

The Midstates Consortium for Math and Science presents

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**Physical Sciences, Mathematics,
and Computer Science**

**November 15 & 16, 2019
The University of Chicago**

Beloit College - Carthage College - Colorado College - Grinnell College
Gustavus Adolphus College - Hope College - Knox College
Lawrence University - Luther College - Macalester College
St. Olaf College - University of Chicago
Washington University in St. Louis



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**Midstates Consortium for Math and Science Undergraduate Research Symposium
Physical Sciences, Mathematics, and Computer Science
The University of Chicago, November 15 & 16, 2019**

**Program Schedule
Friday, November 15**

1:30 pm – 5:30 pm	Graduate School Exploration Seminar Registration @ 1:30, various sessions begin @ 2:00	Eckhardt Research Center 5640 S. Ellis
12:00 pm – 4:45 pm	Midstate Registration	Hyatt Place Chicago South 5225 South Harper Ave
4:45 pm – 5:30 pm	Reception – sponsored by Graduate School Open to all participants – no RSVP needed	Eckhardt Research Center (ERC) Lobby
5:00 pm – 5:30 pm	Registration Continues	ERC 161
5:30 pm – 5:40 pm	WELCOME Stuart Kurtz, Symposium Organizer; University of Chicago Michael Seymour, Director – Midstates Consortium for Math and Sciences; Hope College	Maria Goeppert Mayer Lecture Hall – Kersten 106
5:40 pm – 6:30 pm	Keynote Lecture David Cash, Associate Professor Dept. of Computer Science, The University of Chicago <i>Cryptography from Caesar to Snowden</i>	Kersten 106
6:30 pm – 7:30 pm	Dinner Buffet	Atrium - Gordon Center for Integrative Science (GCIS)
7:30 pm – 8:20 pm	Janet Anderson Lecture Jill Dietz Grace A. Whittier Endowed Chair in Science Dept. of Mathematics, Statistics and Computer Science St. Olaf College <i>Exercise, eat right, and study linear algebra</i>	Kersten 106
Following lecture	Group Picture University shuttles to the Hyatt after group picture	

Saturday schedule continues next page

Saturday, November 16

Begins at 7:00 am	Breakfast Depart for University of Chicago Campus Those with vans or cars will drive to campus. Others will walk or take Hyatt Shuttle. There is locked room for storage of luggage and posters at the meeting site	Hyatt Hotel Hyatt Lobby
8:00 am – 8:30am	Set-up for poster session 1 Check computer set-up for oral presentations	GCIS Atrium
8:30 am – 9:30 am	Poster Presentations Session P1	GCIS Atrium
9:30 am – 9:50 am	Break, remove posters, check set-up for oral presentations in respective rooms	GCIS Atrium
9:50 am -11:25 pm	Session I. Oral Presentations of Student Papers, <i>15 min presentation, 5 min between talks</i> Session I.A (5) 9:50, 10:10, 10:30, 10:50, 11:10 Session I.B (5) Session I.C: (5) Session I.D: (5)	Kersten Room 101 Room 103 Room 105 Room 206
11:30 am– 12:15 pm	Careers at Liberal Arts Colleges	Kersten 206
11:30 pm – 12:45 pm	Lunch Buffet	Baker Dining Hall
12:45 pm – 1:00 pm	Set-up posters for session 2	GCIS Atrium
1:00 pm – 2:00 pm	Poster Presentations Session P2	GCIS Atrium
2:00 pm – 2:15 pm	Remove posters, check set-up for oral presentations	
2:15 pm – 3:30 pm	Session II. Oral Presentations of Student Papers Session II.E: (4) 2:15, 2:35, 2:55, 3:15 Session II.F: (4) Session II.G: (3) Session II.H: (4)	Kersten Room 101 Room 103 Room 105 Room 206
3:30 pm -3:50 pm	Break, set-up for poster session 3	GCIS Atrium
3:50 pm – 4:50 pm	Poster Presentations Session P3	GCIS Atrium
4:50 pm	Remove posters	
4:50 pm – 5:00 pm	Meeting Concludes Complete evaluations – available online Boxed meal to go Shuttle pick up and return to the Hyatt	GCIS Atrium



2019 Keynote Lecture

Cryptography from Caesar to Snowden

David Cash

Associate Professor

Department of Computer Science

The University of Chicago

Abstract: Cryptography has been used to protect communications since the beginning of written history, and today cryptography is an indispensable tool underlying the Internet, cellular networks, automobiles, cryptocurrencies, and other technologies. Modern cryptography is also unique in its application of certain areas of mathematics to computer security, including number theory and algebraic geometry. This talk will introduce some of the central ideas of modern cryptography, and describe how mathematics is applied in the cryptographic systems that we routinely depend on today. It will conclude with discussion of the current political and technical debates on how cryptography should be restricted, including the Snowden revelations and the so-called "Crypto Wars."

