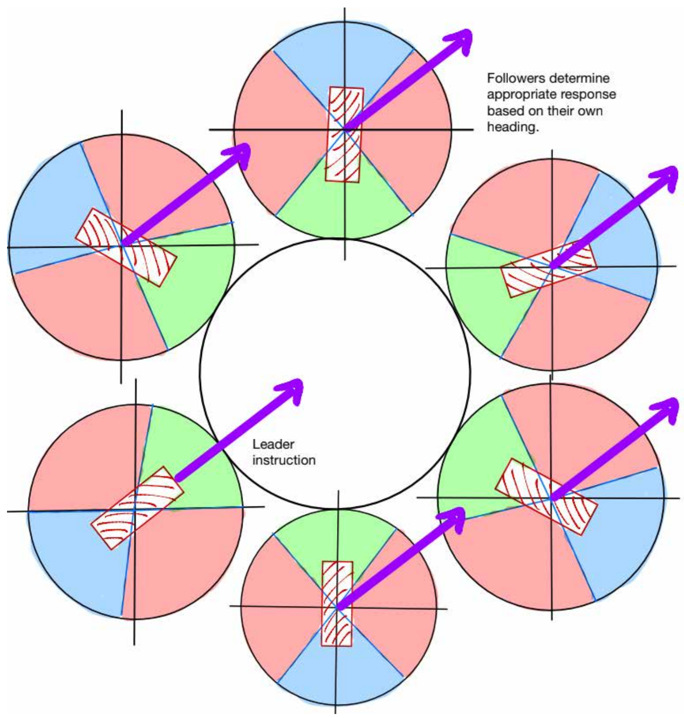
Abstract

Transporting objects is a common task for humans and many species, but large or heavy items pose challenges for individuals. Humans typically use tools and technology to assist with this task. In contrast, ants employ complex cooperative behavior, known as "group retrieval" or "collective object transport," to move objects efficiently as a cohesive group. Studying and mimicking this behavior in robotic systems offers several benefits, including improved scalability up to thousands of units, increased robustness due to the decentralized nature of the system, and heightened adaptability to new situations.

Our system aims to mimic the behavior of ants, which align and combine their forces by pushing and pulling objects towards the direction indicated by an informed leader. This approach is implemented using low-cost, homogeneous robots. Each robot is equipped with a gyroscope to determine its heading accurately and a transceiver for direct communication with other robots. A chosen leader communicates its heading to the group, and each robot then aligns its movement to follow the leader's direction. Our experiments show that this approach allows a swarm of five robots to accurately move larger objects to desired locations, opening the door to potential applications such as moving objects around a warehouse or a construction site. Leader determination can be managed for different tasks, allowing human direction for greater control. Future directions could include an autonomous system with pathfinding algorithms to enable precise navigation in group settings.





Development of the SigCap App for Automated Spectrum Sharing Using ML

Arav Mukherjee
Advanced Wireless Research Experiences (AWaRE)

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Abstract

Though WiFi 6E enables gigabit internet speeds, current 6 GHz spectrum sharing regulations hinder widespread adoption. To ensure unlicensed devices do not interfere with incumbents, outdoor devices must first access an Automatic Frequency Control (AFC) database to obtain permission. Indoor devices can simply lower transmission power. However, since current devices can not differentiate, separate indoor/outdoor access points are mandated. Dr. Ghosh's team discovered a correlation between WiFi/cellular signal and being indoor/outdoors. SigCap was developed and used to automatically record signal measurements, specifying if they were taken indoors/outdoors. Certain Machine Learning (ML) models trained on this data were 99% accurate. My contribution to SigCap aims to address the issues of data accuracy to prevent overfitting, and getting a version of the model to run on-device, despite the computational expense. I added an interactive mapping feature, allowing users to see where each measurement was taken, in terms of any metric. Previously, data accuracy was reduced when users briefly walked through buildings during "outdoor" recordings. Now, they are visually alerted and can easily remove erroneous measurements. Additionally, I am working on implementing an on-device version of the model that can be automatically retrained as new data is received. These additions further demonstrate the feasibility of using a classification model for automated spectrum sharing, even in terms of practical constraints. If devices are able to self-identity, the need for indoor/outdoor specific devices would be eliminated, allowing for the removal of inconvenient restrictions and greater spectrum optimization.

It's Probably Right: Convergence Testing as Validation for Monte Carlo Radiation Transport Methods

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Abstract

Any good implementation of a code that purports to solve a problem must be proven to actually achieve that of which it claims to be capable. The most tangible way of doing this is via a robust suite of tests that, comprehensively, makes use of each feature that is set forth in the code. Here, we propose a set of convergence tests for Monte Carlo / Dynamic Code (MC/DC)[1], an implementation of Monte Carlo methods for, among other applications, neutron transport. The accuracy of Monte Carlo simulations can be tested using convergence testing, wherein the changing of the number of histories run results in a stochastic error decreasing by $O(1/\sqrt{N})$. The tests proposed examine performance of time dependent neutronics given different source configurations – plane initial condition, square initial condition, square source, gaussian initial condition, and gaussian source, which are all variations on the AZURV1 benchmarks[3] – across time. Errors are computed with respect to semi-analytic benchmarks given in [2]. The results of this testing, with an example in Figure 1, were consistent with the expected order of convergence and validated the time dependent performance of MC/DC across a non-trivial amount of time for varied scenarios. This allows for more confident use of this package anywhere in the incredibly diverse set of fields that require the application of neutronics.

References:
1. J. P. Morgan, I. Variansyah, S. Pasmann, K. B. Clements, B. Cuneo, A. Mote, C. Goodman, C. Shaw, J. Northrop, R. Pankaj, E. Lame, B. Whewell, R. McClarren, T. S. Palmer, L. Chen, D. Anistratov, C. T. Kelley, C. Palmer, and K. E. Niemeyer. Monte Carlo / Dynamic Code (MC/DC): An accelerated Python package for fully transient neutron transport and rapid methods development.
2. Bennett, W., & McClarren, R. G. 2022. Benchmarks for Infinite Medium, Time Dependent Transport Problems with Isotropic Scattering. *Journal of Computational and Theoretical Transport*, *51*(4), 205–221.
3. Ganapol, B. D. 2001. Homogeneous Infinite medium time-dependent analytical benchmarks for X-TM transport methods development. Technical Report LA-UR-01-1854. Los Alamos National Laboratory.

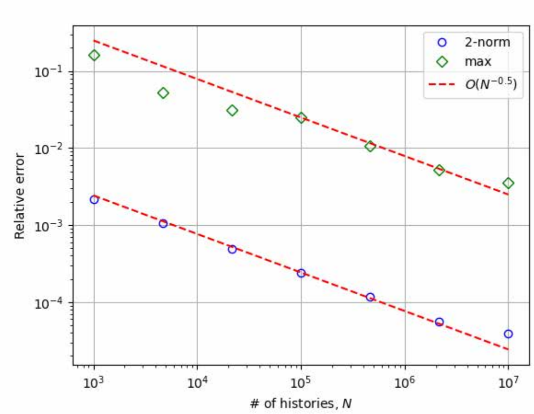

Figure 1. Convergence Plot for Gaussian Source $t_0 = 5$

Determining Energy Transfer in Doped Perovskite-Dye Systems

Sara Murray
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Abstract

Perovskite nanocrystals (NCs) are a promising material for energy harvesting and conversion applications due to their strong absorption and tunable optical properties. Doping with transition metals such as Mn offers an increased quantum yield and a longer excited state lifetime for the host NCs[1]. In this study, we investigate how the exciton and dopant states participate in the Mn doped NC-tricarbocyanine (IR 125) acceptor system.

