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Midstates Consortium for Math and Science Undergraduate Research Symposium

Physical Sciences, Mathematics and Computer Science Washington University in St. Louis

November 11 & 12, 2022

	Program Schedule	
	Friday, November 11	
1:00 – 5:30 pm	Midstates Check-in at Clayton Plaza Hotel 7750 Carondelet Ave, Clayton, MO 63105	Clayton Plaza Lobby
5:30 – 5:45 pm	Introduction and Comments Professor John Bleeke, Symposium Organizer Washington University in St. Louis	Hotel Grand Ballroom
	Ed Hansen, Director Midstates Consortium for Math and Sciences Hope College	
	2022 Janet Anderson Lecture	
5:45 – 6:45 pm	Shonda Kuiper	Hotel Grand Ballroom
6:45 -7:45 pm	Banquet	Hotel Grand Ballroom
7:45 – 8:45 pm	2021 Janet Anderson Lecture Dwight Stoll	Hotel Grand Ballroom
Following lecture	Group Picture	Hotel Grand Ballroom

Saturday, November 12 All Saturday events are at Wrighton Hall, WUSTL campus

Starts at 7:00 am	Breakfast at hotel	Clayton Plaza Lobby
7:45 - 8:00 am Bus leaves at 8:00 & 8:15 am	Load bus and vans. Bring luggage if leaving Saturday. There is a secure room for luggage and posters at the meeting site. Those with vans or cars will drive to campus. Windy City bus will return for final load.	Clayton Plaza Lobby
8:30 – 9:00 am	Coffee, tea, and water available Check rooms for Session I Oral presentations	Outside Wrighton 250
9:00 – 10:00 am	Keynote Speaker—Professor Kade Head- Marsden, Department of Chemistry, Washington University	
10:00 – 11:00 am	Session I Oral Presentations of Student Papers Session I.A: (Mathew Wright) Session I.B: (Margaret Koker) Session 1.C: (Tom Stojsavljevic)	Wrighton Hall Room 250 Room 300 Room 201
11:00 – 11:15 am	Break, set-up posters for Poster Session I Check rooms for Session II Oral presentations	
11:15 am – 12:00 pm	Session 1 Poster Presentations (19)	Rettner Gallery & 3 rd floor
12:00 – 1:40 pm	Lunch and panel discussion on "Life in Graduate School"	Holmes Lounge
1:40 – 1:55 pm	Set-up posters for session 2	Rettner Gallery & 3 rd floor
1:55 – 2:40 pm	Session 2 Poster Presentations (19)	Rettner Gallery & 3 rd floor
2:40 – 3:40 pm	Session II Oral Presentations of Student Papers	Wrighton Hall
	Session II. D: (Stuart Kurtz) Session II. E (Amanda Bowman) Session II. F (Paul Fischer)	Room 250 Room 300 Room 201
3:40 – 3:55 pm	Break, set-up posters for Poster Session III	
3:55 – 4:40 pm	Session 3 Poster Presentations (19)	Rettner Gallery & 3 rd floor
4:40 – 5:00 pm	Meeting Concludes Complete online evaluations, those who ordered will pick-up box meals	Wrighton Hall



2022 Janet Andersen Lecture

The Challenges of Making Decisions with Data

Dr. Shonda Kuiper Professor of Mathematics and Statistics Grinnell College, Grinnell, IA

ABSTRACT

We live in an increasingly data-rich world. With this trend has come an increasing need for people who can understand and analyze data. This growing interest in data has also led to tremendous growth in statistics enrollments at the high school, undergraduate, and graduate levels. While this growing interest in data analysis sounds great, I argue that many researchers are still failing to address core issues that are essential for making data-based decisions. In this talk, I provide examples of the misuse of data in the media and published research. I also discuss examples that demonstrate how easy it can be to inadvertently draw misleading conclusions.

ABOUT DR. KUIPER: Dr. Kuiper has been recognized as a leader in statistics education, developing lab-based curricula that have allowed colleagues across the world to access research-like activities for their students through her National Science Foundation grants, publications, textbook, and Stat2Labs website. She also has an outstanding record as a research mentor for undergraduate students. All of her courses involve group research projects and she encourages her students to submit their projects to the Undergraduate Statistics Project Competition (USPROC). Since 2014, twenty-eight of her groups of students have won USPROC awards, which is more than any other faculty member in the history of the award. Between the summers of 2017 and 2021, she mentored a total in forty-four individual research students as part of Grinnell's Mentored Advanced Projects (MAPs) program. In the last two years, seven groups of her MAPs students have presented their research at professional conferences. Particularly relevant to the Janet Andersen award is the fact that she has mentored student projects from a variety of majors including mathematics, computer science, biology, biochemistry, economics and sociology.

2021 Janet Andersen Lecture



Research in Multi-Dimensional Separations – A Platform for Undergraduate Discovery in Multiple Dimensions

> Dr. Dwight Stoll Professor of Chemistry Gustavus Adolphus College

ABSTRACT

Liquid Chromatography (LC) is one of the most frequently used analytical tools in broad range of study areas ranging from environmental science to biopharmaceutical analysis. It is capable of first separating, and then quantifying and/or identifying, molecules across a remarkable range of properties (e.g., monosaccharides to vaccines). However, in many disciplines there is no end to challenges presented to chromatographers. Many times, biologists, biochemists, environmental scientists and others would like more information than conventional LC can provide. In these cases we turn to two-dimensional LC (2D-LC), a 40-year old technique that has only begun to flourish. In this presentation I will survey our work on 2D-LC over the past decade, and highlight recent advances that are having broad impact on the direction of the field. Additionally, I will provide examples of how our studies of the details of 2D-LC have provided many undergraduates to discover where their passions lie, ranging from computer science to physics and biochemistry. Finally, and perhaps most importantly, I will reflect on the origins of the ideas that have led to the most impactful aspects of our research. Developing the habit of consistently and insistently asking "why" can lead a researcher down unexpected and rewarding paths.

ABOUT DR. STOLL: The writer of the nomination letter for Dr. Stoll noted that "His research lab is not just open to the 'best and the brightest'. He is willing to offer an opportunity to any student who expresses a genuine curiosity about science and even seeks out students who have a glimmer of scientific potential. In other words, Dwight pays attention to his students and realizes their potential before they realize it themselves." One measure of Dr. Stoll's success as a research mentor is that 21 of the roughly 60 undergraduate research students he has worked with have been co-authors on his scientific papers. Another measure of the quality of his scholarly work as a separation scientist focused on liquid chromatography is his appearance on The Analytical Scientist's 'Top 100 Analytical Scientists' 2019 Power List. Dr. Stoll is also known as a skillful and dedicated teacher with strong interests in curricular and pedagogical innovation. He has provided outstanding service to both his scholarly and campus community, particularly during the pandemic crisis of the past year when he served as chair of the COVID Gustavus Adolphus faculty emergency planning committee and held a position on college-wide COVID leadership team



Information about the Janet Andersen Lecture Award

Professor Janet Andersen was a beloved faculty member in the Hope College Mathematics Department and served enthusiastically as the Midstates Consortium Director for five years before her life ended tragically in an automobile accident in November 2005. As a teacher and scholar, Janet was devoted to providing creative, high quality learning experiences for her students, and she herself was always learning as she was teaching. As Consortium Director, she looked for ways to connect with and support natural science faculty, both new and experienced.

To honor Janet's work with students and faculty in her teaching, research and service to the Consortium, the Janet Andersen Lecture Award was established in 2008. Each year, two faculty nominees from Consortium institutions are selected by the Executive Committee to present the Janet Andersen Lecture at one or both of the fall Undergraduate Research Symposia on a topic of his or her expertise.



Keynote Address

Chemistry at The Intersection of Quantum Sciences

> Professor Kade Head-Marsden Department of Chemistry Washington University

ABSTRACT

Accurate modelling of energy transport is critical to understanding important chemical processes such as photosynthetic light harvesting. The molecular complexes involved in these processes are often large and experience complicated environmental interactions, presenting several obstacles for accurate theoretical treatment. One method of approach is through the lens of open quantum systems, where a small subset of the entire complex is treated under the influence of its environment. This perspective can effectively minimize the active space of interest to be treated at a high level of theory, while also capturing environmental interactions and effects. Recent progress in quantum computation has illuminated a complementary method of approaching molecular energy transport. Quantum computers and algorithms offer a route to consider both static and dynamic properties of molecular complexes, with the potential for reduced computational cost. Here, I will discuss progress in both classical and quantum mechanical method development to treat energy transport accurately in molecular and condensed matter systems. The intersection of methods from open quantum systems and electronic structure theory, combined with classical and quantum computational resources, has the potential to provide a unique and holistic perspective on important chemical properties and processes.

	Oral Session i Schedule			
SESSION I.A: 10:00 - 11:00 am Room: 250 Moderator: Mathew Wright				
Session # Presenter Name Institution Title of Presentation				
I.A.1	Thai-Nam Hoang	Beloit College	Wildfire Forecasting with Satellite Images and Deep Generative Model	
I.A.2	Dylan Laurianti John Tobin	Grinnell College	Coarse-Grained Networks	
I.A.3	Khan Henderson	St. Olaf College	Utilizing Awareness of Surroundings to Reduce Network Disruption While Maximizing Coverage in Multi-Robot Exploration	

Oral Session I Schedule

SESSION I.B: 10:00 – 11:00 am Room: 300 Moderator: Margaret Koker			
Session #	Presenter Name	Institution	Title of Presentation
I.B.1	Katelyn Espe	Gustavus Adolphus College	Search for the Z' boson in events with four top quarks at CERN
I.B.2	Aidan Cloonan	University of Chicago	Formulating a selection function for DES galaxy-galaxy strong lense
I.B.3	Benjamin de Jonge	Washington University in St. Louis	Simulating Spectra for the Advanced Particle- astrophysics Telescope
I.B.4	Erin Coleman Anne Monroe	Gustavus Adolphus College	Listening to the radio sounds of space as a method to detect extrasolar moons

SESSION I.C: 10:00 – 11:00 am Room: 201 Moderator: Tom Stojsavljevic			
Session #	Presenter Name	Institution	Title of Presentation
I.C.1	Shannon Kim	University of Chicago	D-RNA selects L-amino acids in a newly characterized aminoacyl-RNA loop ligation
I.C.2	Daniel Lewinsohn	Colorado College	Consensus Label Propagation with Graph Convolutional Networks for Single-Cell RNA Sequencing Cell Type Annotation
I.C.3	Deepthi Kailash	Washington University in St. Louis	Spatial Allocation Rules in the Eukaryotic Cell
I.C.4	Emily Nigro	University of Chicago	Adaptive failure and its impact on taxonomic and morphologic diversification of burrowing marine bivalves

Oral Session II Schedule			
SESSION II.D: 2:40 – 3:40 pm Room: 250 Moderator: Stuart Kurtz			
Session #	Presenter Name	Institution	Title of Presentation
II.D.1	Barry Henaku	Washington University in St. Louis	Good ABC Triples and Good Elliptic Curves
II.D.2	Jessica Cao	University of Chicago	Erdös Distance Problems
II.D.3	Abigail Engbrecht Avi Rajan	St. Olaf College	A combinatorial description of Kostka-Foulkes polynomials in all classical types
II.D.4	Lauren Tsai	University of Chicago	Cardinal numbers and Boolean algebras

SESSION II.E: 2:40 – 3:40 pm Room: 300 Moderator: Amanda Bowman			
Session #	Presenter Name	Institution	Title of Presentation
II E.1	Joseph Geniesse	University of Chicago	Ytterbium-doped lead-free quantum cutting perovskites to improve the efficiency of silicon solar cells
II E.2	Isabella Aase	Gustavus Adolphus College	Comparison of Retention Factors Obtained using Long and Short Columns in Liquid Chromatography
II E.3	Andrew Shanahan	Lawrence University	Capturing Brownian Motion with an Open- source Microscope
II.E. 4	Chengyu Tang	University of Chicago	Novel carbazole-based semi-ladder polymer with optimized photoelectric properties

SESSION II.F: 2:40 – 3:40 pm Room: 201 Moderator: Paul Fischer			
Session #	Presenter Name	Institution	Title of Presentation
II. F.1	Kabir Dubey	University of Chicago	Differentiable Preisach Modeling for Characterization and Optimization of Particle Accelerator Systems with Hysteresis
II.F.2	Erin Beer Kathryn Cash	Gustavus Adolphus College	Researching the potential of activated carbon to reduce inorganic mercury bioavailability in mesocosms
II.F.3	Lauren Bryan	Hope College	Selective Preservation of Structural Carbohydrates During Peat Formation
II.F.4	Annie Corbett	Gustavus Adolphus College	Nonsense-Mediated Decay of CEP3 mRNA

11:15 a.m. – 12:00 noon Room: Rettner Gallery & 3 rd floor hallway			
Poster #	Presenter Name	Institution	Title of Presentation
P1.01	Caitlin Abreu Tanmaie Kailash Han Xie	Grinnell College	Predicting Pathogen Zoonosis with a Multilayer Network
P1.02	Hasif Ahmed	Lawrence University	Network Theory using Quantum Techniques
P1.03	Sullivan Fitz	University of Chicago	Chiral Liquid Crystals in Microfluidic Environments
P1.04	Will Asinger	St. Olaf College	Mapping Japanese satoyama with socio- ecological data
P1.05	Justin Douty	Knox College	Using Audio To Teach Heterogeneous Computing
P1.07	lan Huelsbeck Samantha Ries	Colorado College	Consistent method for the detection of perfluorooctanesulfonic acid utilizing a molecularly imprinted polymer
P1.08	Alexandra Hurd	Macalester College	Measuring charge lifetimes in organic solar cells
P1.09	Khang Vo Huynh	St. Olaf College	Cloud-powered PDC Computation for a Runestone interactive Textbook
P1.10	Shiva Iyer	Washington University in St. Louis	Heat sensing in biological systems using NV defects in Diamonds
P1.11	Julianne Lampert	Washington University in St. Louis	Nanoconfinement of Electrodeposited Nickel Oxide Catalysts in Porous Antimony Tin Oxide
P1.12	Nhan Nguyen	Beloit College	Multi-site stimulation of globus pallidus and subthalamic nucleus in treating biophysical network of Parkinson's disease
P1.13	Mark Jareczek	Washington University in St. Louis	A Survey of New Metals and Demetallation Strategies for Use In Catenane Cross-linked Gels
P1.14	Nicolò Petroccione	Beloit College	Implementation of adaptive multi site local field potential deep brain stimulation in STN and GPe
P1.15	Angelina Minocha	Washington University in St. Louis	Web-Based visualization tool for interpretation of quantitative EPMA imaging
P1.16	Jonah Pratt	Grinnelll College	Design, synthesis, and biological testing of antimicrobial peptide derivatives
P1.17	Will Rosenberg	Washington University in St. Louis	Training a Feed-Forward Neural Network to Solve the S-wave Nucleon-Nucleon Scattering Problem