Biography: David is an associate professor in the Computer Science Department at the University of Chicago. He does research in applied and theoretical cryptography and computer security. Before joining the University of Chicago in 2018, he earned his PhD at Georgia Tech in 2009, and in the intervening years worked at the University of California San Diego, IBM, Ruhr University Bochum, and Rutgers University.



2019 Janet Andersen Lecture
Exercise, eat right, and study linear algebra

Jill Dietz

Grace A. Whittier Endowed Chair in Science
Department of Mathematics, Statistics and Computer Science
St. Olaf College, Northfield, MN

Abstract: Leibniz knew something about both calculus and linear algebra more than 300 years ago, but rigorous development of calculus came about much earlier and has been part of many high school curricula since the 1980s. By contrast, linear algebra in its modern form did not develop until the early 1900s when algebraic axioms (for groups, rings, vector spaces) were formalized. Students do not typically learn linear algebra until college, though one can argue that the subject is just as fundamental as calculus.

Undergraduates majoring in physics, chemistry, neuroscience, computer science, economics and certainly mathematics often take a first course in linear algebra, but there are good reasons to study the subject further. In this talk I will begin with a survey of introductory ideas in linear algebra (matrices, vectors, transformations, eigenvalues, etc), then expand upon them. My goal is to show that delving into the abstract theory of vector spaces leads to bigger and better applications than just row reducing matrices to solve systems of linear equations. The applications are fundamental to the areas of interest of the Midstates Consortium participants.

About Professor Dietz: The nomination letter for Dr. Dietz describes how her active support for undergraduate research (UGR) over the past 23 years has been key in transforming a nascent UGR program into a top priority for the Mathematics, Statistics and Computer Science department at St. Olaf. By expanding her personal research interests to include topics that are accessible at the undergraduate level she is a role model and a catalyst for a culture of research among both faculty and students. The nearly 100 undergraduates mentored by Dr. Dietz are evidence of her impact in this area. Through her development of the Directed Undergraduate Research (DUR) course, mathematics research has become more than a summer or academic year project. The DUR course is now a regular offering in many other disciplines, with academic credit for students and teaching credit for faculty. Dr. Dietz is acknowledged by students to be among the most popular and effective teachers in a department of creative and dedicated educators. Younger faculty benefit from her insights regarding teaching, research and the general challenges of balancing an academic career with life beyond the campus environment. When not on campus, Dr. Dietz loves to be in nature, especially camping and hiking in the mountains, or boating and swimming at “the cabin” up in central Minnesota. Dr. Dietz will be recognized for her contributions to undergraduate research and education by presenting the Janet Andersen Lecture at the 2019 Midstates Consortium Undergraduate Research Symposium in the Physical Sciences, Math and Computer Science.



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.

Janet Anderson Lecture Award Presentations

Year	Biological Sciences and Psychology Recipients	Physical Sciences, Mathematics and Computer Science Recipients
2008	David Hall, Biochemistry Lawrence University	Jeff Wilkerson, Astrophysics Luther College
2009	Ken Yasukawa, Biology Beloit College	Robert Jacobel, Physics St. Olaf College
2010	Sarah Elgin, Molecular Biology Washington University in St. Louis	Graham Peaslee, Nuclear Physics Hope College
2011	William Hammer, Paleo-geology Augustana College	George Lisensky, Materials Chemistry Beloit College
2012	Eric Cole, Biology St. Olaf College	Tim Pennings, Mathematics Hope College
2013	Daniel Hornbach, Biology & Environmental Studies, Macalester College	Bradley Chamberlain, Chemistry Luther College
2014	Phoebe Lostroh, Molecular Biology Colorado College	Kevin Crosby, Physics, Astronomy & Computer Science, Carthage College
2015	Laura Listenberger, Biology and Chemistry, St. Olaf College	Julie Bartley, Geology Gustavus Adolphus College
2016	Maria Burnatowska-Hledin, Chemistry and Biology, Hope College	Andrew Beveridge, Mathematics Macalester College
2017	Julie Legler, Mathematics, Statistics & Computer Science, St. Olaf College	Thomas Varberg, Chemistry Macalester College
2018	Neena Grover, Chemistry and Biochemistry Colorado Collage	Joanne Stewart, Chemistry Hope College
2019		Jill Dietz, Mathematics, Statistics & Computer Science, St. Olaf College