By altering the halide composition (Br/Cl) in Mn-$CsPb(Cl_{1-x}Br_x)_3$, the intensity of the luminescence of the Mn peak can be increased. We found the greatest Mn luminescence with Mn-$CsPb(Cl_{0.7}Br_{0.3})_3$. We demonstrated energy transfer between Mn-$CsPb(Cl_{0.7}Br_{0.3})_3$ and surface bound IR 125, a near-infrared dye, through a combination of steady-state and time-resolved absorption and photoluminescence (PL) studies. PL experiments were used to analyze the magnitude of quenching of Mn-$CsPb(Cl_{0.7}Br_{0.3})_3$ emission as the concentration of IR 125 was increased. Both the Mn and NC peaks were significantly quenched along with a simultaneous emergence of IR 125 emission, indicating the possibility of singlet energy transfer from both the exciton and dopant energy states. The PL decay of the doped NC was taken with and without IR 125 present to determine the rate of energy transfer. Transient absorption spectroscopy was used to analyze the energy transfer kinetics between the doped NC and IR 125 in the picosecond timescale. The results suggest the potential of singlet and/or triplet energy transfer from the exciton and dopant states in the Mn-doped NC donor-acceptor system.

References:

1. Wang, S.; Leng, J.; Sun, Q.; Zhao, C.; Jin, S. Efficient External Energy Transfer from Mn-Doped Perovskite Nanocrystals. *J. Phys. Chem. Lett.* **2021**, *12*, 1475– 1480, DOI: 10.1021/acs.jpclett.1c00017

FDA-approved Drug Screening to Identify Inducers of Ferroptosis as Novel Therapeutic Agents for Advanced Cancers

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Warren Center for Drug Discovery REU

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Brian Blagg, Charles Huisking Professor of Chemistry and Biochemistry and Director of Warren Center for Drug Discovery and Development
Aktar Ali, Associate Research Professor of Chemistry and Biochemistry and Director of Warren Center Biological Screening Core College of Science

Abstract

In recent years, cancer treatment has advanced significantly, however the disease remains one of the leading causes of death. This provides a framework for further studies involving anticancer strategies; in fact, several types of cancer cells have been shown to be susceptible to ferroptosis in other studies. Ferroptosis is a distinct form of programmed cell death that differs from others, such as apoptosis, autophagy, and necrosis. Accumulation of iron-dependent lipid peroxidation and reactive oxygen species causes failure of the cell's antioxidant system and membrane damage of the cell, ultimately leading to cellular death. Glutathione Peroxidase 4 (GPX4) is a selenoprotein and endogenous antioxidant enzyme which has been shown to play a crucial role in ferroptosis induction. We hypothesize that if the GPX4 pathway can be inhibited through drug administration, ferroptosis will be induced in the cell, causing cancer cells to degregate. In this study, we developed an assay for GPX4 synthesis using a nuclease-treated Rabbit Reticulocyte Lysate (RRL) from Promega. We then used this assay to screen FDA-approved drugs from the Warren Family Center for Drug Discovery and Development, to identify if they could induce ferroptosis by inhibiting the GPX4 pathway. From these efforts, we found compounds **9**, **21**, and **25** were revealed to have promising hits of GPX4 inhibition and will be subjected to further investigations.

Essential Characteristics for Determining the Indoor or Outdoor Environment of Devices on the Radio Spectrum

Jincy Njenga
Advanced Wireless Research Experiences (AWaRE)

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Seda Tusha, Postdoctoral Researcher
Monisha Ghosh, Professor of Electrical Engineering
College of Engineering

Abstract

On the radio spectrum, there is a limited number of frequency bands available for all devices to potentially utilize. Spectrum sharing, which allows multiple devices to transmit on a frequency band, can be implemented to optimize the radio spectrum. However, to perform spectrum sharing, devices must be able to classify its environment as indoors or outdoors. To determine a device's environment, I used SigCap, an android application that collects the data of Wi-Fi and cellular signals. I collected data at various indoor and outdoor locations on the Notre Dame campus, and graphed the compiled data. Using the Cumulative Distribution Function (CDF), I analyzed the Received Signal Strength Indicator (RSSI) and Reference Signal Received Power (RSRP) of Wi-Fi and cellular signals. Overall, the CDF graphs indicate that RSSI levels are greater indoors than outdoors, and RSRP is greater outdoors than indoors. It is clear that analyzing RSSI and RSRP are reliable methods for determining a device's environment. Currently, my mentors are working on building a machine learning model that can analyze numerous characteristics of a wireless signal, to produce accurate predictions of a device's environment. Furthermore, advancements in radio spectrum can address challenges regarding spectrum sharing, like Wi-Fi-6E's occupancy of the 6 Ghz band and its effects on incumbents. I aim to measure the RSSI of Wi-Fi signals transmitted by Access Points located inside campus buildings. Based on research conducted by my mentors, I anticipate that RSSI levels are relatively low, suggesting that Wi-Fi-6E's signal interference with incumbent devices is improbable.

Manufacturing an Artificial Residual Limb for Pressure Distribution Analysis in Prosthetic Sockets

Sbeydi Ponce Duarte
Engineering Summer Research Experience (E-SURE)

Faculty Advisor:
Edgar A. Bolívar-Nieto, Assistant Professor of Aerospace and Mechanical Engineering
College of Engineering

Abstract

This research focuses on advancing the understanding and estimation of pressure distribution within prosthetic sockets. Funded by the NIH/NIBIB Trailblazer Award, this project aims to develop a system that utilizes an electronic fabric (e-fabric) and a load cell to accurately capture pressure distribution over extended periods through optimization algorithms. This approach aims to overcome the need for expert calibration and frequent sensor replacement, key limitations of pressure sensors. By extending the duration of pressure distribution monitoring, this study seeks to provide a comprehensive understanding of pressure distribution over extended periods and correlation with prosthetic user discomfort.

The current preliminary stage of project design involves the preparation of a testbed capable of high-pressure socket-like conditions using a tensile machine, a below-knee prosthetic socket, and a custom artificial residual limb using silicone material. Perfecting this preliminary stage is crucial before beginning human subject testing. This endeavor is enriched by extensive research and collaboration efforts with Dr. Edgar A. Bolívar-Nieto's Wearable Robotics Laboratory (WeRoLab) and Prof. Chi Hwan Lee's Sticktronics Laboratory at Purdue University, where PhD student Tianhao Yu is developing the e-fabric.

My primary contribution focuses on the manufacturing process of an artificial residual limb. This involved developing proficiency in crafting a silicone model and using off-the-shelf prosthetic components to represent loading conditions through bone. Challenges such as air bubble entrapment in silicone and alignment issues were addressed through careful problem-solving. Despite these challenges, the overarching goal remains to improve the lives of prosthetic users by advancing prosthetic technology through adaptive problem-solving and strategic decision-making. The integration of e-fabrics and load cells aims to provide a detailed estimation of pressure distribution within the prosthetic socket.

References:

1. Barrutia WS, Bratt J, Ferris DP. A Human Lower Limb Mechanical Phantom for the Testing of Knee Exoskeletons. IEEE Trans Neural Syst Rehabil Eng. 2023;31:2497-2506.
2. Prosthetic and Orthotic Parts - Bulldog Tools, Inc.
3. EcoflexTM 00-31 near ClearTM Product Information. Smooth-On, Inc.
4. NIH 3D - Human Tibia and Fibula, 3d.nih.gov/entries/3dpx-000169.