Poster Session P1

P1.18	Anna Teurman	Gustavus Adolphus College	A Probabilistic Model of Mantle Transition Zone Discontinuities from Auto-picked Precursor Data
P1.19	Alexandria Weary	University of Chicago	Energy of rare gas cluster implosions maximized by cluster size/configuration and ionization variables

1:55 p.m. – 2:40 p.m. Room: Rettner Gallery & 3 rd floor hallway			
Poster #	Presenter Name	Institution	Title of Presentation
P2.01	Jessica Berkman	Washington University in St. Louis	Search for an S-wave Resonance in ⁷ Li just Above the Proton Decay Threshold
P2.02	Shamika Bhandarkar	Washington University in St. Louis	Engineering enhanced Hsp104 NBD1 variant disaggregases using next-generation sequencing-based selections.
P2.03	Tenzin Choedon Stacie Elliott Chanjin Park	St. Olaf College	Dissolvo, an accurate method for estimating mutational signature contributions
P2.04	Andnet DeBoer	Hope College	Multi-unit robotic systems
P2.05	John Georgiades	Washington University in St. Louis	Development of Hydrophobic Cycloguanil Derivatives as Cell Permeable Inhibitors of Bacterial Dihydrofolate Reductase
P2.06	Rowen Glusman Isaiah Escapa, Rachel Kovach- Fuentes	University of Chicago	A Comparative Analysis of Glass Plate Digitization Methods Using Stellar Variability
P2.07	Tuan Huynh	Lawrence University	X-ray Fluorescence (XRF) Analysis on The Coins in the LU Wriston Gallery Collection.
P2.08	Mohammad Tanzil Idrisi	Beloit College	CapsNet for classification of infected vs normal patches in biomedical image segmentation
P2.09	Reagan Keeney	Knox College	Quantifying nationalism online via stance detection
P2.10	Zihao Yu	Grinnell College	FNI App: An expert-centered knowledge dashboard to support multidisciplinary research
P2.11	Tyler Meeks	Grinnell College	Synthesis and characterization of phenylated Ni(II) bis(thiosemicarbazone) compounds for CO2 reduction
P2.12	Tracey Nelson	St. Olaf College	Characterization of Methyl Substituted N2P2 First Row Transition Metal Complexes
P2.13	Phuc Ngo	Beloit College	Is CLIP Fooled by Optical Illusions?
P2.14	Anusha Vajrala	Colorado College	Switching the Reactivity of Pyruvate Formate- Lyase-Activating Enzyme to Epimerization with Single Mutation
P2.15	Andrew Valentini Kaitlyn Prokup Rebecca Dowe	Carthage College	Modeling Binary Compact Object Merger Events Detected by the LIGO and Virgo Gravitational Wave Observatories

Poster Session P2

P2.16	Emilio Rosas Linhard	University of Chicago	Silicon Integrated Microfluidics for Microbial Genomics
P2.17	Ronan Wallace	Macalester College	Using Remote Sensing in Relocating Lubra Village and Visualizing Flood Damages in Nepal
P2.18	Selina Wang, Olivia Lazorik, Gianna Glenn, Shiva Iyer	Washington University in St. Louis	Probing the thermal distribution inside yeast cell using nanodiamond as quantum sensor
P2.19	Diya Gandhi	University of Chicago	Discovery and direct enhanced sampling of solvent-inclusive atomistic CVs using autoencoder embeddings in n- Pentatetracontane(C45) system
P2.20	Brian Sun	Washington University in St. Louis	Amyloid fiber remodeling observed by single- molecule nanoscopy is correlated with the orientation of amyloidophilic dye molecules.

3:55 p.m. – 4:40 p.m. Room: Rettner Gallery & 3 rd floor hallway						
Poster #	Presenter Name	Institution	Title of Presentation			
P3.01	Sadeen Alsabbagh	Beloit College	Sami Calendar and Accurate Time Measurements			
P3.02	Polina Barzova	Washington University in St. Louis	Synthesis of densely functionalized heterocyclic building blocks from chiral lactols			
P3.03	Adam Brohl	Knox College	C Star Programming Language			
P3.04	Sabrina DelBello	Washington University in St. Louis	Cross Correlation of tSZ with Galaxy Density to Constrain the Gas Pressure of the Universe			
	Withdrawn					
P3.06	Federico Fiorda	Gustavus Adolphus College	Pebble Survey Conducted in Jezero Crater, Mars (Sols 350-399)			
P3.07	Bryan Forrest	Hope College	Development of directing groups for rhodium- catalyzed decarbonylation reactions			
	Withdrawn					
P3.09	Diangen Lin	University of Chicago	Accelerating deep learning-mediated protein design with a synthetic sequence evaluation pipeline			
	Withdrawn					
P3.11	Swagat Malla	St. Olaf College	Generalized Fibonacci Polynomial Identities			
P3.12	Sarah Olsen	Washington University in St. Louis	Adding Solubilizing Alkyl Chains to Self- Complementary Urea-Based Arrays			
P3.13	Auras Khanal	Beloit College	Comparative Analysis of First and Second Order Optimization Methods in Neural Networks			
P3.14	Shivani Chatterji	University of Chicago	Understanding the Interactions Amongst Constituents in Suspensions for Tape/Freeze- Cast Battery Separators			
P3.15	Marya Wydra	Lawrence University	Towards a quinoxaline-based anti-parasitic drug via click chemistry			
P3.16	Matthew Yu	Washington University in St. Louis	X-rays from Cygnus X-1 reveal structure of stellar gas			

Poster Session P3

P3.17	Yiren Zhang	Colorado College	Phytochemical Characterization of Ninety-Two Rosinweed (Silphium Integrifolium) Genotypes
P3.18	Steven Labalme	University of Chicago	Site isolation in metal-organic layers enhances photoredox gold catalysis

Abstracts for all Sessions Physical Sciences, Mathematics and Computer Science MCMS Undergraduate Research Symposium, Washington University in St. Louis November 11-12, 2022

All abstracts (poster and oral) are listed alphabetically by presenter last name. Abstracts with multiple presenters appear only once with first listed presenter. An alphabetical list of all meeting participants and their respective poster session or oral presentation number follows the abstracts.

Presenter(s): Isabella Aase
School: Gustavus Adolphus College
Session: Oral II E.2
Title: Comparison of Retention Factors Obtained using Long and Short Columns in Liquid Chromatography
Advisor(s): Dwight Stoll, Chemistry, Gustavus Adolphus College

Abstract HPLC is a method of analytical chemistry that measures the retention time of a compound. This is used to identify, characterize, and purify chemicals in numerous industries. Traditionally, this is done using 100mm columns (composed of a specific chemical environment), and measurements may take hours. By using a shorter 5mm column, these data points can be collected in minutes. Some current results using a short C3-type column followed a different trend in retention factor vs. mobile phase composition than has been found using long C18-type columns. We investigated if the differences were due to column age or a property of the short column. The long C3-type column exhibited a trend similar to the short C3-type column, but the measurements themselves differed. Some compounds had over 50% different retention time between long and short columns. We found that retention time decreased as the column aged. When replaced with a new column, retention time increased to similar to that of early measurements with the original column. However, data using a new short column differed from data using a new long column. This suggests that there may be significant differences between the stationary phases used by manufacturers to prepare long and short columns.

Presenter(s): Caitlin Abreu, Tanmaie Kailash, Han Xie
School: Grinnell College
Session: Poster P1.01
Title: Predicting Pathogen Zoonosis with a Multilayer Network
Advisor(s): Nicole Eikmeier, Computer Science, Grinnell College
Co-Author(s): Luke Klein-Collins, Cheryl Andam, Tavis Anderson,

Abstract The ongoing COVID-19 pandemic demonstrates the need for research into predictive models for pathogen zoonosis that allows healthcare systems to prepare for, and mitigate, the effects of such pandemics. In this work, we hypothesis that zoonotic pathogens jump host species due to either genetic or functional trait similarity between pathogens. To capture interspecies transmission and determine how predictive each hypothesized factor is, we use a multi-layer network consisting of a host and pathogen layer using data on

Staphylococcus Aureus. The host layer shows interspecies transmissions between hosts, whereas the pathogen layer shows genetic similarity between different strains. The multilayer network combines these two networks into one by linking the hosts and the strains that occur in them. While findings in each layer are uninteresting, humans tended to cluster away from all the other hosts in the multilayer network while strains are more central when they are genetically like other strains and occur in many hosts.

Presenter(s): Hasif Ahmed School: Lawrence University Session: Poster P1.02 Title: Network Theory using Quantum Techniques Advisor(s): Scott Corry, Mathematics, Lawrence University Co-Author(s): Brett Schneider

Abstract: Stochastic systems can be represented in networks whose underlying dynamics are explored using techniques we borrow from Quantum Field Theory (QFT). We begin by expressing the observable changes in epidemiological models, chemical reactions and population growth models using differential equations under a deterministic framework. We then introduce the master equation under a probabilistic framework and extend the Anderson-Craciun-Kurtz (ACK) theorem to the case of spatial dynamics. Annihilation and creation operators from QFT are borrowed to track the dynamics in some simple examples of pandemics and chemical reactions. We ultimately investigate properties of the hamiltonian operators used while extending the ACK theorem.

Presenter(s): Sadeen Alsabbagh
School: Beloit College
Session: Poster P3.01
Title: Sami Calendar and Accurate Time Measurements
Advisor(s): Tom Stojsavljevic and Mehmet Dik, Mathematics, Beloit College and Rockford University

Abstract: The Hijri and the Julian calendars are the two calendars in regular use in the Muslim world, corresponding respectively to the lunar and solar calendars. Islamic rituals are directly based on the hijra as the historical landmark marking the beginning of the era for the spread of Islam and the establishment of the new Muslim polity. The Muslim experience of colonization and imposition of the Julian calendar resulted in the marginalization of the Hijri calendar. Consequently, many events are not known by the Muslims by their Hijri date. For time measurements to be accurate, convictions and variables must be consistent such as the zodiac calendar and the length of a year. In the Sami calendar, the constant variables are the synchronization between the sun and moon movement and a third star on the zodiac line based on the time of the year. These movements are consistent and the time discrepancies are accommodated through the addition of a solar month to the Sami Calendar every two years and eight months. This research aims to synchronize the lunar, solar calendars, and the zodiac line to generate new methods to accurately chronicle these events independent of the existing calendar systems.

Presenter(s): Will Asinger **School:** St. Olaf College

Session: Poster P1.04 Title: Mapping Japanese satoyama with socio-ecological data Advisor(s): Paul Jackson, Katherine Tegtmeyer Pak, Environmental science, St. Olaf College

Abstract: Japanese farmers traditionally practice mosaic land use patterns, known as satoyama, that may hold global lessons for sustainable living. Where are satoyama in Japan today? Identifying satoyama systematically across space and time poses difficulties, in part because the scholarly work lacks a quantitative framework and a transdisciplinary perspective. We compile a novel spatially-linked dataset of 200 variables across 150,000 administrative units and analyze nine case studies. Exploring various model-building techniques allows us to (1) connect the social and ecological dimensions of satoyama and (2) define it in contrast to urban areas and deep mountain forests. We train a final multinomial logistic regression model on our case studies, then extend it to classify the entire land area of Japan in order to identify novel satoyama. Incomplete datasets and case studies grounded upon incommensurate interpretations of complex social phenomena limit our model. Additional qualitative research will further our understanding of satoyama's relationship to global sustainability.

Presenter(s): Polina Barzova School: Washington University in St. Louis Session: Poster P3.02 Title: Synthesis of densely functionalized heterocyclic building blocks from chiral lactols Advisor(s): Kevin Moeller, Chemistry Department, Washington University in St. Louis

Abstract: The project's goal is the synthesis of new C-glycosides with defined stereochemistry using electrochemical tools. There are two main incentives in developing a straightforward route to C-glycoside building blocks. Natural C-glycosides are common bioactive molecules, and synthetic C-glycosides are often used as therapeutic targets since they can escape endogenous hydrolytic enzymes. The Miller and Lin Groups developed a method for creating chiral lactols, which can be used as a starting point for synthesis of complex C-glycosides using electrochemical oxidative cyclization reactions. The first step in the synthesis is the Wittig reaction, which introduces an electron-rich double bond. The Wittig reaction is followed by the Mitsunobu reaction that substitutes the alcohol group with sulfonamide. In the last step, the electrical current is applied to oxidize an electron-rich, normally nucleophilic olefin to produce a radical cation that triggers an intramolecular cyclization reaction with the nucleophilic sulfonamide. The reaction is completed by the second oxidation step and trapping of a cation by a methanol. So far, a cyclic pyrrolidine derivative, containing two oxygen substituents along with an aromatic side chain, was successfully synthesized. A similar reaction can be triggered by the oxidation of vinyl sulfide. The sulfur group will be deprotected to yield the aldehyde, which provides a convenient chemical handle for further functionalization of the C-glycosides building blocks.

Presenter(s): Erin Beer, Kathryn Cash **School:** Gustavus Adolphus College

Session: Oral II.F.2

Title: Researching the potential of activated carbon to reduce inorganic mercury bioavailability in mesocosms

Advisor(s): Jeff Jeremiason, Chemistry & Environmental Studies, Gustavus Adolphus College

Abstract: Despite stringent efforts to regulate mercury levels in the environment, contamination in waterways is the most commonly observed source of mercury pollution today. Large-scale remediation of Hg is cost-prohibitive and largely inefficient, thus alternative solutions are needed. Activated carbon (AC) is a chemical intervention being considered as a sediment amendment to manage pollutants in aquatic environments. Utilization of AC by Bussan et al. has shown promising small-scale results in which the reduction of mercury bioavailability was achieved; however, little experimental research has been done using AC in large-scale mesocosms. Our research works to bridge that gap and addresses the potential AC has to reduce mercury bioavailability in mesocosms. The 100gallon mesocosm environments are ecologically and hydrologically diverse and are designed to mimic periodic flushing from tidal-like mixing. Conditions are controlled but complex compared to previous mesocosm studies with single organisms and a static water column. Initial results demonstrated reduced methylmercury concentrations in sediment (solid phase), pore water, surface water, and biota when comparing amended mesocosms to control conditions. Recent preliminary results demonstrate a more modest reduction in methylmercury concentrations in some but not all matrices. Therefore, continued analysis is necessary before definitive conclusions can be made.