Oral Session I. Schedule

Session I.A: 9:30 – 11:25 a.m. Room: Kersten 101			
Session #	Presenter Name	Institution	Title of Presentation
I.A.1 (9:50)	Elijah McMahon	Gustavus Adolphus College	The Environmental Fate of Dicamba
I.A.2 (10:10)	Sarah Mersch	Gustavus Adolphus College	DeepCHALLA sediment core: Atmospheric mercury and lead in Equatorial East Africa over the last 250,000 yrs
I.A.3 (10:30)	Jonny Norwine	Colorado College	Mechanisms of Land Subsidence in Colorado Springs Related to Abandoned Coal Mine Tunnels
I.A.4 (10:50)	Andrea Salazar	University of Chicago	Modeling the role of volcanism in the last 20 million years of global cooling
I.A.5 (11:10)	Sydney Jenkins	University of Chicago	Cloud Characterization with Deep Learning

Session I.B: 9:30 – 11:25 a.m. Room: Kersten 103			
Session #	Presenter Name	Institution	Title of Presentation
I.B.1 (9:50)	Jonathan Rebelsky	Grinnell College	$\text{La}_{(x)}\text{Sr}_{(1-x)}\text{Co}_{(y)}\text{Fe}_{(1-y)}\text{O}_3$ Thin-Film Oxygen Reduction and Evolution Catalysts Grown by Spray Pyrolysis
I.B.2 (10:10)	Adee Athiyaman	Knox College	Synthesis and characterization of heteroleptic copper dimers generated from tetrakis(3-phenylpropionate) dicopper(II) precursor
I.B.3 (10:30)	Kelly Vences	Lawrence University	Investigating the Doublet State Photophysics of the Organic Luminescent Radical BAXPA
I.B.4 (10:50)	Keir Adams	University of Chicago	Characterizing the timescale and voltage dependence of $\text{Cs}_3\text{Bi}_2\text{I}_9$ as high-performing and tunable supercapacitor electrode material
I.B.5 (11:10)	Vennela Mannava	University of Chicago	Nickel-mediated dehydrogenative aryl-aryl homocoupling of a bulky phosphino-pyridine

Session I.C: 9:30 – 11:25 a.m. Room: Kersten 105			
Session #	Presenter Name	Institution	Title of Presentation
I.C.1 (9:50)	Jerrell Cockerham	Colorado College	Polynomial Conversion Involved in Describing Weight q -Multiplicities for Representations of the Exceptional Lie Algebra g_2
I.C.2 (10:10)	Thong Vo	St. Olaf College	The Delicate Details of Filling Space
I.C.3 (10:30)	Kate Herman	Colorado College	Numerical methods for Picard-Lefschetz solutions to the Path Integral
I.C.4 (10:50)	Shelby Klomp	Gustavus Adolphus College	Simulation for radio detection of dark matter photons
I.C.5 (11:10)	Nicholas Vaporciyan	Lawrence University	What Makes A Rainbow?