Gateway 1 Clustering Drone Results

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Abstract

Human error is a significant factor in major incidents involving small Uncrewed Aerial Systems (sUAS). Fuzz testing is a software testing method aimed at detecting vulnerabilities in code; however, applying it to sUAS is dangerous and likely to produce dangerous flights and physical damage. Therefore, HIFuzz testing is conducted across three levels: a fully simulated environment with proxy human agents (L1), a simulated environment with real humans (L2), and a real-world environment with real humans (L3). Level 1 is best suited for running thousands, or even hundreds of thousands, of test cases within a reasonable timeframe due to its simulated environment and simulated human interactions. In contrast, Level 2, while still a simulated environment, involves human testing, which underscores the importance of limiting the number of cases. Transitioning from L1 to L2 through a gateway (G1) analyzes test-case results by using the K-Means clustering algorithm to identify groups of similar failures. Without effective clustering, critical types of failures may be missed and not passed down the testing pipeline to L2. My work involved enhancing the G1 gateway by creating tighter, more separated clusters using the Spherical K-Means clustering algorithm. Additionally, we further defined the criteria to identify failure cases, so that successful outcomes, in which an sUAS completed the mission as expected, could be removed from the results. An interactive application was developed to implement this approach, enabling the user to query the data and to obtain immediate results. The application also dynamically generated visualizations of the cluster data and reported the unique features of each cluster. By improving the cluster techniques of the HIFuzz system and allowing the humans-on-the-loop to better analyze the data, the work plays a pivotal role in identifying the common factors that cause human machine interaction errors in sUAS systems.

References:

[1] Chambers, Theodore, Michael Vierhauser, Ankit Agrawal, Michael Murphy, Jason Matthew Brauer, Salil Purandare, Myra B. Cohen, and Jane Cleland-Huang. "HIFuzz: Human Interaction Fuzzing for Small Unmanned Aerial Vehicles." In *Proceedings of the CHI Conference on Human Factors in Computing Systems*, pp. 1-14. 2024.

Examining Treatment Efficacy in the Pregnant Mom's Empowerment Program: A Transdiagnostic Perspective

Safa Rahman
ND-PREP

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Abstract

The Pregnant Mom's Empowerment Program (PMEP) is an intervention aimed to alleviate symptoms of major depressive disorder (MDD) and post-traumatic stress disorder (PTSD) for pregnant women who are exposed to intimate partner violence. Previous analyses of treatment outcomes indicate PMEP significantly reduces symptoms of MDD but not PTSD among program participants (Miller-Graff et al., 2022). This finding is particularly interesting given the highly comorbid nature of both psychopathologies (Afzali et al., 2017). The current study seeks to further evaluate how PMEP reduced psychopathology by evaluating change at the level of individual symptoms, rather than evaluating change across broader symptom clusters. Multiple regression item-level analyses were conducted on the Center of Epidemiological Studies-Depression (CES-D) and the PTSD Checklist for DSM-5 (PCL-5) questionnaires completed by participants ($N = 137$; $M_{age} = 27.29$, $SD = 6.00$) to evaluate change from pre- to post-intervention. Results indicated that assignment to treatment significantly predicted a reduction in participants' feelings of sadness ($\beta = -.43$, $p = 0.014$), viewing their life is a failure ($\beta = -.35$, $p = 0.028$), and concentration difficulties ($\beta = -.73$, $p = 0.002$), compared to participants in the control group. Interestingly, these symptoms broadly indicate a reduction in negative affect. Therefore, it may be the case that PMEP improves transdiagnostic symptoms across MDD and PTSD by reducing the intensity of negative affect as opposed to promoting positive affect. Future analyses will include running multi-level models to test for within-person differences in transdiagnostic treatment outcomes at post-intervention and additional follow-ups.

References:

Afzali, M. H., Sunderland, M., Teesson, M., Carragher, N., Mills, K., & Slade, T. (2017). A network approach to the comorbidity between posttraumatic stress disorder and major depressive disorder: The role of overlapping symptoms. *Journal of affective disorders*, *208*, 490–496. https://doi.org/10.1016/j.jad.2016.10.037

Miller-Graff, L. E., Paulson, J. L., Hasselle, A. J., Cummings, E. M., & Howell, K. H. (2022). Examining the efficacy of prenatal intervention in reducing IPV revictimization and improving maternal mental health: A quasirandomized controlled trial of the pregnant moms' empowerment program (PMEP). *Journal of Consulting and Clinical Psychology*, *90*(11), 884–898. https://doi.org/10.1037/ccp0000772

Collaboration between Large Language Model and Autonomous Vehicles

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Center for Research Computing (CRC) Internship
(Trusted AI)

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Abstract

This project explores the capabilities of foundational models, commonly known as Large Language Models (LLMs), in their ability to collaborate and strategize to complete complex tasks in conjunction with autonomous vehicles. As the use of specialized local foundational models becomes more widespread, this research aims to deploy a team of multiple local "agents" to achieve high-performance inference and reasoning. These agents can potentially eliminate the need for private data centers, extensive computational networks, or even an internet connection. Moreover, the project investigates the potential of these models to interact with the physical world through robotics, particularly in search and rescue scenarios where the models are tasked with searching, mapping, and locating targets.

A key focus is on the ability of LLMs to control robotics, enhancing and automating complex or hazardous tasks with minimal initial investment and fine-tuning compared to traditional automation processes. This involves enabling foundational models to utilize live data, such as sensor information and live camera feeds, to make real-time decisions and communicate effectively. The research also examines how agents can process sensor data to form coherent recommendations, communicate and divide tasks efficiently, and prioritize information to choose the best course of action.

Successful implementation would represent a substantial advancement, demonstrating that LLMs can offer practical solutions for real-world applications, especially in scenarios requiring quick, accurate responses. This project not only pushes the limitations of what foundational models can achieve in controlled environments but also advances their application in dynamic, real-world settings.

Taxol & Neurodegenerative Diseases: A Connection

Oliver Reyes
ND-PREP

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Abstract

Alzheimer's is a neurodegenerative disease that affects memory, thinking, and behavior. It impacts many people and has various proposed causes. One potential cause is the assembly of a microtubule-binding protein called Tau into filaments that eventually form neurofibrillary tangles. This transformation renders Tau inactive, disrupts microtubule function, and inhibits neuronal transport. Our lab was studying this Tau protein, and unexpectedly saw that adding the chemotherapy drug Taxol to mixtures of microtubules and Tau causes Tau to form filaments. Our lab aims to investigate whether Taxol stabilized Microtubules can induce Tau filament formation in cells as well as test tubes. We will introduce Taxol into mammalian cells that are expressing a version of Tau that is prone to filament formation and observe if Tau filaments form in the cells. If we do observe that Taxol can induce Tau filament formation in the cells, this may raise questions about the use of Taxol as a chemotherapeutic agent. We hope that this does not occur, as it would negatively affect the range of available chemotherapeutic agents, but it could also provide valuable information. Since there is continued debate on the possible relationship between chemotherapeutic agents and neurodegenerative disease, evidence that Taxol promotes filament formation in cells expressing mutant Tau might imply that normal cells have a way to remove the Tau filaments. This could deepen our understanding of neurodegenerative diseases and aid in developing effective treatments.