Presenter(s): Jessica Berkman

School: Washington University in St. Louis

Session: Poster P2.01

Title: Search for an S-wave Resonance in ⁷Li just Above the Proton Decay Threshold **Advisor(s):** Lee Sobotka, Chemistry and Physics, Washington University in St. Louis **Co-Author(s):** Nicolas Dronchi, Robert J. Charity, Anthony Thomas, Jonathan Elson, Jack Bishop, Cody E. Parker, Brian Roeder, Antti Saastamoinen

Abstract: Near threshold resonances play an outsized role in nucleosynthesis and applied nuclear science. The study of nuclei removed from stability has greatly extended the list of resonances very close to decay thresholds. The No Core Shell Model with Continuum (NCSMC) recently predicted an S-wave resonance just above the proton decay threshold of ⁷Li at an excitation energy of 10 MeV [1]. The ⁶He(d,n) ⁷Li reaction was employed at the Cyclotron Institute at Texas A&M to selectively populate this resonance where 4 Δ E-E [Si-Si] telescopes were used to detect and identify the ⁶He+p fragments. For this experiment, the detector design, constraints, and setup are examined as well as some early invariant-mass results. This case of a near-threshold resonance is unique because it is not important for an astrophysical reaction pathway. It is only dependent on the quantum mechanics of the ⁶He+p fragments extended into the continuum

[1] M. Vorabbi, el al., Phys. Rev. C 100, 024304 (2019).

Presenter(s): Shamika Bhandarkar

School: Washington University in St. Louis

Session: Poster P2.02

Title: Engineering enhanced Hsp104 NBD1 variant disaggregases using next-generation sequencing-based selections.

Advisor(s): Meredith Jackrel, Chemistry, Washington University in St. Louis

Abstract: A native yeast protein, Hsp104, is a disaggregase that solubilizes and reactivates proteins trapped in aggregated states. We aim to engineer enhanced Hsp104 variants via mutations in the first nucleotide binding domain (NBD1), with the goal of generating variants that mitigate toxic misfolding of α -synuclein, TDP-43, and FUS implicated in neurodegenerative disorders (e.g., Parkinson's Disease, ALS). Using a comprehensive library of Hsp104 NBD1 variants comprised of mutations to all natural amino acids at each position in NBD1, we have identified variants that counter α -synuclein. TDP-43, and FUS toxicity. To do so, we used next-generation sequencing (NGS) to identify potentiated Hsp104 variants that display substrate specificity, and then validated these hits using a toxicity assay in a yeast model. The NGS revealed a wide range of possible substrate-specific trends across the domain. We find that several potentiated Hsp104 variants chosen from the NGS scan successfully mitigate α -synuclein, TDP-43, and FUS toxicity. We conducted degeneracy tests at positions with enhanced disaggregase activity to investigate the mutability of the protein. We suggest that increasing the substrate specificity of potentiated variants in NBD1 could be applied to generate finely tuned disaggregase therapeutics for fatal neurodegenerative diseases. (special characters required - alpha, α , symbol for α -synuclein)

Presenter(s): Adam Brohl School: Knox College Session: Poster P3.03 Title: C Star Programming Language Advisor(s): Ritwik Bose,Computer Science, Knox College

Abstract: C Star is a Turing complete esoteric programming language based on the mechanics of a Turing machine. The core of the language revolves around a tape, or list, of cells that each hold a single byte of information. The language allows the user to move along the tape, modify bytes, perform conditional operations, and handle data going in and out of the program. Like many other programming languages, C Star has variables, functions, and even polymorphism. The interpreter was written in Python with the aid of ANTLR, which automatically generates a lexer and parser to generate an abstract syntax tree allowing for complex syntax in the language.

Presenter(s): Lauren Bryan
School: Hope College
Session: Oral II.F.3
Title: Selective Preservation of Structural Carbohydrates During Peat Formation
Advisor(s): Michael Philben, Department of Geological and Environmental Sciences and
Department of Chemistry, Hope College
Co-Author(s): Erik Schoonover, Trevor Hile, Rachel Shaw, Ali Koehl, Grace Behrens,

Co-Author(s): Erik Schoonover, Trevor Hile, Rachel Shaw, Ali Koehl, Grace Behrens, Christian Lundy, Madison Smith, Mackenzie Dole, Madeleine O'Donnell

Abstract: Previous studies show the structural carbohydrate "sphagnan" plays a role in slowing the degradation of *Sphagnum* moss, resulting in carbon sequestration in peatlands. Sphagnan

is composed of a galacturonic acid and rhamnose backbone. It is currently unclear whether sphagnan persists beyond early-litter degradation and playsinto long-term preservation of

peatland organic matter. This study analyzed hydrolyzable neutral sugars, using rhamnose as a proxy for sphagnan content, and tracked concentration of rhamnose within moss before and after decomposition, and at different depth intervals within peat cores from southwest Michigan. An increase in relative abundance of rhamnose over moss decomposition was indicated, but little change occurred in rhamnose concentrations in peat cores compared to depth, implying that the degradation of sphagnan occurs at roughly the same rate of other sugars over long periods of time. However, an increase in glucose concentration occurred with depth, alongside decreasing xylose and arabinose abundances, indicating cellulose may be selectively preserved. Our results indicate that sphagnan plays a greater role in the shortterm preservation of *Sphagnum* mosses and sequestration of carbon, but this effect is not as prominent over long-term peat accumulation.

Presenter(s): Jessica Cao School: University of Chicago Session: Oral II.D.2 Title: Erdös Distance Problems Advisor(s): J Peter May, Mathematics, University of Chicago

Abstract Consider n points in a plane. What is the maximum number of pairs of points that are one unit distance apart? What is the minimum number of distinct distances between pairs of points? The former question is referred to as the unit distance problem and the latter is referred to as the distinct distances problem. These questions are considered twin problems proposed by Paul Erdös in 1946. Although simple questions, the search for answers has generated years of research into fields like discrete geometry, combinatorics, and number theory. In this talk, I will discuss known proofs on the current bounds of O(n^4/3}) proven by Spencer, Szemerédi, and Trotter on the unit distance question and \Theta(n/(log n)) (special character needed for big Theta) proven by Guth and Katz on the distinct distance problem. I will begin with an introduction to incidence theory and the methods used to show the bounds mentioned above, which include Székely's crossing inequality method and Guth and Katz's polynomial method. Then, I will show proofs for the best-known bounds and discuss open problems on improved bounds.

Presenter(s): Shivani Chatterji,
School: University of Chicago
Session: Poster P1.14
Title: Understanding the Interactions Amongst Constituents in Suspensions for Tape/Freeze-Cast Battery Separators
Advisor(s): Katherine T. Faber, Department of Applied Physics and Materials Science,
California Institute of Technology
Co-Author(s): Chun-Wei (Vince) Wu, Katherine T. Faber

Abstract: With safety issues at extreme operating conditions and depleting sources of lithium, non-lithium-ion batteries like sodium-ion batteries (SIBs) are promising. However, battery separators – a required component to separate the cathode and anode while still facilitating ion transfer – must be compatible with SIBs. Using tape/freeze-cast separators with tunable pore size, wettability, and ion transfer, the addition of ceramic nanoparticles (alumina, AI_2O_3) as reinforcements were shown to improve the mechanical properties and thermal stability of these separators. We focused on understanding suspensions composed

of alumina powders with or without sulfur, in dimethyl sulfoxide or water, with commercial dispersants used to reduce agglomeration of particles. The stability of these ball-milled suspensions was tested through sedimentation tests and particle size analysis. The compatibility between the solvent and alumina was assessed with a contact angle goniometer. The electrical characteristics of the suspensions were analyzed through electrophoresis deposition, electrical conductivity tests, and zeta potential measurements. The difference between sulfur-containing and pure alumina was explored by running Fourier transform infrared spectrometry and energy-dispersive X-ray spectroscopy. The dispersion of these suspensions were compared in order to provide guidance on the processing of battery separators.

Presenter(s): Tenzin Choedon, Stacie Elliot, Chanjin Park,
School: St. Olaf College
Session: Poster P2.03
Title: Dissolvo, an accurate method for estimating mutational signature contributions
Advisor(s): Jaime Davila, MSCS(Mathematics, Statistics, Computer Science), St. Olaf College

Abstract: The Catalogue of Somatic Mutations in Cancer (COSMIC) contains a curated set of mutational signatures generated from thousands of cancer patients. Different signatures are associated with unique mutational processes, for example, COSMIC SBS4 mutational signature is associated with tobacco smoking and is characterized by an abundance of C>A mutations. We are interested in estimating the contribution of a prescribed number of mutational signatures for a given sample. To solve this problem we proposed a method, dissolvo, based on linear regression with constraints. The constraints correspond to quantile information curated by COSMIC for each represented signature and cancer type. We found that the correlation between Dissolvo's output and the true proportion of sample profiles is 95% and the mean squared error (MSE) is 0.003. The correlation between Dissolvo and fit_to_signatures, a comparable method, is 99%. In conclusion, we provide an R function, Dissolvo, to estimate mutational signature contribution.

Presenter(s): Aidan Cloonan
School: University of Chicago
Session: Oral I.B.2
Title: Formulating a selection function for DES galaxy-galaxy strong lenses
Advisor(s): Anowar J. Shajib; Alex Drlica-Wagner, Kavli Institute of Cosmological Physics; Department of Astronomy and Astrophysics, University of Chicago

Abstract: Strong gravitational lensing is a powerful probe into the mass structures of distant galaxies and galaxy clusters. However, in studies of strong lenses to probe galaxy structure, we must assess whether strong lenses are representative of the general galaxy population or they form a biased subsample. Here, we investigate potential selection biases in a sample of 98 galaxy-scale strong lens candidates, identified in the Dark Energy Survey (DES). We model the surface brightness profile for all lensing galaxies and obtain best-fit values and uncertainties for photometric model parameters. We then draw a population of 8400 non-lensing luminous red galaxies (LRGs) from the DES imaging catalogs and apply our modeling

process to these galaxies. We explicitly draw this population to match our lens sample's distribution in photometric redshift and r-band half-light radius, minimizing self-induced selection bias. Several statistical comparisons between the two populations are then performed using a set of photometric observables from our model posteriors. Incoming results and uncovered selection biases will inform how we may infer properties of galaxy populations from a sample of lenses. We look to improve our techniques for lens-source deblending when fitting lensing galaxy surface brightness profiles, to increase our lens sample size.

Presenter(s): Erin Coleman, Anne Monroe
School: Gustavus Adolphus
Session: Oral II.B.4
Title: Listening to the radio sounds of space as a method to detect extrasolar moons
Advisor(s): Darsa Donelan, Physics, Gustavus Adolphus College

Abstract: The electromagnetic interaction between Jupiter and Io, its closest moon, causes bursts of radio waves that can be observed from Earth. These Io storms can be separated into three categories by the positions of Jupiter and Io into several types, each with distinctive characteristics. This project utilized two 15 meter dipole antennas and a radio receiver connected to a computer running spectrograph software to collect and record the intensity of radio waves across an 8 MHz spectrum during all three types of Io storms. In future, storm data will be used to train a deep learning model to search for extrasolar moons orbiting gas giants. A deep learning model needs a large dataset for training, so it is necessary to take every opportunity to record storm data. This can be difficult due to the timing of observable storms, which are typically in the nighttime or very early morning, as well as the quantity of data required, so this project also made preliminary steps toward incorporating a Raspberry Pi microcomputer to automate data collection.

Presenter(s): Annie Corbett School: Gustavus Adolphus College Session: Oral II.F.4 Title: Nonsense-Mediated Decay of CEP3 mRNA Advisor(s): Jeffrey Dahlseid, Biochemistry and Molecular Biology, Gustavus Adolphus College

Abstract: The appearance of a genetic trait depends on whether the corresponding gene is "expressed", a phenomenon that involves multiple molecular steps and DNA, RNA, and protein molecules. Messenger RNAs (mRNAs) are enzymatically synthesized and are copies of the genetic information stored in DNA that code for the synthesis of proteins, which provide structure, support, and facilitate movement for a cell. In addition to the synthesis of RNA and proteins, degradation of RNA also plays a role in gene expression, ultimately influencing the amount of protein and thus the degree of genetic trait that is apparent. For mRNA degradation, one important mechanism includes deadenylation-independent decapping (also called nonsense mediated decay, or NMD). NMD is a cell surveillance mechanism that accelerates the decay for many aberrant, and some non-aberrant mRNAs. In this study, we analyzed CEP3, a naturally occurring, non-aberrant mRNA degraded by NMD. We will present results testing and describing the enzymes involved and RNA features responsible

for NMD recognition of CEP3. Overall, our goal is to understand the determinants of molecular recognition for NMD.

Presenter(s): Benjamin de Jonge School: Washington University in St. Louis Session: Oral I.B.3 Title: Simulating Spectra for the Advanced Particle-astrophysics Telescope Advisor(s): James Buckley, Physics, Washington University in St. Louis

Abstract: This researched focused on developing a tool to simulate spectra for the currently in development gamma ray telescope Advanced Particle-astrophysics telescope (APT). Due to the unique nature of this endeavor and prior experience/familiarity, it was decided to use the highly programmable ISIS (Interactive Spectral Interpretation System) to perform this research. The process began with simulating particle events on the detector in a Geant4 simulation, then taking that data in the appropriate file formats into ISIS. From there, instrument response files, specifically ancillary response files (ARFs) and response matrix files (RMFs), were constructed from scratch to model APT's simulated effective area and energy resolution respectively. Ultimately, using functions within ISIS such as 'fakeit' and these response files, spectra were simulated for several astrophysical sources to show the advantages of APT in detecting such objects. Further simulation, such as looking into the dark-matter self-interaction cross section, is worth looking into. Moreover, moving the simulation to a more user-friendly environment (such as XSPEC or a website) would make it more accessible.

Presenter(s): Andnet DeBoer School: Hope College Session: Poster P2.04 Title: Multi-unit robotic systems Advisor(s): Miguel Abrahantes, Engineering, Hope College

Abstract: This work is intended to lay the foundation for a versatile multi-unit robotic system capable of implementing and testing advanced algorithms designed for robots operating on the ROS network. This system uses three Yujin Kobuki robots each equipped with a Raspberry Pi for processing and communication via a secure Wi-Fi network. The system implementation was run through an experiment in which each robot was equipped with two high-frequency ultrasonic sensors mounted at such an angle as to leave a blind spot in the robot's forward view. A simple obstacle avoidance program was written that failed in the instances when an object resided fully in the robot's blind spot. The robots were placed in an enclosure with cubes randomly scattered around and the program was allowed to run to completion. The blind spot in the ultrasonic sensor array allowed the robots to collide with the cubes and manipulate them creating interesting results. By the end of the experiment, all cubes were pushed against the walls of the enclosure or pushed against another cube. This demonstrates the ability of simple commands to achieve a higher-level task when working within a versatile multi-unit robotic system.