Session I.D: 9:30 – 11:25 a.m. Room: Kersten 206			
Session #	Presenter Name	Institution	Title of Presentation
I.D.1 (9:50)	Mattias McMullin	Lawrence University	Tuning of Photonic Band Gap Superconducting RF Cavities
I.D.2 (10:10)	Pei Robins	Lawrence University	Measuring the Frequency Response of a Harmonic Potential and Gaussian Potential
I.D.3 (10:30)	Salamong Xiong	Macalester College	SuperCDMS: Energy Calibration of a Cryogenic Ge HV Particle Detector
I.D.4 (10:50)	Hope Lee	University of Chicago	High Quality Factor SiGe Optical Ring Resonators for Microwave to Optical Quantum Transduction
I.D.5 (11:10)	Tianle Liu	University of Chicago	ProtoDUNE: measuring electric field in the drift direction using cathode-anode crossing muons

Oral Session II. Schedule

Session II.E: 2:15 - 3:30 p.m. Room: Kersten 101			
Session #	Presenter Name	Institution	Title of Presentation
II.E.1 (2:15)	Mesut Caliskan	University of Chicago	The Hubble Constant from the Lensed Gravitational Waves
II.E.2 (2:35)	Hanjue Zhu	University of Chicago	Galaxy-Halo Connection in the Cosmic Reionization on Computers Simulation
II.E.3 (2:55)	Austin Stover	Washington University in St. Louis	Photonic Crystal Fibers Improve Light Collection in a Gamma-ray Telescope
II.E.4 (3:15)	Jason Tang	Washington University in St. Louis	Optimization of small-pixel CZT detectors for hard X-ray astronomy

Session II.F: 2:15 - 3:30 p.m. Room: Kersten 103			
Session #	Presenter Name	Institution	Title of Presentation
II.F.1 (2:15)	Runqi Huang	University of Chicago	Stretchable Organic Electrochemical Transistor for Implantable Bioelectronics
II.F.2 (2:35)	Fabian Dauzvardis	Beloit College	Emulsion Polymerization, Size Determination, and Self-Assembly of Monodispersed Poly (methyl methacrylate) Nanospheres for Photonics
II.F.3 (2:55)	Makenzie Mullan, Gunnar Goetz	Carthage College	Micellar-Facilitated Peptide Coupling Reactions in Continuous-Flow Conditions
II.F.4 (3:15)	Lily Liu	University of Chicago	Modeling Systems of Drop Carrier Particles Using Energy Minimization

Session II.G: 2:15 - 3:30 p.m. Room: Kersten 105

Session #	Presenter Name	Institution	Title of Presentation
II.G.1 (2:15)	Ishaan Tibrewal	Grinnell College	Driving Performance Under Influence of Cannabis and Alcohol During Secondary Task Engagement
II.G.2 (2:35)	Sanjeeda Shutrishna	Gustavus Adolphus College	Modeling of altruistic suicide in E.Coli Bacteria
II.G.3 (2:55)	Filip Belik	Gustavus Adolphus College	A Study of the Propagation of Health Related Habits on Twitter
II.G.4 (3:15)	Open time		

Session II.H: 2:15 - 3:30 p.m. Room: Kersten 206

Session #	Presenter Name	Institution	Title of Presentation
II.H.1 (2:15)	Tyler Walker	Colorado College	Computational screening and optimization of small molecules for African sleeping sickness
II.H.2 (2:35)	Amy Crawford	Gustavus Adolphus College	2D-LC/HRMS for direct structure characterization of small molecule drugs
II.H.3 (2:55)	Uriya Jankurazova	Lawrence University	De-noising Data for Topological Data Analysis
II.H.4 (3:15)	Alexander Cohen	University of Chicago	Coarse-grained simulations of conjugated polymers and graph-theoretic measures for exciton transport