Hydrogel Biomimetic Polymers for High-throughput Prostate Cancer Organoid Culture

Kamilah Richardson
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

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Abstract

Prostate cancer (PC) is the 4th most common form of cancer and 70% of men who develop metastatic PC have a survival rate of 33%[1]. Hence, it is essential to understand the progression of metastatic PC. While 2D culture is commonly used to study cellular mechanisms, 3D cultures are more favorable as they better mimic cell-cell interactions, tissue-like structures, and tumor microenvironment conditions. The inverted colloidal crystal (ICC) scaffold is a more refined, reliable, and exemplary 3D culture platform that produces a high quantity of size-controlled tumor spheroids, compared to the traditional hanging drop method[2,3]. In this work, we use ICC scaffolds to create a high quantity of reliable and consistent prostate cancer spheroids using a bone metastasis PC cell line, LNCaP-TR-BOM, and a control PC cell line, LNCaP-TR, to investigate the metastasis of PC. The analysis showed that the ICC scaffold is more favorable for spheroid formation than the hanging drop method. After creating, growing, and comparing the spheroids to the hanging drop method, we consistently found that the ICC scaffold formed a high quantity of uniform spheroids in larger quantities, was a less time-consuming procedure, and was more thorough for analysis. These findings are crucial for PC research because having a tumor cell model that accurately mimics the tumor microenvironment of PC cells *in vitro* allows for a better analysis of metastatic PC. Additionally, since this tumor cell model allows for accurate drug screening and testing, this model can effectively test novel treatments for metastatic PCs.

References:

[1]Carpenter, R.; Macres, D.; Kwak, J.-G.; Daniel, K.; Lee, J. Fabrication of Bioactive Inverted Colloidal Crystal Scaffolds Using Expanded Polystyrene Beads. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7099427/ (accessed 2024-07-15).
[2]Lee, J.; Cuddihy, M. J.; Cater, G. M.; Kotov, N. A. Engineering Liver Tissue Spheroids with Inverted Colloidal Crystal Scaffolds. https://www.sciencedirect.com/science/article/pii/S0142961209005353?via%3Dihub (accessed 2024-07-15).
[3]Prostate Cancer Statistics: World Cancer Research Fund International. https://www.wcrf.org/cancer-trends/ (accessed 2024-07-12).

Real-Time Analyses in Monoclonal Antibody Production Using Functionalized Membranes

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Abstract

Therapeutic monoclonal antibodies (mAbs) modulate immune responses in autoimmune diseases, neutralize infections, and hinder the growth of cancer cells. mAb synthesis occurs in fermentation broths, and monitoring of mAb composition and concentration is vital for efficient production and quality control. Enzyme Linked Immunosorbent Assays (ELISAs) can quantify mAb concentrations during and after their production. However, these assays typically take hours to complete and cannot provide real-time monitoring. This research focuses on engineering new methods for capturing and analyzing mAbs within five minutes using porous affinity membranes. Flow through micron-sized pores in the membranes enables mAb capture in minutes through binding to affinity sites. Subsequent flow-based binding of a fluorescently labeled secondary antibody gives a fluorescence signal whose intensity depends on the concentration of the initial mAb.

This method uses glass-fiber membranes modified with polyelectrolytes to immobilize oxidized Fc-III-4C (oFc20), a short peptide that binds strongly to mAbs in their Fc-region. Membranes in 96-well plates enable parallel analyses and determination of fluorescence using a plate reader. This summer research is investigating ways to increase the sensitivity of analyses of mAbs and other proteins. By attaching either gold nanoparticles or fluorescent beads to the secondary antibody, digital counting of these individual objects could lead to much lower detection limits. However, such methods require extremely low non-specific adsorption, which is an ongoing challenge.

References:

1. Yang, Junyan, Raluca Ostafe, Christopher J. Welch, Brandy Verhalen, Ivan L. Budyak, and Merlin L. Bruening. "Rapid Quantitation of Various Therapeutic Monoclonal Antibodies Using Membranes with Fc-Specific Ligands." *Analytical Chemistry*, vol. 95, no. 22, 2023, pp. 8541-8551. DOI: 10.1021/acs.analchem.3c00531.
2. Maniya, Nalin H., and Sonu Kumar, et al. "An Anion Exchange Membrane Sensor Detects EGFR and Its Activity State in Plasma CD63 Extracellular Vesicles from Patients with Glioblastoma." *Communications Biology*, vol. 7, no. 1, 2024, pp. 677. DOI: 10.1038/s42003-024-06385-1.

Drone Voice Interfaces Using Large Language Models

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Abstract

Drones are indispensable tools across a variety of applications, especially in urgent scenarios like search and rescue operations where rapid response is crucial. However, the effectiveness of drones is often compromised by complex user interfaces that delay critical maneuvers. Typically, the pilot-in-command (P.I.C) must juggle focusing on intricate drone operations with monitoring its status, a demanding task that significantly hampers efficiency. With the advent of artificial intelligence (AI) technologies, the interaction paradigms between humans and machines are evolving. Leveraging large language models (LLMs) and AI can transform drone interfaces, enhancing operational efficiency by enabling voice commands for direct information retrieval and action initiation, thus minimizing the need for manual interface navigation. For instance, setting up a geo-fence could transition from manual map inputs to verbal instructions, allowing the P.I.C to maintain attention on the drone's flight rather than the interface. This shift towards AI-enhanced interfaces represents a significant advancement in drone technology, promising to optimize response times and streamline operations. By integrating AI, especially voice-activated controls, into drone systems, we can substantially reduce the cognitive load on operators, thereby increasing both the speed and safety of mission-critical deployments. As we continue to refine these technologies, the future of drone operations will likely see a dramatic shift towards more autonomous, reliable, and user-friendly systems, ultimately broadening the scope of their application and effectiveness in real-world scenarios.

WhatsApp Grocery Assistant: Providing Product Recommendations That Are Affordable and Healthy

Roman Sally
CSE Summer Enrichment Program

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Ronald Metoyer, Vice President and Associate Provost for Teaching and Learning; Professor of Computer Science and Engineering
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Abstract

Balancing a healthy and affordable diet is a challenge for many Americans who must consider multiple factors such as price, ingredients, nutritional value, and personal dietary goals when purchasing food products. This project aims to address these challenges by developing and testing a WhatsApp chatbot that provides real-time, customized grocery product recommendations based on a user's grocery list items and dietary goals. We designed the chatbot interface to interact with the user to collect information regarding dietary goals and prompt the user to enter shopping list items. We employ an optimization strategy to recommend items that minimize the total cost of the items in the list while considering dietary goals and constraints. Through the WhatsApp messaging capability, we provide specific product recommendations to the user based on inventory and dietary goals. The user is also able to message with the chatbot to explore product alternatives for any item. To refine the system, we plan to conduct interviews with local community members to validate the design and understand how our chatbot can support a users list building and shopping. Their feedback will help identify the strengths and weaknesses of the WhatsApp chatbot, guiding necessary improvements.