Presenter(s): Sabrina DelBello **School:** Washington University in St. Louis **Session:** Poster P3.04 Title: Cross Correlation of tSZ with Galaxy Density to Constrain the Gas Pressure of the Universe

Advisor(s): Andrina Nicola, Physics, Washington University in St. Louis

Abstract: In this project, our goal is to use cosmological tools and theory to set a constraint for the gas pressure of the universe. To do this, we are using the cross-correlation between the thermal Sunyaev-Zel'dovich effect (tSZ) and galaxy density by computing their spherical harmonic power spectra. By cross-correlating maps of the tSZ with maps of the galaxy density, we can put constraints on the thermal gas pressure and energy in the Universe and thus learn about astrophysical processes governing galaxy evolution and baryonic feedback effects. The CMB is relic electromagnetic radiation left over from the early universe. The tSZ is a secondary anisotropy of the Cosmic Microwave Background (CMB) that occurs when CMB photons undergo inverse Compton scattering with free, hot electrons in the intra-cluster medium. To compute the cross correlations, we are using data from the Atacama Cosmology Telescope (ACT) and the Hyper-Suprime Cam (HSC). ACT is a US National Science Foundation-funded telescope located in the Atacama Desert that saw first light in October of 2007. The HSC survey is an optical survey ran by the astronomical communities of Japan, Taiwan and Princeton University, and measures the positions and shapes of millions of galaxies.

Presenter(s): Justin Douty School: Knox College Session: Poster, P1.05 Title: Using Audio To Teach Heterogeneous Computing Advisor(s): David Bunde, Computer Science, Knox College

Abstract: As the speed of modern generations of computer processors approaches its limits, new hardware capabilities must be added to keep up with the industry's increasing demand for performance and energy efficiency in computing. This emerging style of heterogeneous computing requires new and innovative approaches to traditional computer programming to take advantage of this hardware, leading to a shift in the modern computing landscape. Many schools lack sufficient coverage of these concepts, leaving computer science-oriented students less prepared to excel in modern industry.

Over the summer, I focused on helping to diversify the materials available on heterogeneous computing, in which I designed a classroom-friendly assignment that involves the use of graphics cards (GPUs), and the MIDI audio format to generate music. Its purpose is to introduce students to GPU programming using CUDA, demonstrate the performance increase when using heterogeneous programming styles over their sequential counterparts, and show how GPU programming can be applied to use cases other than processing computer graphics. I hope this project can help capture interest in computer science, and expand the reach of heterogeneous computing concepts in schools.

Presenter(s): Kabir Dubey
School: University of Chicago
Session: Oral II. F.1
Title: Differentiable Preisach Modeling for Characterization and Optimization of Particle Accelerator Systems with Hysteresis
Advisor(s): Young-Kee Kim, Physics, University of Chicago

Abstract: Future improvements in particle accelerator performance are predicated on increasingly accurate, online modeling of accelerators. Hysteresis effects in magnetic, mechanical, and material components of accelerators are often neglected in online accelerator models used to inform control algorithms, even though reproducibility errors from systems exhibiting hysteresis are not negligible in high precision accelerators. In this work, we combine the classical Preisach model of hysteresis with machine learning techniques to efficiently create non-parametric, high-fidelity models of arbitrary systems exhibiting hysteresis. We demonstrate that our technique accurately predicts hysteresis effects in physical accelerator magnets. We also experimentally demonstrate how these methods can be used in situ, where the hysteresis model is combined with a Bayesian statistical model of the beam response, allowing characterization of hysteresis in accelerator magnets solely from measurements of the beam. Furthermore, we explore how using these joint hysteresis beam models allows us to overcome optimization performance limitations when hysteresis effects are ignored.

Presenter(s): Abigail Engbrecht, Avi Rajan
School: St. Olaf College
Session: Oral II.D.3
Title: A Combinatorial Description of Kostka-Foulkes Polynomials in all Classical Types
Advisor(s): Adam Schultze, Mathematics, St. Olaf College
Co-Author(s): Martin Liu

Abstract: In the mathematical area of algebra, we often use certain polynomials to classify (or even just count) abstract structures. One such family of polynomials are the Kostka-Foulkes polynomials and they come in four types: A, B, C and D. It has long been known that these polynomials have non-negative integer coefficients (so each coefficient is either a positive integer or zero). This was explicitly shown for the Kostka-Foulkes polynomials of type A through the use of a statistic called charge. However, it has been a long standing problem to explicitly show this non-negativity in types B, C and D. In this paper, we consider a recently developed statistic on Kostka-Foulkes polynomials which is equivalent to the charge statistic in type A, but was designed to extend to the other types more easily. We conclude by showing computer evidence for the non-negativity of these polynomials for all types when restricted to a special case.

Presenter(s): Isaiah Escapa, Rowen Glusman, Rachel Kovach-Fuentes
School: University of Chicago
Session: Poster P2.06
Title: A Comparative Analysis of Glass Plate Digitization Methods Using Stellar Variability
Advisor(s): Richard G. Kron, Astronomy and Astrophysics, University of Chicago
Co-Author(s): William Cerny, Michael N. Martinez, Amanda Muratore, Ali Chapman, Audrey
Paris Scott, Daniel Babnigg, Aafia Sait,

Abstract: Stellar variability can occur for a variety of interesting astrophysical reasons, and over a wide range of timescales. Much of what we know about variability comes from decadelevel observational data; however, analog data present on photographic plates spans more than 100 years. With access to this century-old data from Yerkes Observatory, we have developed a suite of methods which enable us to derive precise magnitude measurements crucial to determining a classification and source of a star's variability.

In this work, we build on our previous findings and compare digitizations of astronomical photographic plates using a graphic arts scanner and a DSLR camera, both of which were chosen due to their financial and operational accessibility. We investigate the astrometric and photometric performances using precise measurement on a variable star and detail advantages and disadvantages attendant on each method of capture. We also illustrate critical improvements to our analysis methods, particularly on our work with Plate 8 in E. E. Barnard's Photographic Atlas of Selected Regions of the Milky Way (1927), and demonstrate how these improvements can be applied to the digitization and analysis of other types of plates, including spectra.

Presenter(s): Katelyn Espe School: Gustavus Adolphus College Session: Oral I.B.1 Title: Search for the Z' boson in events with four top quarks at CERN Advisor(s): Mark Kruse, Physics, Duke University

Abstract: The ATLAS Collaboration at the European Council for Nuclear Research (CERN) seeks out New Physics Beyond the Standard Model, including a search for the Z' boson in four top quark events. An extension of the current Z' boson search is conducted by considering same-sign dilepton (electron or muon) channels. A preliminary approach to sorting the detectable decay particles based on their kinematic properties is investigated to propose a method for determining the particles associated with the Z' boson decay in four top quark events.

Presenter(s): Federico Fiorda
School: Gustavus Adolphus College
Session: Poster P3.06
Title: Pebble Survey Conducted in Jezero Crater, Mars (Sols 350-399)
Advisor(s): Julie K. Bartley, Department of Environment, Geography, and Earth Sciences, Gustavus Adolphus College
Co-Author(s): Aileen Yingst

Abstract: Understanding the processes that formed the martian surface in Jezero Crater is key to interpreting the geology and past habitability of the planet. As part of its geological investigation, the Perseverance rover acquires surface images during each sol (martian day) that the rover travels. Images acquired along Perseverance's traverse from sol 350 to 399 were examined to characterize surface pebbles larger than 5.25 mm (25 pixels; Yingst et al., 2016). Grain size, shape, and texture were then analyzed to determine whether systematic changes in grain size, shape, or composition occurred along the traverse. Preliminary analysis indicates that median grain size varies between 6 and 10.5 mm but displays no clear spatial trend over the traverse. Angularity shows an overall decrease across the studied traverse sols. These preliminary results suggest some variation in local bedrock, sediment source, and/or mechanism of sediment transport within Jezero Crater.

Presenter(s): Sullivan Fitz

School: University of Chicago Session: Poster P1.03 Title: Chiral Liquid Crystals in Microfluidic Environments Advisor(s): Juan de Pablo, Pritzker School of Molecular Engineering, University of Chicago Co-Author(s): Tadej Emersic

Abstract: Liquid crystals are complex anisotropic fluids that form a variety of liquid mesophases, best known for display applications. In contrast to the physical properties of conventional isotropic fluids, which are widespread in state-of-art microfluidic research and technology, microfluidic flows of anisotropic liquid crystals have recently gained considerable attention with several perspectives and potential applications such as ultrafast optical modulation, defect-guided transport of colloidal particles, and tunable stream shaping. The main advantage of these approaches lies in the very diverse and intriguing dynamics that arise from inherent coupling interactions between the fluid flow, molecular orientational order, viscosity, and geometric or topological constraints. We study experimentally the flow and non-equilibrium structures of chiral nematic liquid crystals in chemically functionalized microfluidic channels through polarizing optical microscopy. We demonstrate that the chiral structures and flow are highly sensitive with respect to the chirality of the system, surface anchoring, mechanical perturbations, and imposed temperature gradients. By tailoring the chirality, driving pressure, and temperature, we can form intriguing structures in chiral liquid crystal bulk, which we believe may have important implications for sensing applications in the future

Presenter(s): Bryan Forrest School: Hope College Session: Poster P3.07 Title: Development of directing groups for rhodium-catalyzed decarbonylation reactions Advisor(s): Jeffrey B. Johnson, Chemistry, Hope College Co-Author(s): Jazmin Aguilar-Romero, Mary Kapitula, and Grace Stalions

Abstract: Selective metal-catalyzed C-C bond activation is useful in constructing and simplifying pathways to synthesize complex molecules. Consequently, several methods of C-C bond activation have emerged in the past few decades. Previous work has utilized rhodium-catalyzed decarbonylation to form new C-C bonds from pyridyl ketone starting materials, where the nitrogen on the pyridine ring acts as a directing group. Though this reaction is easily replicated and gives high yields, the need for a pyridine directing group limits the range of molecules that can be synthesized. The goal of this project is to develop new directing groups to increase the scope of this decarbonylation reaction. To this end, various ketones with amine-containing moieties were tested, and the most success was found with heterocycles containing closely situated nitrogen atoms.

Presenter(s): Joseph Geniesse
School: University of Chicago
Session: Oral II.E.1
Title: Ytterbium-doped lead-free quantum cutting perovskites to improve the efficiency of silicon solar cells
Advisor(s): Eray Aydil, Chemical and Biomolecular Engineering, New York University

Abstract: Advancements in silicon solar cell efficiency have plateaued in the last two decades, primarily due to poor external quantum efficiency in the blue-ultraviolet (UV) region. Ytterbium-doped compounds have garnered attention as solar spectral shifting materials, which can improve solar cell efficiency by converting blue-UV photons into near infrared (NIR) photons. Furthermore, quantum cutting (QC) materials are able to convert each blue-UV photon into two NIR photons. However, current leading QC materials utilize lead which is toxic and the photoluminescence quantum yield (PLQY) of these materials decreases at high photon fluence, thus developing lead-free QC materials is of interest.

Double perovskites that substitute divalent lead octahedra with alternating monovalent and trivalent octahedra have emerged as promising QC hosts. We investigated this class of materials, depositing ytterbium-doped $A_2B^{1+}B^{3+}X_6$ (A=Cs, Rb; $B^{1+}=Ag$, Na; $B^{3+}=Bi$; X=Br, Cl) thin films using physical vapor deposition. We found that ytterbium-doped Rb2AgBiBr6 had low PLQY. We determined that ytterbium-doped Cs₂NaBiBr₆ is thermodynamically unstable and forms (Cs₂Na)Bi₂Br₉. Conversely, ytterbium-doped Cs₂NaBiCl₆ is stable, but does not have a high PLQY. Finally we synthesized ytterbium-doped Cs₂AgBiBr₆ thin films with a PLQY of 95% which is a significant improvement over the highest previously reported PLQY of 28% from lead-free materials.

Presenter(s): John Georgiades

School: Washington University in St. Louis

Session: Poster P2.05

Title: Development of Hydrophobic Cycloguanil Derivatives as Cell Permeable Inhibitors of Bacterial Dihydrofolate Reductase

Advisor(s): Timothy Wencewicz, Chemistry, Washington University in St. Louis

Co-Author(s): Angela Poffenberger, Carrie E. Lasky, Twila A. Mason, Kelly Flentie, Christina L. Stallings, James E. Champine, Marvin J. Miller, Bruce A. Hathaway,

Abstract: Dihydrofolate reductase (DHFR) is a critical component in the metabolic backbone of life, catalyzing the reduction of 7,8-dihydrofolate to 5,6,7,8-tetrahydrofolate, an essential cofactor in the biosynthesis of multiple nucleic and amino acids. Critically, DHFR is the only source of 5.6.7.8-tetrahydrofolate in the cell and has relatively low sequence similarity between humans and bacteria, making it an excellent target for drug development. Indeed, multiple FDA-approved DHFR inhibitors exist. However, it has been 60 years since a new DHFR inhibitor has entered the clinic for use as an antibacterial. Developing novel antifolates could play a key role in combatting the global antibiotic resistance crisis. We screened a library of compounds built from the scaffold of the antimalarial cycloguanil for their antibacterial activity against multiple pathogens. Most notably, 1-(4-chlorophenyl)-2,4diamino-1,3,5-triazines with a 6-nonyl substitution showed activity against multiple ESKAPE pathogens, including P. aeruginosa, A. baumannii, E. coli, S. aureus, and E. faecium as well as M. tuberculosis. It has previously been demonstrated that such a hydrophobic moiety may allow a dual action against both DHFR and the bacterial membrane. We aim to understand the enzyme kinetics of these inhibitors against DHFR in several of these organisms and investigate their mechanism of action.

Presenter(s): Diya Gandhi **School:** University of Chicago **Session:** Poster P2.19 **Title:** Discovery and direct enhanced sampling of solvent-inclusive atomistic CVs using autoencoder embeddings in n-Pentatetracontane(C45) system **Advisor(s):** Andrew Ferguson, Pritzker School of Molecular Engineering, University of Chicago

Abstract: This project utilizes Molecular Enhanced Sampling with Autoencoders (MESA) to perform dimensionality reduction and backpropagation to determine CVs (Collective Variables) to describe a polymer system. Here we used Pentatetracontane (C45) as a test system and then performed enhanced sampling directly in the CVs. The goal of this project was to use PIVs (Permutation Invariant Vectors) to generate better CVs to describe our system and allow our system to sample more structural conformations and free energy space. PIVs are generated by passing an abridged adjacency matrix of interatomic distances through a switching function that parametrizes them from a range of 0 to 1. These PIV values are then passed as an input into an autoencoder that is trained to learn CVs. Initially we ran an unbiased training allowing the system to train without outside influence. Then we ran three biased runs of the system where we used well tempered metadynamics, an enhanced sampling method, to increase exploration along our CVs. This method deposits gaussian potentials at decreasing heights along CV space to allow the system to explore more free energy conformations until the system reaches convergence. This process allowed us to learn more about the C45's conformations and solvent contributions.