Poster Sessions Schedule

Poster Session 1: 8:45 a.m. – 9:45 a.m. Room: GCIS Atrium			
Poster #	Presenter Name	Institution	Title of Presentation
P1.01	Alexander Liebl	Gustavus Adolphus College	Synthesizing peptides for identifying PfGCN5 bromodomain recognition for specific acetyl-modified histone tail marks
P1.02	Alexandra Nisenoff	University of Chicago	Study of University of Chicago affiliates' vulnerability to password-guessing attacks
P1.03	Andrew Boldt, Jonathan Ramirez	Carthage College	Radical Functionalization Using Photoredox Catalysis
P1.04	Asa Kalish	Washington University in St. Louis	Robust organelle size control in <i>Saccharomyces cerevisiae</i>
P1.05	Bryce Cook	Grinnell College	Synthesis and Biological Evaluation of Lugdunin Analogues
P1.06	Caroline Burkhardt	Hope College	Iterative Learning Techniques for Improved Performance of Bio-Inspired Control Law
P1.07	Emily Saari	Gustavus Adolphus College	Synthesis and optimization of drug-like molecules for inhibition of the PfGCN5 bromodomain
P1.08	Evan Unruh-Friesen	Macalester College	Detrital Zircon Geochronology: The blueschist facies sequences of Baja California
P1.09	Grace Tews	Carthage College	Synthesis of Gamma-Cyclodextrin Based Metal Organic Frameworks (MOFs) to Improve Water Quality
P1.10	Hannah McCall	Washington University in St. Louis	Supernova Cosmology without Spectroscopy
P1.11	Innes Maxwell	Lawrence University	Developing an Integrated Light Source in Band Gap Photonic Crystals
P1.12	João Francisco Shida, Fangjian (Roy) Wu	University of Chicago	Design of a Cesium Vapour Pressure Gauge Based on Electronic Thermionic Emission
P1.13	Kathryn Stein	St. Olaf College	G-Quadruplex Stability in Aqueous Cosolute Solutions
P1.14	Kavya Devgun	St. Olaf College	Development of an optical system to determine impurity content & composition in a snowpack
P1.15	Keegan Proctor	Knox College	Synthesis of Heteroleptic Copper Dimers of Various Alkoxybenzoates and 8-Carbon Carboxylates
P1.16	Zuofu Huang, Kieu-Giang Nguyen	Macalester College	Clustering Longitudinal Categorical Data
P1.17	Leonardo Ferreira Guilhoto	University of Chicago	Numerically Solving The Generalized Dirichlet Problem Using Stochastic Calculus
P1.18	Linh Tran	St. Olaf College	CSinParallel Platform Benchmarking Project

P1.19	Nicole Chavarria	Colorado College	Geospatial and Temporal Mapping of per-Fluorinated Alkyl Substances in Colorado Springs Via EPA Method 537.1
P1.20	Serena Rolland	Luther College	Nanocrystal ligand substitution: a mechanistic study
P1.21	YiLi Luo, Tanvi Jindal	Grinnell College	A latent variable approach for evaluating collision scenarios with application to driving simulator time-series data
P1.22	Ying Wang	Colorado College	The Inverse Problem for Rational Equivariant Cohomology
P1.23	Xiaohe Jia	University of Chicago	Isolation of Displaced Leptons from Long-lived Slepton Decays
P1.24	Aldo Portillo	Knox College	Ligand Exchange in Copper Tetramer Complexes with Axial Caprolactam: Synthesis and Characterization of Novel Copper Tetramers with Bridging Carboxylate Ligands

Poster Session 2: 1:15 p.m. - 2:15 p.m. Room: GCIS Atrium			
Poster #	Presenter Name	Institution	Title of Presentation
P2.01	Adam Rivkin	University of Chicago	Multidimensional Database Reconstruction from Range Query Access Patterns
P2.02	Allie Goldman	Lawrence University	Progress Toward a Pyrene-derived Redox-active Ligand for use in Coordination Polymers
P2.03	Amy Sorge	Carthage College	Development of Flow Chemistry Experiments for the Organic Chemistry Curriculum
P2.04	Arsalan Bin Najeeb	Knox College	Facial Recognition Assignment on the Raspberry Pi
P2.05	Chankyung Jung	St. Olaf College	Improving the Usability of Two-Parameter Persistence Software
P2.06	Conor Broderick	Macalester College	Organic Electronic Materials Synthesis: Progress Toward n-Cationic Naphthalene Diimides
P2.07	Elvis Haisa	St. Olaf College	Developing and implementing technology to investigate the effects of temperature gradients on snow grain growth
P2.08	Emma Daggett Jonathan Rustad,	St. Olaf College	Temperature dependence of the optical properties of cesium lead halide perovskite nanocrystals
P2.09	Eric Salisbury, Jacob VanderRoest, Erik Schoonover	Hope College	Carbon-Carbon Bond Activation: ortho-fluoro Pyridyl Ketones in Substitution-Decarbonylation Reactions with Boronic Acids
P2.10	Gabriella Griffen	University of Chicago	Optimizing the Reversible Phosphate-Binding of a New Micelle-Based Material