Flow-Induced Stress on Red Blood Cells for Single-Cell Health Monitoring

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Gabriel R. Burks, Assistant Professor of Chemical and Biomolecular Engineering
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Abstract

Sickle Cell Disease (SCD) is a rare blood disease that can lead to many health complications due to genetic mutations of red blood cell (RBC) hemoglobin. In particular, SCD causes RBCs to morph into a crescent or sickle-shape during deoxygenation cycles. This cycling gradually increases the concentration of tactoids, sticky gel-like hemoglobin structures that cause RBCs to agglomerate, thus blocking blood vessels and preventing normal flow of healthy blood. Moreover, these morphological changes lead to a change in the modulus of the cells. Theory suggests an increase in cell modulus can be related to tactoid concentration, serving as a marker for an RBC's state of health. Recent microfluidic techniques have granted the ability to trap single RBCs within a pressure-driven flow field through thin channels to induce stress. Here, an effective approach to trap RBCs without introducing secondary damage to the cell and a methodology for determining single cell modulus is reported. A 3D-printed four-channel microfluidics Stokes trap was fabricated with 1 mm channels for particle trapping. RBCs collected from live mice were preserved using ethylenediaminetetraacetic acid (EDTA) and separated from whole blood through centrifugation. Highly concentrated bulk RBCs were diluted for particle trapping using phosphate-buffered saline. Thickening agents were then added to the RBC solutions to increase viscosity which promoted greater trapping efficiency. Optical microscopy shows that particle trapping is an appropriate method to capture RBCs without causing morphological changes. Further image analysis was conducted via LabView to determine the modulus of RBCs for further studies.

Investigating Low States in Intermediate Polars

Sierra Sanne
Summer Research Opportunities Program (SROP)

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Peter Garnavich, Professor, Department of Physics and Astronomy
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Abstract

We investigate 45 confirmed intermediate polars' ATLAS and TESS absolute magnitude light curves for low states, during which they fade unpredictably and for anywhere from days to months. We find that nearly one-fifth of these systems show either definite or possible low states, which we define as a sustained fade of 0.5 magnitudes or more. While some of these low states have been previously reported, many are newly identified. One of these systems, MU Cam, was serendipitously observed by TESS while it started to fade into a low state, one of the first instances there has been TESS data that captured the beginning of a low state in an intermediate polar. Using a 2D power spectrum of the TESS data, we investigate how MU Cam's mode of accretion changes in response to the reduced mass-transfer rate during that low state. We also compare the properties of IP low states with low states in non-magnetic cataclysmic variables and find that the VY Scl and intermediate polar populations have similar orbital period and absolute magnitude distributions, although the VY Scl stars have deeper low states than intermediate polars. Our results expand upon previous investigations of low states in intermediate polars and serve as the most comprehensive search undertaken for low states in intermediate polars.

Pressing Matters: Using the Novel Paradigm, "PressMORE," to Evaluate Social Motivation in Preschoolers

Julia Savino
College of Science Summer Undergraduate Research Fellowship (COS-SURF)

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Abstract

Early autism interventions rely on social or tangible rewards to teach functional behavior. However, willingness to work for these rewards varies. We developed PressMORE, a child-friendly progressive ratio task, to measure this willingness. We measured the child's 'breakpoint', or maximum number of times they willingly pressed a button for a reward (short bubble display; Fig 1). Children completed PressMORE twice: first independently (nonsocial condition), then with caregiver encouragement (social condition). Additionally, the parent-report Social Responsiveness Scale-2 (SRS-2) was used to quantify autistic characteristics. We aim to 1) assess the feasibility of PressMORE in 3 to 5-year-olds, 2) analyze the effect of caregiver encouragement, and 3) explore the relationship between breakpoint and SRS-2 T-score.
All participants (n=20, ages 3;0 to 5;11) successfully completed the task. Total button presses ranged from 2 to 2541. The mean breakpoint was higher in the social (M=49.6, SD=24.8)) than the nonsocial condition (M=29.5, SD=19.1; $t(38)=2.87$, $p=0.007$). No significant correlation was observed between changes in breakpoint and SRS-2 T-scores (r=0.247, p = 0.32).

These results demonstrate feasibility of PressMORE for 3–5-year-olds. Participants exerted more effort when encouraged by their caregiver; in this small sample of mostly neurotypical children, the increase was not correlated with autistic characteristics. Future directions include collecting additional data, and testing PressMORE in younger toddlers and autistic children to understand social motivation in a developmental disorder characterized by differences in social motivation.

Figure 1. PressMORE setup

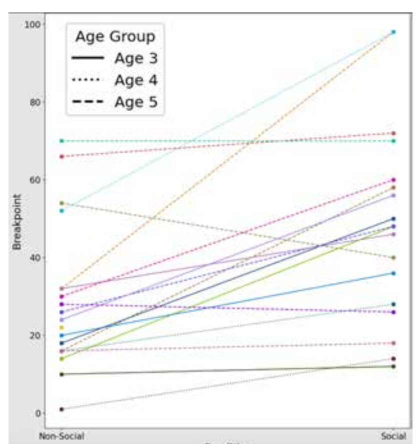

Figure 2. Spaghetti plot of non-social to social breakpoints for each participant

Construction and Characterization of Functional Polymeric Membranes for Continuous Stress Indicator Sensing

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NDnano Undergraduate Research Fellowship (NURF)

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College of Science, College of Engineering

Abstract

As a rise in individuals turn towards wearable devices for monitoring and collecting personal health data ranging from heart rate to stress levels, longevity of the biosensors continuously collecting accurate data has become increasingly relevant. Issues in performance arise due to the continuous exposure to excreted sweat, in which an assortment of unwanted molecules and proteins can non-specifically absorb on the interface of these sensors, decreasing the accuracy of valuable data readings as time progresses. This project focuses on the elimination of such sensor fouling though developing a biocompatible nanostructured membrane functionalized with an antifouling zwitterionic polymer brush.

Using a spin coater, a P(HEMA-GMA-TFEMA-OEGMA) copolymer synthesized within the lab was evenly spread onto a silicon wafer creating a thin membrane. These membranes were transferred onto a polyvinylidene fluoride (PVDF) support via a sacrificial transfer process, allowing for the evaluation of the relationship between membrane throughput versus applied pressure. With control measurements determined, the zwitterionic polymer brush sulfobetaine methacrylate was grown on the membrane through a surface-initiated ARGET ATRP method. Continued assessment of permeability for these enhanced membranes was obtained allowing for comparison with the previously collected data for the control HEMA membrane. These further measurements will help define whether the zwitterionic layer leads to a reduction in fouling on the membrane surface without significantly inhibiting permeability selectivity.

Characterization of CNTN2 in Inner Ear Neuron Development

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Abstract

The inner ear, comprised of the cochlea and vestibular organs, is important for functioning senses of hearing and balance respectively. Cochlear and vestibular neurons carry information from these inner ear organs to the brain for processing. Thus, inner ear neurons are critical for normal inner ear functions. Disorders such as deafness can be due to abnormal development or damage to the inner ear neurons. To develop treatments, normal development must first be understood. Our interest was determining what gene(s) are involved in the process of inner ear neurons forming connections with their sensory organ targets. This project investigated the location and timing of cell adhesion protein, CNTN2 in chickens from embryonic (E) day 2 to E6.5, during the process of pathfinding. Immunohistochemistry was used to visualize the CNTN2 protein. Immunofluorescent staining evidence from our lab demonstrates that CNTN2 is expressed in inner ear neurons of the chick during the process of pathfinding. These findings suggest that CNTN2 may play a role in axonal pathfinding of inner ear hair cell targets. These hair cell targets are significant in relaying sensory information to the brain for processing. As aforementioned, problems with inner ear neurons can disrupt this natural process and lead to hearing loss or vestibular disorders. A better understanding of the expected interaction between inner ear specific genes and their sensory targets will hopefully lead to the ability to identify and treat abnormalities in this process.