Presenter(s): Barry Henaku School: University of Washington in St. Louis Session: Oral II.D.1 Title: Good ABC Triples and Good Elliptic Curves Advisor(s): Alexander Barrios, Mathematics, University of St. Thomas

Abstract: The Modified Szpiro Conjecture, which is an open statement about elliptic curves, is equivalent to the ABC conjecture. This equivalence gives us a dictionary that moves between good ABC triples and good elliptic curves. This summer, we introduced infinite families of good ABC triples, generalized known results, and showed that there are infinitely many good isogeny classes of elliptic curves with a 12-isogeny

Presenter(s): Khan Henderson
School: St. Olaf College
Session: Oral I.A.3
Title: Utilizing Awareness of Surroundings to Reduce Network Disruption While Maximizing Coverage in Multi-Robot Exploration
Advisor(s): Elizabeth Jensen, Mathematics, Statistics and Computer Science, St. Olaf College
Co-Author(s): Khang Vo Huynh, Ethan Kilmer

Abstract: Multi-robot exploration encompasses a variety of applications including deep sea, space, and search and rescue. In many of these, maintaining communication between robots can be crucial. However, communication networks can experience interference and partitioning from external networks or physical objects. Many proactive algorithms focus on the distance between the robots, but proximity to physical objects can have notable and unexpected effects as well. We created multiple scenarios to assess and analyze this effect

using Turtlebot3 mobile robots and Raspberry Pi Zero W stationary agents in a wireless adhoc network. We measured the strength and reliability of communication using round-trip time and transmit quality, and object proximity using LiDAR. After collecting data from multiple indoor and outdoor scenarios, we used a neural network and a decision tree to train classifiers on the robot's overall state. The robots will then use these to autonomously determine their path as they attempt to maximize the exploration coverage while minimizing disruptions to the communication network.

Presenter(s): Thai-Nam Hoang School: Beloit College Session: Oral I.A.1 Title: Wildfire Forecasting with Satellite Images and Deep Generative Model Advisor(s): Mehmet, Dik, Department of Mathematics & Computer Science, Beloit College Co-Author(s): Sang, Truong T. & Chris, Schmidt

Abstract: Wildfire prediction has been one of the most critical tasks that humanities want to thrive at. While it plays a vital role in protecting human life, it is also difficult because of its stochastic and chaotic properties. We tackled the problem by interpreting a series of wildfire images into a video and used it to anticipate how the fire would behave in the future. However, creating video prediction models that account for the inherent uncertainty of the future is challenging. The bulk of published attempts are based on stochastic image-autoregressive recurrent networks, which raise various performance and application difficulties such as computational cost and limited efficiency on massive datasets. Another possibility is to use entirely latent temporal models that combine frame synthesis with temporal dynamics. However, due to design and training issues, no such model for stochastic video prediction has yet been proposed in the literature. This paper addresses these issues by introducing a novel stochastic temporal model whose dynamics are driven in a latent model to beat previous state-of-the-art approaches on the GOES-16 dataset. Results are compared using various benchmarking models.

Presenter(s): Ian Huelsbeck, Samantha Ries

School: Colorado College

Session: Poster P1.07

Title: Consistent method for the detection of perfluorooctanesulfonic acid utilizing a molecularly imprinted polymer

Advisor(s): Eli Fahrenkrug, Chemistry and Biochemistry, Colorado College

Abstract: Per- and polyfluoroalkyl substances (PFAS) are a family of pollutants that are of considerable importance to water purity and safety globally. The EPA currently utilizes solid phase extraction liquid chromatography-tandem mass spectrometry and other costly methods for the detection of PFAS in water. This research aims to develop novel sensor technology that uses electropolymerized molecularly imprinted polymers (MIP's) in concert with voltametric measurements for cheap and on-site detection of PFAS compounds. In this work, we used cyclic and differential pulse voltammetry to systematically evaluate electropolymerization parameters that directly impact binding affinity of one particularly potent PFAS compound, perfluorooctanesulfonic acid (PFOS). These data suggest there are two

experimental parameters that can be externally controlled to tune the binding thermodynamics of the PFAS compound with the imprinted polymer. To our knowledge, these results represent the first explicit report for controlling PFAS binding equilibria to the MIP/electrode interface, which will be invaluable in developing multiplexed sensors going forward.

Presenter(s): Alexandra Hurd
School: Macalester College
Session: Poster P1.08
Title: Measuring charge lifetimes in organic solar cells
Advisor(s): Brian Collins, Physics and Astronomy, Washington State University
Co-Author(s): Awwad Alotaibi, Acacia Patterson, Obaid Alqahtani, Brian A. Collins

Abstract: Printable and flexible solar panels are promising sources of cheap, large-scale renewable energy. Polymer inks are deposited onto sheets of plastic to form thin layers of carbon-based solar cells. Despite the efficiency of printable manufacturing, there are some limitations to these solar cells. First, toxic halogenated solvents have historically been necessary to dissolve polymers to make ink. Additionally, charges must be separated in the cell for a certain amount of time for the cell to efficiently convert light to energy. Many of these organic solar cells have high rates of charge recombination, which shortens their lifetimes of separation. Here, we use a transient photovoltage (TPV) technique to measure these charge lifetimes in cells made from two different organic solvents. The first solvent is toxic, halogenated dichlorobenzene (DCB), typically used to make organic solar cells. The other is a less toxic, non-halogenated solvent, carbon disulfide (CS2). By varying the processing methods in this way, we find that cells made from CS2 have longer charge lifetimes and higher efficiencies than those made with DCB. This indicates that moving forward, we may be able to decrease the toxicity of organic solar cell manufacturing and simultaneously improve the efficiency of the devices, bringing this powerful method of capturing solar energy to the forefront of sustainable design.

Presenter(s): Tuan Huynh School: Lawrence University Session: Poster P2.07 Title: X-ray Fluorescence (XRF) Analysis on The Coins in the LU Wriston Gallery Collection. Advisor(s): Margaret K. A. Koker, Physics Department, Lawrence University

Abstract: XRF (X-ray fluorescence) is a non-destructive analytical technique used to determine the elemental composition of materials. XRF analyzers determine the chemical composition of a sample by measuring the fluorescent (or secondary) x-ray emitted from a sample when it is excited by a primary x-ray source. It is a great technology for qualitative and quantitative analysis of material composition because each element in a sample emits a distinct set of characteristic fluorescent x-rays (often referred to as "a fingerprint"). The primary goal of this research is to apply this method of analysis to investigate objects of unknown origin or with open inquiries, clarifying processes for dating or establishing authenticity. Lawrence University's Wriston Gallery coins collection includes both well-known and unknown specimens. By studying XRF data collected on the ancient coins of the renowned Buerger collection, we can establish a database of information to assess the

authenticity, origin, or dating of unknown specimens. We also seek to examine the efficiency of this analysis method.

Presenter(s): Khang Vo Huynh School: St. Olaf College Session: Poster P1.09 Title: Cloud-powered PDC Computation for a Runestone interactive Textbook Advisor(s): Richard Brown, Computer Science, St. Olaf College Co-Author(s): Anway De, Thong Vo

Abstract: In today's Big Data world, Parallel and Distributed Computing (PDC) plays a significant role in improving general performance of computers. Consequently, PDC has become an expected part of computer science (CS) education, beginning as early as the first course in CS. However, learning PDC requires specialized computational resources, such as computers with many cores for parallel computation and computer clusters for distributed computing. We describe a strategy for compiling and carrying out PDC computations automatically on demand, on available cloud computing resources using technologies such as Docker containers and Kubernetes. This strategy will support backend computations for an online interactive Runestone textbook intended to supplement early CS courses, in which students will be able to modify and experiment with various types of PDC code (currently OpenMP and MPI, in C or Python language) and receive rapid custom-computed results. Future work includes scaling our backend strategy to support thousands of simultaneous users on demand, assessing performance of these backend computations, and extending the strategy by adapting containers for other forms of PDC, including OpenACC (with GPU computations) and Apache Spark.

Presenter(s): Mohammad Tanzil Idrisi
School: Beloit College
Session: Poster P2.08
Title: CapsNet for classification of infected vs normal patches in biomedical image segmentation
Advisor(s): Mehmet Dik, Mathematics, Beloit College

Abstract: Medical Image Segmentation is one of the standard starting points for predicting any disease and preparing for higher procedures in the medical field. This paper talks about CapsNet a better framework and architecture for the classification of Infected vs Normal Patches in a biomedical image However before we used CNN for the classification of CT Scans and MRI, which required extensive data augmentation and a large dataset to identify detailed spatial relations between image instances. It's been a while since institutions started practicing the recent new architecture CapsNet that has accomplished better strength in representation learning by supplanting pooling layers with dynamic routing and convolutional stride, which has shown potential results on popular tasks such as classification, recognition, segmentation, and natural language processing in medical image segmentation. Here, we also created an efficient algorithm and extensive method to increase the efficiency by its loss functions and doubling the types of capsule instances in COVID-19 image segmentation. This will also work better with Lung cancer's histologic image classification and other biomedical and normal classifications. Therefore, Capsule Networks are promising candidates when it comes to the classification of small datasets in comparison to their counterparts. Presenter(s): Shiva Iyer, Olivia Lazorik, Selena Wang
School: Washington University in St. Louis
Session: Poster P1.10
Title: Heat sensing in biological systems using NV defects in Diamonds
Advisor(s): Erik Henriksen, Shankar Mukherji, Chong Zu, Physics, Washington University in St. Louis

Abstract: Nitrogen-Vacancy defects in diamonds are fluorescent at specific frequencies of light. The fluorescent path of the electron in the defect can be manipulated using microwaves, allowing the electron to de-excite via a non fluorescent pathway. This decrease in fluorescence can be measured and the frequency at which it occurs (center frequency) displays a temperature dependence, allowing it to serve as a heat sensor in biological systems.

Presenter(s): Mark Jareczek

School: Washington University in St. Louis

Session: Poster P1.13

Title: A Survey of New Metals and Demetallation Strategies for Use In Catenane Crosslinked Gels

Advisor(s): Prof. Jonathan Barnes, Chemistry, Washington University in St. Louis

Abstract: A unique approach to building materials that change properties in response to external stimuli, involves cross-linking metal-coordinating catenanes (mechanically interlocked rings) in organogels.

Our group has shown that viscoelastic properties of an organogel change with presence or absence of a coordinated tetrahedral Cu(I) metalated catenane crosslinker.

Work to be presented here characterizes the use of different tetrahedral metal centers in catenane cross-linked gels, and the possible changes in material properties as a result. Two new demetallation strategies (metal ion removal methods) were also explored, as previously used demetallation methods were hypothesized to cause gel degradation.

From relevant precedent and convenience, two 2,9-Bis(4-methoxyphenyl)-1,10phenanthroline ligands were used to simulate catenane-metal binding. 1H NMR spectroscopy and isothermal calorimetry (ITC) were employed to confirm formation of Cu(I), Zn(II) and Ag(I) homoleptic phenanthroline complexes and estimate dative bond strength. Using cyclic voltammetry and potentiometry, conditions for electrochemical demetallation of Cu(I) were found. Chemical demetallation of Zn(II) from the phenanthroline complex was also tested.

More sensitive conditions for demetallation and a spread of different metals to insert into gels will expand the tunability and use of catenane crosslinked materials.

Presenter(s): Deepthi Kailash

School: Washington University in St. Louis Session: Oral I.C.3

Title: Spatial Allocation Rules in the Eukaryotic Cell

Advisor(s): Shankar Mukherji, Physics, Washington University in St. Louis

Abstract: Uncovering the functional rules by which the eukaryotic cell controls the size of its organelles is a fundamental problem in cellular biophysics. Here we aim to elucidate one

such rule, namely how the budding yeast Saccharomyces cerevisiae coordinates the size of its organelles with the size of the cytoplasm within which they reside. By combining quantitative fluorescence microscopy with tools from synthetic cell biology, we directly engineer cells to exhibit a wide range of cytoplasmic spatial availability and monitor the response of organelle size to varying spatial constraints. In contrast to the mitochondria, lipid droplets, and endoplasmic reticulum, we observe that vacuolar sizes exhibit a strong response to decreasing cytoplasmic availability. We observe that with a significant amount of condensate in cells (>1%), the vacuolar volume starts to decrease as cell size increases, the opposite relationship to what is observed in the cells with an insignificant amount of condensate (<1%) and previously reported observations. Our data suggest the hypothesis that the vacuole potentially plays a key role in buffering variation in the cytoplasmic volume even as the size of the cell as a whole changes.

Presenter(s): Reagan Keeney School: Knox College Session: Poster P2.09 Title: Quantifying nationalism online via stance detection Advisor(s): Ritwik Bose, Computer science, Knox College

Abstract: This project aims to explore stance detection as a method of quantifying and tracking nationalism on the internet. The systems being prioritized in computer science are highly applicable to the study of political behavior, but the field as it stands is largely research conducted with older methods of analysis. This creates an opportunity for novel findings in areas of political research that have been unreasonable to study previously. The data used in the project was collected from Twitter during periods of political polarization in specific countries when nationalist discourse is particularly salient, and filtered by relevant keywords to minimize extraneous data points. Using this data, domain/belief pairs are constructed based on relevant topics or groups. These pairs can then be examined in the context of the various ideologies within the country of study. More specifically, the data from stance detection can be used to characterize the in/out group dynamics that are ever-present in research concerning nationalism. This research seeks to expand on the pre-existing literature on political computation while also showcasing the advantages of stance detection applied to political research due to the added specificity it allows.

Presenter(s): Auras Khanal School: Beloit College Session: Poster P3.13 Title: Comparative Analysis of First and Second Order Optimization Methods in Neural Networks Advisor(s): Mehmet Dik, Beloit College

Abstract: Artificial Neural Networks are fine tuned to yield the best performance through an iterative process where the values of their parameters are altered. Optimization is the preferred method to determine the parameters that yield the minima of the loss function, an evaluation metric for ANN's. Optimization efficiency is imperative to reduce the use of computational resources and time when training Neural Network models. However, the process of finding an optimal model which has minimum loss faces several obstacles, the most notable being regions in the loss function such as saddle points and local minima that

reduce the efficiency and rate of convergence to the minima of the loss function. This paper reviews and compares the intuition and effectiveness of existing optimization algorithms such as Gradient Descent, Gradient Descent with Momentum, RMSProp and Adam that implement first order derivatives, and Newton's Method that utilizes second order derivatives for convergence, in reducing or eliminating such challenges. It also explores the possibility to combine and leverage first and second order optimization techniques for improved performance and a general formula to determine and govern the integration of these techniques.