P2.11	Hannah Wilkins	Grinnell College	Semi-Synthesis and Biological Activity of Enoxolone Derivatives
P2.12	Hanqing Li	Colorado College	Stochastic Models of Feed Forward Loops in Gene Regulatory Networks
P2.13	Jennifer DeJong, Yilin Chen	Macalester College	Signal Processing on the Permutahedron: New Analysis Tools for Ranked Choice Data
P2.14	Jessica Bigley	Washington University in St. Louis	Characterizing UBQLN2, an ALS-associated gene, in a yeast model system and defining its genetic modifiers
P2.15	Kathryn Hanggi	Luther College	Dopamine Quantification using HPLC for Biological Applications
P2.16	Matthew Venzke	Gustavus Adolphus College	Electrochemical Reduction of Nitro Groups: From Bioanalysis to Lightweight High-Energy Density Cathodic Materials
P2.17	Max Huang	Washington University in St. Louis	Low voltage Muon telescope based on plastic Scintillators and wavelength shifting fibers
P2.18	Maya Lengvenis	Gustavus Adolphus College	Midrange wireless power transfer using strongly coupled resonant printed circuit boards
P2.19	Nicholas Weigle, Elliott Berens	Hope College	Chemical defenses in the seeds of pioneer plants
P2.20	Samuel Alves-Czachor	Grinnell College	Synthesis and characterization of molybdenum(V) imido complexes
P2.21	Siddhant Singh	Macalester College	Laser Excitation Spectra of Niobium and Tantalum Hydride
P2.22	Sonja Katt	Carthage College	Synthesis of ZIF-8 Metal Organic Framework to Improve Water Quality
P2.23	Frederick Lehman	Knox College	Synthesis and characterization of Mn(II) carboxylate caprolactam adducts

Poster Session 3: 3:45 p.m. - 4:45 p.m. Room: GCIS Atrium

Poster #	Presenter Name	Institution	Title of Presentation
P3.01	Shauna Capron	Gustavus Adolphus College	Measuring the Success of Sustainable Land Use Practices in Seven Mile Creek Watershed
P3.02	Yu Wu	Colorado College	Reactivity of Malonic Acid Half Thioester Derivative with Benzyne Precursor under Base Catalyst Conditions
P3.03	Maia Cohen	Washington University in St. Louis	Methods for finding supernova grains
P3.04	Anway De	St. Olaf College	Improving the Usability of Two-Parameter Persistence Software
P3.05	Alexandru Florea	Gustavus Adolphus College	In Situ Determination of pH Changes Inside HPLC Columns

P3.06	Dreycen Foiles, Runyao Yin	Grinnell College	Improving the Sensitivity of LSPR Biosensors for Microtubule Nucleation Detection
P3.07	Amy Imdieke	St. Olaf College	Quantifying the Effects of Cosolutes on the Stability of Bulged RNA Duplexes
P3.08	Emmet Katzer	Carthage College	Correlations Between Different UV Environments and DIB Strengths
P3.09	Madeline Kroeger, Jam Hamza, Michaela Lindemann, Noah Mayer	Luther College	Synthesis and characterization of new unsymmetrical diglycolamide ligands for rare earth metal extraction
P3.10	Chase Snodgrass	Grinnell College	Analysis of Noise Enhanced Propagation in a Mechanical Array
P3.11	Lisa Lin	University of Chicago	Chemical Consequences of Giant Impacts on Proto-Uranus
P3.12	ALain Brilliant NIshimwe	Luther College	Quantifying atomic scale wear with an atomic force microscope
P3.13	Yu Nishio	Grinnell College	Synthesis of Lugdunin and Lugdunin Derivatives
P3.14	Sami Pathak	Washington University in St. Louis	Mathematical modeling of thin-filament regulation and its application to understanding modulators of cardiac contraction
P3.15	Logan Caraco	Macalester College	Making the Blockly library accessible via touchscreen
P3.16	Chris Seong	St. Olaf College	Synthesis of Novel PNNP Ligands and their First Row Transition Metal Complexes
P3.17	William Setterberg	Macalester College	Diamond-Based Optical Magnetic Sensing of Superconductors
P3.18	Jared Siegel	University of Chicago	Smoothed Particle Inference Studies of Supernova Remnant Abundances
P3.19	Terrell Solberg	Hope College	Preparation of a PEDOT-based redox mediator for the electrochemical detection of glucose
P3.20	Tiffany Suwatthee	University of Chicago	Electrostatic Effects on the Binding of Milk Fat Globule EGF Factor 8 to Phospholipid Membranes
P3.21	Sophia Tajnai	Carthage College	Developing Light Sheet Microscopy at a Small Liberal-Arts College
P3.22	Haocheng Wang	St. Olaf College	HiPerCiC: Custom Web Applications and Infrastructure