Designing a Controller for a Knee Exoskeleton to Assist in Sit-to-Stand Motion

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Engineering Summer Research Experience (E-SURE)

Faculty Advisor:
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Abstract

Sit-to-stand transitions can be physically demanding for older adults which makes them and their caregivers a high risk for developing back injuries [1], [2], [3], [4], [5]. ELVIA (Elastic Locomotion Via Instrumented Apparel) is currently a passive exoskeleton that acts as a parallel spring to passively assist users in sit-to-stand motion. The goal of the research this summer was to design a control law that can eventually be implemented with electric motors to add an active component to ELVIA.

The framework and overall concept of the controller were the main progress this summer. Designing a controller for an exoskeleton is challenging for a variety of reasons. One of the main challenges is that the controller must work in conjunction with the user, which often involves estimating the user's intent so that the exoskeleton can be controlled in accordance with what the user wants to do. This controller will use an estimate of the Center of Mass (CoM) position in the future to determine user intent. After that, it will use impedance control to track the CoM trajectory to determine impedance parameters that will result in a torque applied to the exoskeleton.

References:

[1] R. W. Bohannon, "Measurement of Sit-to-Stand Among Older Adults," *Top. Geriatr. Rehabil.*, vol. 28, no. 1, pp. 11–16, Jan. 2012, doi: 10.1097/TGR.0b013e31823415fa.
[2] A. Garg and B. Owen, "Reducing back stress to nursing personnel: an ergonomic intervention in a nursing home," *Ergonomics*, vol. 35, no. 11, pp. 1353–1375, Nov. 1992, doi: 10.1080/00140139208967398.
[3] A. Garg, B. Owen, D. Beller, and J. Banaag, "A biomechanical and ergonomic evaluation of patient transferring tasks: bed to wheelchair and wheelchair to bed," *Ergonomics*, vol. 34, no. 3, pp. 289–312, Mar. 1991, doi: 10.1080/00140139108967314.
[4] S. Hignett, "Work-related back pain in nurses," *J. Adv. Nurs.*, vol. 23, no. 6, pp. 1238–1246, Jun. 1996, doi: 10.1046/j.1365-2648.1996.13423.x.
[5] A. P. Dawson, S. N. McLennan, S. D. Schiller, G. A. Jull, P. W. Hodges, and S. Stewart, "Interventions to prevent back pain and back injury in nurses: a systematic review," *Occup. Environ. Med.*, vol. 64, no. 10, pp. 642–650, Jan. 2007, doi: 10.1136/oem.2006.030643.

Synthesis of Substrate-Immobilized Gold Nanoplates using $NaAuCl_4$

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NDnano Undergraduate Research Fellowship (NURF)

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Abstract

Noble metal nanoplates are a unique class of two-dimensional (2D) nanomaterials whose planar geometry serves as one of the most important nanoscale building blocks.[1] In addition to that, Au nanoplates are highly studied because of their unique properties like plasmonic response and catalytic activity, bringing a wide variety of applications in a great range of reactions and technological devices. The above is achieved thanks to the possibility of performing functionalizations on the surface of the nanostructure such that they express a specific desired response.[1]

Obtaining these attractive gold nanostructures requires the presence of specific conditions and reagents, starting with seeds with planar defects that promote planer growth through a break in symmetry.[2,3] Likewise, the presence of a reducing agent and a gold precursor is necessary. The gold precursor acts as a source of gold that feeds the seeds to increase their size. The reducing agent plays the role of reducing Au^{3+} to Au^0.[2] The synthesis of nanoplates has previously been studied using Brij S100 and $HAuCl_4$ as the reducing agent and Au precursor, respectively.[4]

The purpose of this project is to compare this synthesis to one that uses $NaAuCl_4$ and Brij S100, thus modifying the pH and optical properties of the growth solution. These parameters are likely to determine the size distribution and growth rate.[2] Studying the properties of this new growth solution by performing wavelength-dependent syntheses will provide a better understanding of the mechanism responsible for the light-driven growth of Au nanoplates.

References:

(1) Neal, R. D.; Hughes, R. A.; Preston, A. S.; Golze, S. D.; Demille, T. B.; Neretina, S. Substrate-Immobilized Noble Metal Nanoplates: A Review of Their Synthesis, Assembly, and Application. *Journal of Materials Chemistry C*. Royal Society of Chemistry October 14, 2021, pp 12974–13012. https://doi.org/10.1039/d1tc01494c.

(2) Langille, M. R.; Personick, M. L.; Mirkin, C. A. Plasmon-Mediated Syntheses of Metallic Nanostructures. *Angewandte Chemie - International Edition*. December 23, 2013, pp 13910–13940. https://doi.org/10.1002/anie.201301875.

(3) Golze, S. D.; Hughes, R. A.; Rouvimov, S.; Neal, R. D.; Demille, T. B.; Neretina, S. Plasmon-Mediated Synthesis of Periodic Arrays of Gold Nanoplates Using Substrate-Immobilized Seeds Lined with Planar Defects. *Nano Lett* **2019**, *19* (8), 5653–5660. https://doi.org/10.1021/acs.nanolett.9b02215.

(4) Demille, T. B.; Neal, R. D.; Preston, A. S.; Liang, Z.; Oliver, A. G.; Hughes, R. A.; Neretina, S. Epitaxially Aligned Single-Crystal Gold Nanoplates Formed in Large-Area Arrays at High Yield. *Nano Res* **2022**, *15* (1), 296–303. https://doi.org/10.1007/s12274-021-3473-1

Tackling Bone Metastasis in Prostate Cancer

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Biological Sciences Research Experiences for Undergraduates (BioREU)

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Abstract

Prostate cancer is the second-leading cause of cancer death in men, with bone metastasis occurring in about 90% of cases. The mechanisms underlying bone metastasis are not well-understood, highlighting the importance of elucidating key players involved. Our preliminary results indicate the involvement of the PRC2 protein complex, which catalyzes histone three methylation. High methylation levels are strongly correlated with bone-metastatic (BoM) cells, which form spheroid structures in 2D and 3D culture.

qRT-PCR analysis was performed on eight genes thought to be strongly correlated with the differentially expressed genes. Several inhibitory drugs were tested at various concentrations. BoM cells were seeded into polyHEMA-coated 96-well plates, which were incubated at 37 C for 24-48 hrs. Spheroids will serve as a proxy to measure drug efficacy. A resazurin assay was performed post-incubation to measure cell viability. The RNA-seq profile was uploaded to OCTAD (a drug discovery tool) to determine potential drug targets.

qRT-PCR results indicate two genes are overexpressed in BoM cells, and OCTAD analysis provided an output of around 1600 drugs that may reverse gene expression in BoM cells. Drug testing is currently an ongoing process, and we expect to see a reduction of spheroid formation in BoM cells.

Due to the exploratory nature of this project, a significant knowledge gap remains in understanding the mechanisms driving bone metastasis. Further validation and testing are required to determine pathways and other factors involved. We plan to obtain an RNA-seq profile with more biological replicates and an ATAC-seq profile to determine epigenomic.

From Diversity to Discovery:
The Power of Cross-Cultural Collaboration in Research

Peyton Shrader
Summer Research Opportunities Program (SROP)

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College of Arts and Letters

Abstract

Cross-cultural collaboration is essential to enhancing research around the world, as it fosters innovation, enhances problem-solving, strengthens communication, and provides a deeper level of trust by bringing together diverse perspectives and expertise. While a “normal” summer research experience usually includes one specifically identified project, I had the privilege of playing a pivotal role in three projects that showcased why cross-cultural collaboration is imperative in the world of research today.