Presenter(s): Zihao Yu
School: Grinnell College
Session: Poster P2.10
Title: FNI App: An expert-centered knowledge dashboard to support multidisciplinary research
Advisor(s): Priscilla Jimenez, Computer Science, Grinnell College
Co-Author(s): Muqi Guo, Priscilla Jimenez

Abstract: Nowadays, academic search engines use established methods to discover and score academic contributions and researchers. However, when researching emerging topics, these former methods are not helpful; the search becomes overwhelming and time-consuming, especially for academics in new research areas or novice researchers.

To facilitate this process and evoke multidisciplinary research by connecting disparate academic fields, we propose FNIApp, a dashboard that allows stakeholders to interact with keywords and authors' visualization networks—helping them identify key contributors or seek potential collaborations. FNIApp shows the rank of researchers based on a new index, ""FNI"" (Field Networking Index), which identifies prominent scholars in emerging fields by analyzing their publication content.

FNIApp, developed in Shiny, connects two components: 1) A wrapper written in Python for accessing publication information and that applies NLP models to generate the datasets to visualize, and 2) Two interactive visualizations written in D3.js. Users can choose between two academic search engines, Google Scholar -for a simplified visualization- and Scopus -for a visualization that includes the FNI. In addition, users can provide a BibTex or CSV file containing a curated list of publications to visualize. We tested the FNIApp with the resulting dataset from a search using the keywords ""religion & science.

Presenter(s): Steven Labalme
School: University of Chicago
Session: Poster P3.18
Title: Site isolation in metal-organic layers enhances photoredox gold catalysis
Advisor(s): Wenbin Lin, Department of Chemistry, University of Chicago
Co-Author(s): Haifeng Zheng, Yingjie Fan, Yang Song, Justin S. Chen, Eric You, Wenbin Lin

Abstract: Among the most useful chemical processes are carbon-carbon bond-forming reactions. Homogeneous photoredox gold catalysis enables running many difficult such reactions — and with little waste — but such setups suffer from a high degree of catalyst deactivation and a low degree of interaction between the photosensitizer and the gold catalyst. However, our research finds that metal-organic layers (MOLs), ultrathin nanoscale

lattices that combine the best parts of homogeneous and heterogeneous catalysis, can improve such systems in both of these areas by over two orders of magnitude.

In this study, we synthesized a novel MOL, Hf-Ru-Au, which comprises gold-based catalysts and ruthenium-based photosensitizers affixed to a Hf-BPY lattice. Under visible light and at room temperature, Hf-Ru-Au effectively catalyzed allenoate-, alkene-, and alkyne-based cross-coupling reactions with aryl diazonium salts.

Hf-Ru-Au afforded comparable yields to the homogeneous control with significantly lower catalyst loadings, had higher turnover numbers, and was recyclable. Altogether, there was a 14-200 fold increase in activity. Mechanistic studies suggest that this improvement comes from site-isolation of gold catalysts and proximity-enhanced synergistic effects between them and the ruthenium photosensitizers.

Presenter(s): Shannon Kim

School: University of Chicago Session: Oral I.C.1 Title: D-RNA selects L-amino acids in a newly characterized aminoacyl-RNA loop ligation Advisor(s): Jack W. Szostak, Chemistry, University of Chicago Co-Author(s): Aleksandar Radakovic, Jack W. Szostak

Abstract: Biology adheres to molecular asymmetry to an extent that homochirality is considered a requisite for the earliest living systems. L-amino acids and D-sugars (in nucleic acids) are almost exclusive throughout biology, but purely chemical synthesis pathways for these molecules (which necessarily predate biological synthesis pathways) yield an even split of both enantiomers. Thus, the origins-of-life field has outstanding interest in mechanisms for symmetry breaking. Numerous investigations on the origins of homochirality have yielded explanations including magnetic fields, crystallization, and the Soai reaction. However, proposed mechanisms tend to target molecules of a single species or synthesis pathway. Such mechanisms are significant only because chemical reactions with an enantioenriched species are assumed to propagate asymmetry throughout chiral molecules. We experimentally suggest such proliferation of asymmetry through an enantiopreferential and self-amplifying aminoacylation reaction which forms a closed RNA stem loop with an amino acid-bridged backbone. Our results demonstrate five-fold preference for L-amino acids with oligomers of D-RNA. We determined that enantioselectivity occurs most prominently in the loop-closing step based on experiments which isolated individual kinetic steps. Because aminoacylation is the cornerstone of RNA-coded protein synthesis, the enantiopreference observed here offers a chemical axis for the selection of L-amino acids in a D-RNA world.

Presenter(s): Julianne Lampert
School: Washington University in St. Louis
Session: Poster P1.11
Title: Nanoconfinement of Electrodeposited Nickel Oxide Catalysts in Porous Antimony Tin Oxide
Advisor(s): Bryce Sadtler, Chemistry, Washington University in St. Louis
Co-Author(s): Ashlynn Berry

Abstract: Solar fuel cells take advantage of sunlight as an energy source to drive electrochemical reactions. One such reaction is water oxidation, a key component in the green production of hydrogen fuel. An effective, low-cost, earth-abundant catalyst is required

to make hydrogen fuel production economically viable. We hypothesized that the use of porous substrates would induce a beneficial effect known as nanoconfinement, increasing the activity and stability of nickel oxide (NiOx) catalysts. Nanoporous antimony tin oxide (ATO) substrates were synthesized, and NiOx was successfully electrodeposited using a pulsed potential technique. Systematic experiments testing the effects of deposition potential, pulse times, and cycle number on the resulting activity for water oxidation were used to determine the optimal deposition conditions. Scanning electron micrographs show that the NiOx catalyst was deposited within the pores of the substrate, and not on the surface. An activation procedure using redox cycling to convert the as-deposited NiOx particles into their catalytically active form consistently yielded effective samples, as evidenced by activity and stability testing. Modifications were made to the ATO synthesis procedure to fabricate non-porous substrates, and preliminary stability tests showed improved results for samples deposited within porous substrates compared to non-porous ones. This project establishes synthetic and experimental methods that will be used to quantify the effects of nanoconfinement on water oxidation catalysts.

Presenter(s): Dylan Laurianti, John Tobin School: Grinnell College Session: Oral I.A.2 Title: Coarse-Grained Networks Advisor(s): Nicole Eikmeier, Computer Science, Grinnell College

Abstract: The complexity of real-world dynamical systems presents a computability problem for network models. This research explores coarse-graining approaches to reducing the complexity of a network while preserving dynamic behavior. A number of properties make the coarse-graining problem difficult: the performance of any algorithm over the set of all networks is independent of the algorithm, exact evaluation of candidate coarse-grainings requires computation of dynamics of the uncompressed network, and it is intractable to compute the dynamics of all possible coarse-grainings. Therefore, practical progress on the coarse-graining of specific classes of networks and dynamics requires experimental patternfinding on the behavior of different algorithms. This research develops a suite of highperformance tools in the Julia language for large-scale experimentation and visualization of results.

Presenter(s): Daniel Lewinsohn
School: Colorado College
Session: Oral I.C.2
Title: Consensus Label Propagation with Graph Convolutional Networks for Single-Cell RNA
Sequencing Cell Type Annotation
Advisor(s): 1. Donald F Conrad 2. Cory B Scott; 1. Division of Genetics 2. Mathematics and

Computer Science; 1. Oregon Health and Science University 2. Colorado College

Abstract: Single-cell RNA sequencing (scRNA-seq) data, annotated by cell type, is useful in a variety of downstream biological applications, such as profiling gene expression at the single-cell level. However, manually assigning these annotations with known marker genes is both time-consuming and subjective. We present a Graph Convolutional Network (GCN) based approach to automate the annotation process. Our process builds upon existing labelling approaches, using state-of-the-art tools to find highly-confident cells through consensus and

spreading these confident labels with a semi-supervised GCN. Using simulated data and two scRNA-seq datasets from different tissues, we show that our method improves accuracy over a simple consensus algorithm and the average of the underlying tools. We also demonstrate that our GCN method allows for feature interpretation, pulling out important genes for cell type classification. We present our completed pipeline, written in Pytorch, as an end-to-end tool for automating and interpreting the classification of scRNA-seq data.

Presenter(s): Diangen Lin
School: University of Chicago
Session: Poster P3.09
Title: Accelerating deep learning-mediated protein design with a synthetic sequence evaluation pipeline
Advisor(s): Arvind Ramanathan, Data Science and Learning Division, University of Chicago & Argonne National Laboratory
Co-Author(s): Alexander Brace, Maxim Zvyagin, Carla M. Mann

Abstract: Deep learning has the potential to accelerate protein design to aid in drug discovery, vaccine development, and other industrial applications. However, deep learning models are difficult to interpret due to large numbers of parameters, so systematic evaluation schemes are required to assess model validity. Here, we build an open-source pipeline that assesses the performance of a Generative Pre-trained Transformer 2 (GPT-2) model. The GPT-2 model was trained on known malate dehydrogenase (MDH) gene sequences and generates new sequences that explore the MDH protein family space. We find a Pearson correlation coefficient of -0.97 (p-value = 0+) when comparing the embedding L2 distance and the pairwise global alignment score on held-out test sequences, indicating that GPT-2 learns the semantic similarity between highly similar sequences and maps them closely together in the embedding space. Furthermore, visualization of high-dimensional sequence embeddings using Uniform Manifold Approximation and Projection (UMAP) reveals clear clustering on GC-content, sequence length, molecular weight, and isoelectric point. These results demonstrate that GPT-2 can effectively learn important properties of nucleotide sequences and generate diverse sequences within a protein family. Our evaluation pipeline provides a streamlined process to gain insights into the performance of transformer models and accelerate the protein design process.

Presenter(s): Swagat Malla School: St Olaf College Session: Poster P3.11 Title: Generalized Fibonacci Polynomial Identities Advisor(s): Matthew Wright, Matthew Richey; Mathematics; St. Olaf College Co-Author(s): Aryaman Joshi, Joey Glampe

Abstract: The Fibonacci sequence 0,1,1,2,3,5,8,... is a popular sequence of numbers computed with initial conditions $F_0=0$, $F_1=1$ and the recurrence as $F_n=F_{n-1}+F_{n-2}$. It is well known that the Fibonacci numbers satisfy certain polynomial identities: for odd p, $F_{pn} = c_1(F_n)^p + c_2(F_n)^{p-1} + ... + c_{p-1}F_n + c_p$. We extended this to generalized Fibonacci sequences defined $G_0=a$, $G_1=b$ and the recurrence as $G_n = rG_{n-1} + sG_{n-2}$. It is not apparent from the literature which generalized Fibonacci sequences have similar identities. We computationally explored over 50,000 combinations of these relationships by setting up and solving finite

linear systems, then tested the solutions to see which ones led to polynomial identities involving an infinite number of relationships. Having identified potential polynomial identities, we were able to prove (using a combinatorial identity known as Waring's formula) certain identities for generalized Fibonacci sequences.

Presenter(s): Tyler Meeks School: Grinnell College Session: Poster P2.11 Title: Synthesis and characterization of phenylated Ni(II) bis(thiosemicarbazone) compounds for CO2 reduction Advisor(s): Maisha Kamunde-Devonish, Chemistry, Grinnell College

Abstract: With significant recent increases in anthropogenic carbon dioxide emissions, it has become crucial that effective processes for atmospheric CO2 removal are studied. Currently, popular methods of removal involve "trap-and-transform" methodology, in which carbon dioxide is trapped from the atmosphere and reduced to 'value-added' products. However, current catalysts capable of performing this reduction often fail to exhibit concomitantly a) reliable product selectivity, b) high-yield, and c) facile synthetic pathways. Previous research suggests that a specific copper (II) bis(thiosemicarbazone) transition metal compound catalyst was able to photo- and electrochemically reduce carbon dioxide to methanol with respectable yield. The aim of this project is to synthesize phenylated derivatives of Ni(II) bis(thiosemicarbazone) compounds to investigate their catalytic potential as CO2 reductants. Four phenylated derivatives were successfully synthesized and characterized via 13C/1H NMR, IR, UV-Vis spectroscopy, and cyclic voltammetry.

Presenter(s): Angelina Minocha School: Washington University in St. Louis Session: Poster P1.15 Title: Web-Based visualization tool for interpretation of quantitative EPMA imaging Advisor(s): Ryan Ogliore Physics, Washington University in St. Louis

Abstract: Modern imaging techniques produce data in the form of large mosaics, wherein every pixel contains valuable mineralogic information. These heavy data files are challenging for most computers to load and process, furthermore access to lunar and other extraterrestrial samples is limited. In 2021, a set of virtual tools was developed to display large electron and qualitative x-ray images of meteorite thin sections (R. C. Ogliore, 2021). Here, we expanded the utility of this tool to enable the extraction of quantitative EPMA data and the presentation of optical, electron and x-ray images. To reduce image distortion, we improved image registration by using a combination of manual and automatic control points selection that allows all image modalities to be registered to high-resolution back-scattered electron (BSE) images. We created three methods of data extraction: single-pixel selection, rectangular region selection, and polygonal region selection. Each of the three methods allows the user to retrieve quant data in the form of weight percentages of 10 common oxide compounds. This tool allows more researchers to study rare samples without the need for expensive technology. With a strong internet connection and a computer, scientists will be able to study the minerology of various samples from any location in the world.

Presenter(s): Tracey Nelson
School: St. Olaf College
Session: Poster P2.12
Title: Characterization of Methyl Substituted N2P2 First Row Transition Metal Complexes
Advisor(s): Elodie Marlier, Chemistry, St. Olaf College
Co-Author(s): Claire Egesdal, Calvin Raymer, Logan Flom, Maddie Logelin, Michelle Soltis, Daron Janzen

Abstract: Industrial catalysis involves the use of second and third row transition metals due to their highly reactive nature and ability to donate electrons. The low abundance and high cost of these metals increase the need for an economical and sustainable alternative. In order to investigate first row transition metals as viable substitutes, a family of N2P2 ligands has been synthesized. The N2P2 binding pocket is created from a β -diketiminate backbone connected to phosphine pendant arms using phenyl linkers. The ligands have been metallated with late first row transition metals Co(II), Ni (II), Cu(I) and Zn(II). Additionally, the influence of sterics on the ligand binding mode has been investigated by introducing methyl substituents on the phenyl linkers. From characterization metals, a wide range of geometries and binding modes of the first row transition metal complexes will be discussed.