Abstracts for all Sessions
Physical Sciences, Math and Computer Science
MCMS Undergraduate Research Symposium, University of Chicago
November 15-16, 2019

All abstracts (poster and oral) listed alphabetically by presenter last name. Abstracts with multiple presenters appear only once with first listed presenter. Session index follows list.

Presenter(s): Keir Adams, University of Chicago

Session: Oral I.B.4 (10:50)

Title: Characterizing the timescale and voltage dependence of Cs₃Bi₂I₉ as high-performing and tunable supercapacitor electrode material

Advisor(s): Neil Robertson, Chemistry, The University of Edinburgh

Co-Author(s): Keir Adams, John Mallows, Tianyue Li, Dimitrios Kampouris, Job Thijssen, Neil Robertson

Abstract: Supercapacitors classify as either electric double layer capacitors (EDLCs) or pseudocapacitors depending on their predominant charge storage mechanisms: whereas EDLCs boast high power densities by rapidly polarizing/depolarizing electrolyte on charged electrodes, pseudocapacitors attain significantly higher energy densities by employing slower Faradaic reactions on the electrodes' surfaces and near-surface pores. To develop a flexible supercapacitor with tunable electrochemical behavior, we assemble a symmetric Cs₃Bi₂I₉-based supercapacitor that supplements predominantly EDLC-type electrostatic charge accumulation at higher potentials (0.3-0.6 V) with Faradaic charge adsorption/desorption at lower potentials (0.0-0.2 V). Due to its varied charge storage mechanisms, the supercapacitor attains maximum gravimetric and areal capacitances of 280 F/g and 2.4 F/cm², representing orders of magnitude improvement over previously reported X₃Bi₂I₉-based devices, while still achieving 88% capacitance retention after 5000 charge-discharge cycles. We thoroughly characterize the timescale and voltage dependence of the charge storage mechanisms through cyclic voltammetry, galvanostatic charge-discharge cycles, and electrochemical impedance spectroscopy. In particular, we perform equivalent circuit simulations at both high (0.4 V) and open circuit potentials to attribute Ohmic loss, charge transfer resistance, and capacitive behaviors to electrochemical processes including Faradaic ion adsorption/desorption, mass diffusion and pore penetration, and electron transfer at timescales ranging from 150 kHz to 0.01 Hz.

Presenter(s): Samuel Alves-Czachor, Grinnell College

Session: Poster P2.20

Title: Synthesis and characterization of molybdenum(V) imido complexes

Advisor(s): Martin Minelli, Chemistry Department, Grinnell College

Abstract: Mo(VI) imido complexes of the type Mo(NAr)(sma)L (Ar=2,6-diisopropylbenzene; smaH₂=N-salicylidene-2-aminothiophenol; L=catecholate, (OO) 2; 2-mercaptophenolate, (SO) 3; 1,2-benzenedithiolate, (SS) 4; 2-amidophenolate, (NO) 5; 3-amidonaphthalate, 6; 1,2-amidonaphthalate, 7; 2-amidothiophenolate, (NS) 8) have been isolated and characterized. Compounds 2, 3, and 4 show a reversible one-electron reduction in their cyclic voltammogram. In these complexes, L is bound in two equatorial positions. In complexes 5-8, where L is coordinated in an equatorial and axial position, no reversible electrochemical reduction is possible. Chemical reduction with a one-electron donor (cobaltocene) can produce Mo(V) complexes for all seven compounds. These Mo(V) complexes have been isolated and characterized.

Presenter(s): Adee Athiyaman, Knox College

Session: Oral I.B.2 (10:10)

Title: Synthesis and characterization of heteroleptic copper dimers generated from tetrakis(3-phenylpropionate) dicopper(II) precursor

Advisor(s): Thomas W. Clayton Jr., Chemistry, Knox College

Co-Author(s): Thomas W. Clayton Jr.