The three projects included (1) assisting on Dr. Bleck’s book manuscript about informal civil society clubs in Mali by cross-checking references within the bibliography and editing the text when needed, (2) anonymizing and organizing data from 79 interviews with civil society leaders conducted in Mali regarding activists’ strategies conditions of political uncertainty, and (3) coordinating a cross-cultural team that included two students from Côte D'ivoire who are working on these projects for the ISLA African Governance Innovations lab under the supervision of Dr. Bleck.

Collaborating with two international students on various research projects has allowed me to reflect on the importance of effective cross-cultural collaboration, no matter the barriers. Collaboration is built upon intercultural relationships and intercultural trust, two ideas that are vital from the first day collaboration begins. When collaboration is successful, cross-cultural teams have an advantage when it comes to increased creativity and profitability, with profitability meaning increased dissemination of knowledge. With this in mind, effective cross-cultural collaboration can create successful, innovative knowledge and ultimately, change the world of research today, no matter the field, for the better.

Effect of Extracellular Matrix Age and Cellular Age on Mammary Fibroblasts

Alexandra Stormer
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

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Abstract

Breast cancer is the most commonly diagnosed type of cancer in women[1], and about 80% of all cases are diagnosed in women over the age of fifty[2], proving age to be a large factor in the development of this disease. There are many different biological factors that change in a person's body as they age, so determining which of these changes have a part in the increased likelihood of developing breast cancer is crucial to understanding and treating the disease. One specific cellular component that has noticeable changes as a person ages is the extracellular matrix (ECM). Here we report the production of cancer-associated proteins of mammary fibroblasts seeded on young and aged ECMs in order to understand how the aging of the ECM can cause cells to show more cancer-like behavior. We show that aged cells seeded onto young ECMs produced an increased amount of matrix metalloproteinase-9 (MMP9), implying that aging of the ECM does not increase the presence of MMP9s. We also show that the levels of matrix metalloproteinase-2 (MMP2) in the cells seeded on both the young and aged ECMs were roughly the same, indicating that the aging of the ECMs likely does not have an impact on the production of MMP2s. We also show that aged cells seeded onto aged ECMs produce the most lysyl oxidase (LOX). Aged cells seeded onto young ECMs produced the second highest amount of LOX, followed by young cells seeded onto aged ECMs, showing that the increased production of LOX is more likely related to the aging of cells rather than the ECM. Together, these results show that the expression of cancer-like behavior of cells may be due to cell aging more so than aging of the ECM.

References:

[1] Benz CC. Impact of aging on the biology of breast cancer. *Critical Reviews in Oncology/Hematology*. 2008;66(1):65-74. doi:10.1016/j.critrevonc.2007.09.001
[2] Thomas GA, Leonard RCF. How Age Affects the Biology of Breast Cancer. *Clinical Oncology*. 2009;21(2):81-85. doi:10.1016/j.clon.2008.11.006

Spectrum LLM Project for Wireless Spectrum Documents and Data

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International Summer Undergraduate Research Experience (iSURE)

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Paul Brenner, Sr. Associate Director, Center for Research Computing; Professor of the Practice
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Abstract

The electromagnetic spectrum is essential for a nation, serving as the foundation of modern communication systems, including radio, television, mobile phones, and the internet. Proper management and allocation of this spectrum ensure reliable and efficient communication, vital for both personal and business purposes. Furthermore, military and defense operations significantly depend on the spectrum for secure and effective communication, navigation, radar, and surveillance systems, making its availability critical for national security. To ensure the spectrum's efficient and effective use for current and future needs, the National Telecommunications and Information Administration (NTIA) published a National Spectrum Strategy and solicited public input on its development and implementation. By April 17, 2023, NTIA received over 130 written comments. To help professionals efficiently extract relevant information from a large number of wireless spectrum documents and data, this research aims to develop a RAG (Retrieval-Augmented Generation) LLM (Large Language Model) tool to assist professionals in related fields. We created a web page for the LLM tool using Django and linked it to the OpenAI Assistant API, which utilizes models, tools, and documents to respond to user queries. The LLM tool will leverage vector stores built on the OpenAI API platform, containing official NTIA documents, to provide answers regarding wireless spectrum regulations, comments and data. Within the web page, users can create multiple chat sessions (threads) and rename them based on the query's subject. Users can also upload files and ask questions related to these files, though the files are not retained. All queries and answers are stored in the backend administration page, where the administrator can filter chats by user, time, and other criteria. Additionally, administrators can upload documents to the vector store.

Solving Captchas via Computer Vision Techniques in Multimodal LLM

Mrunal Vibhute
International Summer Undergraduate Research Experience (iSURE)

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Abstract

Captcha (Completely Automated Public Turing test to tell Computers and Humans Apart) is a test designed to verify human presence and prevent automated abuse and malicious activities on a website. These captchas are major obstacles to automated data collection from Dark Web Marketplaces, often requiring human intervention [1]. This research explores automating captcha solving using multimodal Large Language Models (LLMs) like ChatGPT (GPT-4) and Claude.ai. Traditional machine learning and deep learning methods often fall short in this task, necessitating advanced LLMs that can understand and execute multi-step captcha-solving processes.

We use Selenium for automation and a combination of computer vision techniques, such as image filtering [2] and pattern recognition, and prompts with various levels of details to guide the LLMs. The process starts with the program opening the target website and capturing screenshots of captcha images. The LLMs are made to solve the image related tasks, recognize text, find missing characters, and solve the captcha. Preliminary results show that while initial understanding of scrambled/unscrambled images and text recognition by LLMs can have errors, refining the prompts significantly improves accuracy.

Our goal is to create a system that integrates LLM capabilities to solve captchas, reducing the need for human intervention and making data collection more efficient. The findings from this study could revolutionize the way automated data collection systems interact with web content, offering a novel approach to overcoming captcha barriers using a blend of AI-driven language models and computer vision techniques.

References:

1. Kate Connolly, Anna Klempay, Mary McCann, and Paul Brenner. 2023. Dark Web Marketplaces: Data for Collaborative Threat Intelligence. Digital Threats 4, 4, Article 49 (December 2023), 12 pages. https://doi.org/10.1145/3615666
2. York Yannikos, Julian Heeger, "Captchas on Darknet Marketplaces: Overview and Automated Solvers" in Electronic Imaging, 2024, pp 330-1 - 330-6, https://doi.org/10.2352/EI.2024.36.4.MWSF-330

Custom GPT for Wireless Spectrum Regulation

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International Summer Undergraduate Research Experience (iSURE)

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Paul Brenner, Sr. Associate Director, Center for Research Computing; Professor of the Practice
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Abstract

This research project aims to enhance user comprehension of spectrum regulation by developing a custom assistant utilizing the OpenAI GPT-4 model. The assistant is specifically designed to provide detailed responses to spectrum regulation queries, with test questions sourced from the NTIA Redbook and FCC comments. A comparative analysis was conducted to evaluate performance accuracy across three versions of the GPT model: Assistant GPT (custom-built), Free Version GPT, and Personal Paid GPT. To facilitate user interaction, a web-based interface and database were developed using Python Django. This platform allows users to ask regulation-related questions, select from different assistant versions, and access responses stored in distinct vector store files. Additionally, the system includes administrative functionalities for managing questions and answers, enabling comprehensive analysis.
The study results reveal significant differences in accuracy and response quality among the three versions of GPT. The customized Assistant GPT, optimized through prompt engineering and configured to answer questions based on the uploaded file vector stores rather than hallucinations by adjusting the temperature index, demonstrated superior performance. This improvement was achieved by employing a specific selection of documents uploaded to the vector store. This project underscores the potential of customized AI solutions in specialized domains, emphasizing the importance of customizability and accuracy in tools designed for regulatory understanding.