Presenter(s): Phuc Ngo School: Beloit College Session: Poster P2.13 Title: Is CLIP Fooled by Optical Illusions? Advisor(s): Mehmet Dik, Department of Mathematics, Beloit College Co-Author(s): Phillip Isola, Swami Sankaranarayanan

Abstract: Recent large machine learning models have achieved impressive performance on perception tasks such as classification or object detection, especially on unseen data. While it is unclear if they model the human cognitive process, they provide a compelling framework for case study and analysis. In this work, we test one such hypothesis: To what extent do large vision language models mimic the human cognitive system? We attempt to answer this question by focusing our attention on the ability of such models to perceive optical illusions. We analyze the CLIP model as a visual system, presenting stimuli in the form of image and text prompts and observing how the model's classification score changes under different illusory strengths. Our results show that CLIP is fooled by different types of illusions relating to lightness and geometry.

Presenter(s): Nhan Nguyen School: Beloit College Session: Poster P1.12 Title: Multi-site stimulation of globus pallidus and subthalamic nucleus in treating biophysical network of Parkinson's disease Advisor(s): Thomas Stojsavljevic, Mathematics

Abstract: Parkinson's disease (PD) is a neurodegenerative disorder that causes arduous problems to patients such as but not limited to tremors, muscle stiffness, and impaired

balance. Despite there having been treatments from drug therapies with tradeoffs, deep brain stimulation (DBS) is currently favorable in treating PD. In this paper, we investigate a Parkinson's biophysical network model targeting the basal ganglia circuit which has been developed in the form of mathematical equations. Moreover, we studied the past computational network model and improvised our own approach to stimulating both the subthalamic nucleus (STN) and external globus pallidus (GPe). Specifically, we successfully broke the Parkinsonian state in our multi-site adaptive constant deep brain stimulation (acDBS) protocol. Although our approach yielded different and complex results, it opened a novel methodology for future treating PD.

Presenter(s): Emily Nigro

School: University of Chicago

Session: Oral I.C.4

Title: Adaptive failure and its impact on taxonomic and morphologic diversification of burrowing marine bivalves

Advisor(s): David Jablonski, Department of the Geophysical Sciences, University of Chicago Co-Author(s): Katie S. Collins, Stewart M. Edie, Nicholas M. A. Crouch

Abstract: Why are some clades more diverse than others? One hypothesized mechanism for achieving greater diversity is the development of key adaptive traits, which release taxa from intrinsic or extrinsic evolutionary constraints. The molluscan Class Bivalvia, with its extensive fossil record, provides a rich dataset for the study of key innovations and diversification. Bivalve shells preserve a record of their soft-part anatomy, including presence/absence of the siphon, a snorkel-like tube that allows them to live deeper within soft sediments to escape predation and disinterment. Siphons have been postulated to be a key innovation, leading to a radiation of burrowing species into new niches. In this study, we compare the morphological traits and diversification through time of two burrowing bivalve clades with similar shell forms and life positions: the ancient asiphonate Archiheterodonta and the younger, siphonate Veneridae. We measure shell size, width, and volume in these two groups to test the impact that a single trait, i.e. siphons, has had on diversity and disparity. We find that Archiheterodonta are on average thicker-shelled than Veneridae, suggesting a compensatory adaptation to life at the sediment-water interface. This tradeoff may have limited morphologic and taxonomic diversification, rendering the asiphonate condition an adaptive failure.

Presenter(s): Sarah Olsen School: Washington University in St. Louis Session: Poster P3.12 Title: Adding Solubilizing Alkyl Chains to Self-Complementary Urea-Based Arrays Advisor(s): Vladimir Birman, Chemistry, Washington University in St. Louis Co-Author(s): Ruth Son

Abstract: Stimuli-responsive polymers represent an exciting new development in current materials and technologies. Self-Complementary Urea-Based Arrays (SCUBAs) consist of polymeric chains that are constructed from reversible covalent bonds between precursors, which may then dimerize through a reversible intermolecular hydrogen-bond network. While SCUBAs have been successfully synthesized, one inherent problem in their planar structure is the resulting insolubility in most organic solvents. Here, we attach nonpolar solubilizing alkyl chains to the SCUBA backbone to improve solubility and test the effects of adding a

substituent group. Different alkyl groups were added to the commercially available starting material 2,4-pentanedione, and the established synthetic route was tested to investigate its applicability once a greasy side chain was introduced. We found that the identity of the substituent makes a significant difference in the utility of the current synthetic pathway, with impacts on yields and the intermediates formed. In addition, longer alkyl chains were confirmed to confer increased solubility to SCUBA precursors, demonstrating the promise of solubilizing SCUBAs through this approach. The solubility can potentially be further improved through testing different side chains.

Presenter(s): Nicolò Petroccione School: Beloit College Session: Poster P1.14 Title: Implementation of adaptive multi site local field potential deep brain stimulation in STN and GPe Advisor(s): Thomas Stojsavljevic, Mathematics and Computer Science, Beloit College

Abstract: In the past two decades, deep brain stimulation (DBS) - through a surgically implanted electrode to the subthalamic nucleus (STN) - has become a widely used therapeutic option for the treatment of Parkinson's disease and other neurological disorders. The current form of DBS is the conventional high frequency stimulation (HF) that has several drawbacks. To overcome the limitations of HF, researchers have been developing closed-loop and demand controlled, adaptive stimulation protocols wherein the amount of current that is delivered can be turned on and off in real time in accordance with a biophysical signal. Computational modeling of DBS in neural network models are an increasingly important tool in the development of new protocols that aid researchers in animal and clinical studies. In this computational study we seek to implement a novel technique of DBS where we jointly stimulate the subthalamic nucleus (STN) and globus pallidus external (GPe) in an adaptive fashion. We use the inter-spike firing of the neurons as a biomarker to control external stimulation. Our results show that our protocol induces breaks in the synchronized bursting neuronal activity of the STN and GPe which is hypothesized to cause failure of thalamocortical neurons to respond properly to excitatory cortical inputs.

Presenter(s): Jonah Pratt School: Grinnell College Session: Poster P1.16 Title: Design, synthesis, and biological testing of antimicrobial peptide derivatives Advisor(s): Erick K. Leggans, Chemistry, Grinnell College

Abstract: The overuse and simplicity of currently available antimicrobial and antibiotic drugs has led to a sharp increase in infections from resistant bacteria. To combat this growing issue, new antibiotics, especially ones that have more complex modes of action, need to be identified, studied, and produced efficiently. We are particularly interested in antibiotic candidates isolated from natural products. Antimicrobial peptides (AMPs) are one class of antibiotic candidates that are commonly isolated from natural products and have recently shown promise for treating resistant bacteria. AMPs are most commonly synthesized from readily available amino acids, and other easily obtainable reagents making synthesis costeffective. By synthesizing derivatives of AMPs in fragments, we are able to elucidate structure-activity relationships (SAR), develop methodology for potential future production, and perform biological testing to determine any strong antibiotic candidates.

Presenter(s): Kaitlyn Prokup, Andrew Valentini, Rebecca Dowe
School: Carthage College
Session: Poster P2.15
Title: Modeling Binary Compact Object Merger Events Detected by the LIGO and Virgo Gravitational Waves Observatories
Advisor(s): Jean Quashnock, Physics & Astronomy, Carthage College
Co-Author(s): Andrew Jocham, Will Schuster, Chance Hoskinson

Abstract: In this investigation, we model multiple neutron star and black hole merger events detected in the LIGO-Virgo Collaboration. We use Kepler's Laws and Newtonian mechanics to model an infalling system of two objects with equal masses. We predict the expected increase in frequency or "chirp" of the infalling binary and compare that to what is found in the LIGO-Virgo database (presented in an adjacent poster). In the initial period during which the Newtonian approximation is valid, we find reasonable agreement between our model and the results from the LIGO-Virgo Collaboration, thus verifying the basic physics of the infall. We also estimate the amount of gravitational wave energy emitted during the entire process. This provides a better understanding of the nature of these merger events and why gravitational waves are emitted by these merging compact objects.

Presenter(s): Emilio Rosas Linhard
School: University of Chicago
Session: Poster: P2.16
Title: Silicon Integrated Microfluidics for Microbial Genomics
Advisor(s): Supratik Guha, Molecular Engineering, University of Chicago
Co-Author(s): Oni Basu, Vamsi Krishna Nittala, Suryakant Mishra, Allison Hohreiter

Abstract: The fast-growing field of single cell genomics is establishing novel techniques with applications in medicine, research, and industry. Profiling certain mammalian cells using RNA-Seq is now possible, but sequencing single microbial cells remains a challenge. Specifically, many microbial cells are small in size (\sim 1 µm), have thick cell walls, and contain miniscule amounts of RNA. This project seeks to create a reproducible technology that can lyse a wide range of bacteria, fungi, and other microbes. Research involves establishing the optimal parameters for the fabrication of a microfluidic device and analyzing the resulting effluent. The device is composed of a micro-fabricated silicon chip with sharp tip arrays driven by a piezoelectric drive. Fluid containing microbial cells is sent through the device connected to the silicon chip, mechanically crushing cells as they flow through. Resulting fragments are analyzed using image tools and RNA sequencing. The set-up has been tested with plastic beads, with the intention of improving efficiency before microbial experimentation. Research also involves refining the set-up, further experimentation with different silicon chips and smaller beads, further image analysis, and integration of microbial cells. Plastic beads of sizes varying from 3µm to 10µm have been successfully crushed using the device.

Presenter(s): Will Rosenberg **School:** Washington University in St. Louis **Session:** Poster P1.17 **Title:** Training a Feed-Forward Neural Network to Solve the S-wave Nucleon-Nucleon Scattering Problem

Advisor(s): Maria Piarulli, PhysicsWashington, University in St. Louis **Co-Author(s):** Alessandro Lovato, Krishnan Raghavan, Saori Pastore

Abstract: Our research goal is to develop a neural network that accurately predicts nucleonnucleon scattering observables to replace the computationally expensive numerical solution of the Schrodinger equation. Such a network has applications in Bayesian inference methods used to address the optimization problem of nuclear interaction models. This research serves as a starting point towards that goal. We construct a feed-forward neural network that takes a potential as a discrete function of the distance between nucleons (r) and outputs the S-wave phase shift as a discrete function of the laboratory energy (E). The model is trained, validated, and tested on varying Woods-Saxons potentials. The goal of this project is to determine the most effective model parameters and architecture to create a well-generalized network for Woods-Saxon potentials. This network can be built upon to solve for systems with non-zero angular momentum (I > 0) and other potentials through further research. The most accurate neural network achieved contained 100 input nodes, r ranges [0, 10), 350 output nodes, E ranges [0, 350), and one hidden layer with 187 nodes. This network implemented a tanh() activation function and used the Stochastic Gradient Descent optimization algorithm.

Presenter(s): Andrew Shanahan School: Lawrence University Session: Oral II E.3 Title: Capturing Brownian Motion with an Open-source Microscope Advisor(s): Douglas Martin, Physics, Lawrence University Co-Author(s): Keegan Mencke

Abstract: Modern day microscopes tend to be expensive, require much training to use, and focus on specific types of microscopies. The goal for this project is to create an affordable, easy to use microscope that can be used in the classroom to train students across branches of science. This microscope is open-source and designed to be used for teaching and research-grade data collection. Modifiability via 3D printing is beneficial to locations where budget and resupply are problems. All the mechanical and optical parts can all either be 3D printed, CNC machined, or readily purchased. The electronics are based on an open-source circuit board and chip design that is purchasable from PCB assemblers. The software to control the microscope is μ Manager, which is also an open-source platform. Ultimately the microscope will be capable of fluorescence, brightfield, and darkfield imaging. The presentation will be about both the construction of the microscope, and the first fluorescent experiment that was performed.

Presenter(s): Brian Sun

School: Washington University in St. Louis

Session: Poster P2.20

Title: Amyloid fiber remodeling observed by single-molecule nanoscopy is correlated with the orientation of amyloidophilic dye molecules.

Advisor(s): Matthew D. Lew, Electrical & Systems Engineering, Washington University in St. Louis

Co-Author(s): Weiyan Zhou, Tianben Ding, Tara S. Porter, Tingting Wu

Abstract: Nanoscale dynamics of peptides implicated in chronic ailments such as Alzheimer's disease are of great interest to biomedical scientists. Single-molecule orientation-localization microscopy (SMOLM) resolves the organization of amyloid aggregates by determining the position and orientation of individual Nile blue (NB) molecules transiently bound to these structures. However, it remains unknown whether the orientations of these dyes as they bind to amyloid fibrils can simultaneously quantify their growth and decay tendencies.

Herein, we report the structural dynamics of amyloid-beta 42 (AB-42) fibers imaged using SMOLM. AB-42 fibers are subject to laser irradiation in the presence or absence of Thioflavin T, and the orientations and rotational diffusion of transiently bound NB labels are measured in 2 to 4-minute intervals. We discover that increases in rotational diffusion and the variance of NB orientations are associated with decaying AB-42 segments. The opposite is true of growing segments. Stable fibers are associated with insignificant changes in NB rotational diffusion and dipole orientation. These relationships between segment growth and decay and SMOLM measurements can be represented using a nonlinear model.

To our knowledge, our study is the first to correlate the rotational dynamics and orientations of amyloidophilic dyes with time-series growth and decay of amyloid fibers.

Presenter(s): Chengyu Tang School: University of Chicago Session: Oral II.E. 4 Title: Novel carbazole-based semi-ladder polymer with optimized photoelectric properties Advisor(s): Luping Yu, Chemistry Department, University of Chicago Co-Author(s): Yachu Du, Eric Zhao

Abstract: We are synthesizing a series of novel carbazole-based ladder and semi-ladder polymers that exhibit high photoluminescence. Ladder-type polymers have covalent piconjugated backbones that facilitate coherent electron delocalization, but they also have strong intermolecular packing in condensed phases that reduce photoluminescence through non-radiative decay. We propose to address this challenge by tuning the semi-ladder polymers into coiled foldamers that have H-aggregation but keep a decent amount of intermolecular distance such that photoluminescence remains high. We have designed a conjugated weak donor-weak acceptor carbazole-based semi-ladder monomer, and introduced bulky alkyl groups to both the monomer and co-monomers to tune H-aggregation.We are also experimenting with one-step syntheses of ladder polymers using Friedlander condensation. The study of these polymers and synthesis techniques could contribute to pushing the boundary between light emission and charge transport, generating potential materials for organic light emitting transistors and diodes, as well as developing novel high efficiency synthetic approaches to ladder-type polymers.

Presenter(s): Anna Teurman
School: Gustavus Adolphus College
Session: Poster P1.18
Title: A Probabilistic Model of Mantle Transition Zone Discontinuities from Auto-picked
Precursor Data
Advisor(s): Scott Burdick, Geology, Wayne State University

Abstract: Earthquakes release large waves of energy that travel through the Earth similar to ripples in water. As they encounter boundaries between different materials, these waves may be reflected. Several such boundaries occur in the Earth's mantle, about 410 and 660km below the surface. Here, high temperatures and pressures force mineral phase changes. The depth of this transition varies by region, depending on the temperature and rock composition. To map temperature and composition, we use recordings of earthquakes to compare waves that bounce off the Earth's surface from below and waves that bounce off the discontinuities at 410 and 660km depth. Previously, data from several seismometers was necessary to measure the depths of the discontinuities. A new machine learning algorithm allows us to analyze data from single seismometers. This results in more measurements covering a greater area of the mantle. To create maps of the discontinuities that take the uncertainty of these measurements into account, we use a new method that generates many maps of depths that fit the measurements, then finds the mean values and error bars. This study provides information about mineral transitions in the mantle that will help further knowledge of the Earth's tectonic history and mantle circulation.

Presenter(s): Lauren Tsai School: University of Chicago Session: Oral II.D.4 Title: Cardinal numbers and Boolean algebras Advisor(s): Beniada Shabani, Mathematics, University of Chicago

Abstract: Over the course of the past century, the Continuum Hypothesis has been something of a mystery. Introduced in 1878 by Cantor, this hypothesis proposes that there is no set with cardinality between the natural numbers and the real numbers. The works of Cohen and Gödel, when taken together, prove that the Continuum Hypothesis is independent of the Zermelo-Fraenkel axioms of set theory. So, in search of a solution to this problem of the independence of the Continuum Hypothesis, mathematicians have attempted to find axioms that resolve the question of its truth. One such axiom is an extension of Martin's Axiom called "Martin's Maximum," presented by Foreman, Magidor, and Shelah.

To begin to understand the foundations of this axiom and of the Continuum Hypothesis in general, one must have familiarity with the cardinal numbers and Boolean algebras, among other concepts. In this talk, I will construct the cardinal numbers from the ordinal numbers. I will also briefly introduce the notion of a Boolean algebra.

Presenter(s): Anusha Vajrala
School: Colorado College
Session: Poster P2.14
Title: Switching the Reactivity of Pyruvate Formate-Lyase-Activating Enzyme to Epimerization with Single Mutation
Advisor(s): Joan Broderick, Chemistry/ Biochemistry, Montana State University
Co-Author(s): Maike Lundahl

Abstract: Epimerases and glycyl-radical-enzyme activating enzymes (GRE-AEs) are two subclasses of the radical S-Adenosyl-L-methionine (SAM) enzyme superfamily that can modify peptides. Characterized epimerases have a cysteine residue that may allow for stereoselective quenching of a carbon-centered radical. GRE-AEs like pyruvate-formate-lyase activating enzyme (PFL-AE) catalyze the activation of their natural substrate, by

installing a stable glycyl radical on the Gly734 residue of its inner loop. PFL-AE can activate peptides that mimic this Gly-loop (RVSGYAV) or contain a D-Ala residue replacing the glycine, yielding in a C α based radical. Whenever the C α -radical is formed, one equivalent of dAdoH and either L-Ala peptide or D-Ala peptide is formed. Here, we used site directed mutagenesis to switch the reactivity of PFL-AE into an epimerase. We first reacted a D-Ala peptide with WT PFL-AE to determine if PFL-AE can naturally act as an epimerase. We then introduced the D16C mutation to enable stereoselective quenching of the C α radical. In the HPLC assays of PFL-AE D16C, we detected L-Ala peptide and dAdoH, however, we observed a decrease in turnover when comparing WT PFL-AE to PFL-AE D16C. Further studies are needed to determine if this mutation increased PFL-AE's radical quenching ability by switching PFL-AE into a competent epimerase.

Presenter(s): Ronan Wallace

School: Macalester College

Session: Poster P2.17

Title: Using Remote Sensing in Relocating Lubra Village and Visualizing Flood Damages in Nepal

Advisor(s): Susan Fox, Mathematics, Statistics, and Computer Science, Macalester College

Abstract: As weather patterns change worldwide, isolated communities impacted by climate change go unnoticed. In Himalayan Mustang, Nepal, indigenous Lubra village faces threats of increasing flash flooding. Compared to one flood per monsoon season, flash flooding has grown to three to five floods over the last decade. After every flood, residual concrete-like sediment hardens across the riverbed, causing its elevation to rise. As the elevation increases, this sediment encroaches on Lubra's agricultural fields and homes, making them more vulnerable to flood damage. In the last monsoon season alone, the village witnessed floods swallowing several fields and damaging two homes. To investigate this issue further, first, we look to in-person interviews with the community to understand their needs and perspective in relocating the entire village. Then, we utilize remote sensing techniques to digitally 3D model flood damages and the village itself. These models digitally document the village before floods wipe it out entirely, as well as communicate flood damages and proposed village locations. The architecture development team uses these models to understand terrain and village layout for village development, avoiding costly site visits. Lastly, we explore redirecting flood flow, predicting riverbed elevation trends, and visualizing flood damages further through detailed 3D modeling.

Presenter(s): Selina Wang, Olivia Lazorik, Gianna Glenn, Shiva Iyer

School: Washington University in St. Louis

Session: Poster P2.18

Title: Probing the thermal distribution inside yeast cell using nanodiamond as quantum sensor

Advisor(s): Chong Zu, Eric Henriksen, Shankar Mukherji, Department of Physics,

Washington University in St. Louis

Abstract: Quantum sensors based on solid-state spin defects has recently emerged as probes for a myriad of signals, including magnetic field, strain, and temperature. In fact, nanodiamond with nitrogen-vacancy centers(NV centers) has been a versatile tool to explore various phenomena in physical and biological system. Our group is interested in using

nanodiamond as quantum sensor to probe the thermal distribution inside the yeast cell. Over the past four months, we have been experimenting on nanodiamonds with NV centers in various dimensions in a wide-field optical setup. We primarily use electron-spin resonance(ESR) spectrum as a reflection of signals probed by nanodiamonds. On a bulk diamond with shallow NV centers embedded near the surface, we observed the strain effect on ESR spectrum. Diamond polishing can achieve surface roughness under 1 nm, and as a result, the surface is highly strained. Recently we have been using 140 nm diamonds to probe the local temperature in the yeast cell. We have observed that the nanodiamond has been a promising sensor in the biological environment of yeast cell and the local thermal distribution can be unveiled with control on the movement of diamond using an optical tweezer.

Presenter(s): Alexandria Weary

School: University of Chicago

Session: Poster P1.19

Title: Energy of rare gas cluster implosions maximized by cluster size/configuration and ionization variables

Advisor(s): Edward Ackad, Physics, Southern Illinois University Edwardsville

Abstract: This project aims to maximize the energy of imploding rare gas clusters through manipulation of the number of particles, their initial configuration, and ionization to create the ideal conditions for maximizing fusion. We used computer models of imploding, hollow, rare gas clusters in this experiment. Kinetic, potential, and total energies were calculated and recorded for each colliding ion pair at every time frame (we define a colliding pair as being less than 3.0 angstroms apart). We then plotted the energies of all contributing pairs against each timestep in the implosion. We also created scatter plots to show how the integrations of the energy plots changed with respect to variables such as cluster size/configuration and the presence/intensity of a second laser. We found that clusters with larger empty shells yield more energetic implosions. Furthermore, introducing a second laser into the system decreases the time over which the implosion occurs (greater intensity yields shorter implosions), but does not increase the system's peak energy. We conclude that greater spaces between the shells of the cluster allow the system to have more energetic implosions, which promotes fusion. However, using a second laser heats the electron plasma and thus inhibits the implosion.

Presenter(s): Marya Wydra
School: Lawrence University
Session: Poster P3.15
Title: Towards a quinoxaline-based anti-parasitic drug via click chemistry
Advisor(s): Stefan Debbert, Chemistry, Cornell University

Abstract: The search for new drug candidates to treat the widespread parasitic infection schistosomiasis is motivated by the growing drug resistance of Schistosoma mansoni for the current treatment, Praziquantel. Quinoxaline compounds have shown promise as effective treatments, but they require an improvement in bioavailability which may be achieved by the addition of polar functional groups. This research moves toward a quinoxaline-based drug candidate by functionalizing 2,3-dichloroquinoxaline with a variety of polar substituents to synthesize a diverse family of potential drug candidates. Most notably, a copper-catalyzed

click reaction in aqueous solvent was performed to produce an alcohol-substituted 1,2,3triazole functionality with a quinoxaline base. This synthesis utilizes the versatility of click chemistry to bring quinoxaline compounds closer to being successful drugs for the treatment of schistosomiasis.

Presenter(s): Matthew Yu School: Washington University in St. Louis Session: Poster P3.16 Title: X-rays from Cygnus X-1 reveal structure of stellar gas Advisor(s): Michael A. Nowak, Physics, Washington University in St. Louis

Abstract: Cygnus X-1 is a black hole which is part of a High Mass X-ray Binary system, or HMXB. In HMXBs, a black hole or neutron star accretes gaseous matter from a supergiant companion star, releasing X-rays in the process. In the case of Cygnus X-1, some of these X-rays are absorbed as the companion star to Cygnus X-1 passes across our line of sight. The depth and timescale of these absorption events, or dips, depends on the size and speed of denser pockets of gas in the companion's atmosphere. By making plots of intensity vs. time and color vs. color (ratios of intensity in different energy channels), it appears that Cygnus X-1 shifts between two states every few years as expected—one characterized by low-energy X-rays and higher intensity, and the other characterized by high-energy X-rays and lower intensity. Absorption events occur predominantly when the source is in the hard state. Furthermore, a few of the plots suggest that dips can occur on timescales of a few hundred seconds or as short as tens of seconds. The range in possible dipping timescales may be associated with variation in the size and speed of clouds in the star's atmosphere.

Presenter(s): Yiren Zhang School: Colorado College Session: Poster P3.17 Title: Phytochemical Characterization of Ninety-Two Rosinweed (Silphium Integrifolium) Genotypes Advisor(s): Murphy Brasuel, Chemistry & Biochemistry, Colorado College Co-Author(s): Ayush Chitrakar1, Blaze Johnson2, Alex Griffin2, Ebony Murrell2

1Department of Chemistry/Biochemistry, Colorado College, Colorado Springs, Colorado 2The Land Institute, Salina, Kansas

Abstract: Silphium integrifolium is a common sunflower-like perennial prominent in the Midwest. Due to the ability of S. integrifolium to grow on minimum resources, it is targeted as an alternative for oilseed production. Terpenoids synthesized by the plant are hypothesized to provide insect tolerance. These traits have the potential to result in a green crop for oilseed production. In this study, methods for the extraction of biologically active terpenoids from S. integrifolium leaves were explored and optimized. Air-dried leaves from 92 different genotypes were extracted with isopropyl alcohol using a heated ultrasonic-assisted technique. The extracts were then run on a GC-MS to characterize the terpenoids. The genotypes were all from the Midwest but varied in the region they are native to, eastern, central, or western Midwest. The genotypes also varied in their insecticidal activity, which was determined by a fall armyworm-based bioassay. Chemometric characterization of phytochemical data from the GC-MS included the multivariate techniques of cluster and principal component analysis. The analysis determined that each genotype has a unique

chemical fingerprint that can be used to establish the likely native region of each S. Integrifolium genotype. Furthermore, an inverse correlation was found between the bioassays and the terpenoid concentrations.

All Students Presenting at MCMS Undergraduate Research Symposium, Washington University in St. Louis Physical Sciences, Math and Computer Science November 11-12, 2022

Beloit College: Sadeen Alsabbagh, Thai-Nam Hoang, Mohammad Tanzil Idrisi, Auras Khanal, Phuc Ngo, Nhan Nguyen, Nicolò Petroccione

Carthage College: Kaitlyn Prokup, Andrew Valentini, Rebecca Dowe

Colorado College: Ian Huelsbeck, Daniel Lewinsohn, Samantha Ries, Anusha Vajrala, Yiren Zhang

Grinnell College: Caitlin Abreu, Tanmaie Kailash, Dylan Laurianti, Tyler Meeks, Jonah Pratt, John Tobin, Zihao Yu

Gustavus Adolphus College: Isabella Aase, Erin Beer, Katy Cash, Erin Coleman, Annie Corbett, Katelyn Espe, Federico Fiorda, Anna Teurman

Hope College: Lauren Bryan, Andnet DeBoer, Bryan Forrest

Knox College: Adam Brohl, Justin Douty, Reagan Keeney

Lawrence University: Hasif Ahmed, Tuan Huynh, Andrew Shanahan, Marya Wydra

Macalester College: Alexandra Hurd, Ronan Wallace

St Olaf College: Will Asinger, Tenzin Choedon, Stacie Elliott, Abigail Engbrecht, Khan Henderson, Khang Vo Huynh, Swagat Malla, Tracey Nelson, Chanjin Park, Avi Rajan

University of Chicago: Jessica Cao, Shivani Chatterji, Aidan Cloonan, Kabir Dubey, Isaiah Escapa, Sullivan Fitz, Diya Gandhi, Joseph Geniesse, Rowen Glusman, Shannon Kim, Rachel Kovach-Fuentes, Steven Labalme, Diangen Lin, Emily Nigro, Emilio Rosas Linhard, Chengyu Tang, Lauren Tsai, Alexandria Weary

Washington University in St, Louis: Polina Barzova, Jessica Berkman, Shamika Bhandarkar, Benjamin de Jonge, Sabrina DelBello, John Georgiades, Barry Henaku, Shiva Iyer, Mark Jareczek, Deepthi Kailash, Julianne Lampert, Angelina Minocha, Sarah Olsen, Will Rosenberg, Brian Sun, Selina Wang, Matthew Yu

Participating Faculty

John Bleeke, Washington University in St. Louis, Chemistry Department Rik Bose, Knox College, Computer Science Department Amanda Bowman, Colorado College, Chemistry Department Barbara Breen, Grinnell College, Physics Department Paul Fischer, Macalester College, Chemistry Department Francesc Ferrer, Washington University in St. Louis, Physics Department Joe Fournier, Washington University in St. Louis, Chemistry Department Jennifer Heemstra, Washington University in St. Louis, Chemistry Department Vera Kazakova, Knox College, Computer Science Department Margaret Koker, Lawrence University, Physics Department Shonda Kuiper, Grinnell College, Statistics Department Stuart Kurtz, University of Chicago, Computer Science Department and College Master **Physical Sciences** Richard Mabbs, Washington University in St. Louis, Chemistry Department Shankar Mukherji, Washington University in St. Louis, Physics Department Michael Nowak, Washington University in St. Louis, Physics Department Jean Quashnock, Carthage College, Physics Department Tom Stojsavljevic, Beloit College, Mathematics and Computer Science Department Dwight Stoll, Gustavus Adolphus College, Chemistry Department Tim Wencewicz, Washington University in St. Louis, Chemistry Department Matthew Wright, St. Olaf College, Mathematics Department