Social Psychology and Research Question Development

Diana Whitfield
Summer Research Opportunities Program (SROP)

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Abstract

During my internship, I focused on the research process in social science, particularly in social psychology and organizational behavior. The two key research questions I had considered were: accusations of sexism and racism and coworkers' perception of managerial reactions to such incidents of discrimination. The research I conducted was based on journal references, using snowballing and keyword searches. Afterwards, I funneled unnecessary resources by keeping useful-sounding article names and discarding the rest. I also researched the responses to and causes of workplace dismissal incidents.

Additionally, I spent time researching the implementation of Senate Bill 1577, which allows students up to five mental health or behavior days without a medical note. The bill requires the opportunity to make up work missed and requires students be directed to school personnel after the second mental health day. I reviewed articles that have documented the positive correlations between burnout, influenced by anhedonia and cynicism, and depression, with heightened substance use and suicide rates. In comparison, findings were noted between US and Spain for similar heightened drug use for self-medication in post-COVID-19 pandemic. This allowance of mental health days supported by the certified school professional will provide the elimination of the need for medical leave and enhance the mental health outcome and academic performance of the individual.

These preliminary findings are just the start of my inquisitive nature which I will use as an inclination to pursue graduate studies and contribute more information to the knowledge repositories for mental health problems in educational domains.

Investigating a Neurological Imbalance of Excitation and Inhibition in Kabuki Syndrome Type 1

Isabella Wiebelt-Smith
Biological Sciences Research Experiences for Undergraduates (BioREU)

Mentor, Faculty Advisor:
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Christopher Patzke, John M. and Mary Jo Boler Assistant Professor,
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Abstract

Kabuki Syndrome is a rare neurodevelopmental disorder that causes facial deformation, developmental delay, and intellectual disability. 50-70% of cases are caused by a mutation in *KMT2D* and are considered to be Kabuki Syndrome Type 1 (KS1). *KMT2D* codes for a lysine-specific methyltransferase that operates as part of the ASCOM complex to promote open chromatin states. The Patzke lab has shown that neurons from a KS1 mouse model have increased synapse counts and higher amounts of the vesicular GABA transporter. We hypothesize that the KS1 genotype leads to an imbalance of excitation and inhibition as well as changes in presynaptic and postsynaptic terminal counts in mouse neurons.

In order to investigate this hypothesis, we infected KS1 mouse neurons with a lentivirus to express a fluorescent calcium reporter protein. We then used calcium imaging of these neurons to examine their electrical network activity. These results show an increase in asynchronous calcium transients. Additionally, we are currently using immunocytochemistry to determine levels of the inhibitory neuron markers Necab1, Somatostatin, and Parvalbumin.

By characterizing the KS1 phenotype in neuronal cell culture, we are contributing to the knowledge base surrounding this rare disease and eventual development of therapies to rescue the phenotypes observed. This information also provides insight into the impacts of disruption of the ASCOM complex, whose elements are associated with Kabuki Syndrome Type 2, Spastic Paraplegia, Retinoblastoma, AIDS Dementia, and Rubenstein Taybi syndrome.

For Us By Us: A Multi-step Approach to Developing a Community-Based Suicide Prevention Program for Black Youth and Families

Sequoia Williams
Research Access and Mentoring Program (RAMP)

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Frank Spesia, Associate Director of Community Health and Clinical Partnership;
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Taylor R. Nicoletti, Assistant Clinical Professor, Department of Psychology
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Abstract

Suicide rates in the U.S. have risen by 33% in the past two decades (Centers for Disease Control and Prevention, 2021). Although nearly all demographic groups have been affected, an especially steep increase (66%) has occurred among 10- to 17-year-old Black American youth (CDC, 2021; Hedegaard, Curtin, & Warner, 2020). Namely, Black youth are significantly more likely to die by suicide than their non-Black same-age peers (Sheftall, et al 2022).

Factors such as a family history of suicide, a pediatric diagnosis of ADHD, and exposure to systemic racism, interpersonal discrimination, and violence uniquely amplify the risk of suicidal behavior among Black youth (Baffoe-Bonnie, 2013) The historical mistrust of the healthcare system, stemming from unethical practices like the Tuskegee syphilis study, often leads Black youth to seek support from religious and community elders rather than mental health professionals (Assan et al., 2020).

To bridge the gap in the literature and meet the need for prevention programming, researchers partnered with the Boys and Girls Club of St. Joseph County and local community youth and adults to develop a suicide prevention initiative called Connect to Protect. This poster aims to demonstrate the multi-step process of developing C2P from a community-based research participatory lens. The process generally included three primary steps in development and collaboration with three groups: 1. Expert Advisory Board, 2. Adult Community Advisory Board, and 3. Youth Community Advisory Board.

A Job Well Done: Promoting Ethical Decisions Through Work Meaningfulness

Jemima Yoon
Summer Research Opportunities Program (SROP)

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Jason Colquitt, Franklin D. Schurz Professor of Management, Management & Organization
Mendoza College of Business

Abstract

Interpersonal relationships can influence the ethicality of decision making processes in both positive and negative ways. Previous research has often focused on how unethical behavior is driven by moral disengagement or specific personality traits. Our research examines the role of work meaningfulness in mediating the effect that close coworker relationships have on unethical decision making. We find that the closer people are to their coworkers, the more meaning they find in their work, reducing unethical decisions. This is likely because people are more engaged with their work when they find it meaningful. We also find that ethical leadership significantly moderates the relationship between meaningful work and unethical decision making such that the relationship is more negative when ethical leadership is high and less negative when ethical leadership is low. Our research suggests that organizations should focus on cultivating closer relationships between employees and more clearly communicating ethical values through their leadership to promote more ethical decisions in the workplace.

Electrodialysis for the Recovery of Rare-Earth Ions Utilizing Bare and Coated Nafion Membranes

Oscar Zavala
Soft Materials for Applications in Sustainability and Healthcare (SMASH) Engineering REU

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Abstract

Rare-earth elements (REEs), composed of 15 lanthanides plus Y and Sc, are important components of high-flux magnets, optical fibers, fluorescent lamps, and catalytic converters.The demand for REEs has dramatically increased during the past few decades, mostly because of their use in green technologies such as electric vehicles (Dy and La), wind power (Nd), and energy-efficient lighting (La, Gd, Tb, and Eu). In nature, REEs occur together in numerous ores and accessory minerals as either minor or major constituents. Isolating the REEs from other elements using techniques such as multi-stage solvent extraction processes produce copious amounts of contaminated water and require many steps. Membrane-based ion separations are potentially attractive because they may occur continuously without the need for additional reagents, and they may have low energy costs. We proposed a new electrodialysis model that combines a bare nafion membrane and a polyelectrolyte coated nafion membrane to selectively separate rare earth metals from from monovalent cations with high electrodialysis selectivity. In our electrodialysis setup, both REEs and impurities can pass through the first bare nafion membrane, but only the impurities can go through the polyelectrolyte coated membrane so that high selectivity can be achieved in the accumulation cell. Moreover, the concentration of rare earth metals can reach to ten times higher than its original feed solution in the accumulation cell. We anticipate our method can be a starting point for efficient and environmental-friendly separations of REEs. For example, after dissolving REE ores from nature, this method can isolate REEs from monovalent cations such as Na and K effectively. In this way, we can have pure REEs for downstream production of various electric devices.

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