Abstract: Liquid crystals are anisotropic fluids that feature characteristics of both solids and liquids – organization and fluidity. Liquid crystals have numerous applications such as in biotechnology, electronics, and even renewable energy sources. Copper (II) carboxylate complexes were first discovered in 1938 to feature liquid crystalline properties. Since then numerous homoleptic copper (II) carboxylate liquid crystals have been identified. These homoleptic long chain carboxylates have been thoroughly investigated, but there are no reported heteroleptic carboxylate liquid crystals in the literature. In this project, tetrakis(3-phenylpropionate)dicopper(II) was synthesized from copper (II) chloride dihydrate and sodium 3-phenylpropionate in water. Through axial site addition of caprolactam and TPPO, room temperature liquid crystals were produced. The lability of the 3-phenylpropionate ligand (and carboxylate ligands in general) was utilized to synthesize novel heteroleptic copper (II) dimers. The effect of branching on the melting point and the range of thermal stability of these liquid crystals was investigated. New compounds are characterized through thermal studies, FT-IR spectroscopy, polarized optical microscopy, and elemental analysis. Crystallization of heteroleptic TPPO adducts is in process; suitable crystals will be sent for analysis by X-ray diffraction.

Presenter(s): Filip Belik, Gustavus Adolphus College

Session: Oral II.G.3 (2:55)

Title: A Study of the Propagation of Health Related Habits on Twitter

Advisor(s): Louis Lei Yu, Department of Mathematics and Computer Science, Gustavus Adolphus College

Co-Author(s): Jeffery Engelhardt, Louis Lei Yu

Abstract: There has been a rise in the growth of online social networks in recent years. They allow users to generate and access a vast array of real-time content and facilitate the propagation of ideas. One type of content frequently generated and shared is related to health and exercises. Our study examines how individuals' periodic health and exercise habits can change and propagate due to the influence of health-related content in online social networks, in particular, Twitter. First, to be able to identify whether individuals' tweets are about health and exercises, we tested multiple machine learning algorithms and found that the Neural Network classifier outperforms that of Naive Bayes, Decision Trees, Random Forests, and Support Vector Machines. Next, we selected 10,000 accounts in Twitter and monitored them over a 12 weeks period. We analyzed the change in users' periodic health and exercise habits in relation to that of their followees and found that there is a correlation between the habits of users who are linked; this is due to both social influence and social selection. And, stronger connections lead to stronger correlations in habits. Finally, users are more likely to be socially influenced by others whom they have stronger connections with.

Presenter(s): Jessica Bigley, Washington University in St. Louis

Session: Poster P2.14

Title: Characterizing UBQLN2, an ALS-associated gene, in a yeast model system and defining its genetic modifiers

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

Abstract:

Background: Amyotrophic Lateral Sclerosis (ALS) is a progressive neuromuscular disease that destroys nerve cells and is characterized by the formation of protein aggregates in upper and lower motor

neurons. There is no clear cause of ALS, though recent studies have identified mutations in key genes that are associated with its development. The UBQLN2 gene encodes ubiquilin-2, a protein responsible for proteasomal degradation of ubiquitinated proteins. Mutations to UBQLN2 are associated with ALS, and lead to the aggregation and cytosolic accumulation of UBQLN2. Our lab has shown that heat shock protein 104 (Hsp104) can suppress the toxicity of multiple ALS-associated proteins by reversing their misfolding. I am investigating the toxicity of UBQLN2 and its mutants in a yeast model system to better understand its association with ALS.

Methods: The UBQLN2 gene and ALS-associated variants were PCR amplified and inserted into a yeast vector under the control of a galactose inducible promoter. The UBQLN2 variants were then transformed into yeast to assess their toxicity. Hsp104 variants were then assessed for modification of UBQLN2 toxicity.

Results: UBQLN2 was found to be toxic in yeast. Hsp104 suppresses this toxicity. **Conclusion:** My results suggest that UBQLN2 is toxic in yeast and Hsp104 has the ability to rescue this toxicity.

Presenter(s): Andrew Boldt, Jonathan Ramirez, Carthage College

Session: Poster P1.03

Title: Radical Functionalization Using Photoredox Catalysis

Advisor(s): Susan Stevenson, Chemistry, Carthage College

Abstract: Photoredox catalysis is a powerful tool used to form carbon radicals. These highly reactive carbon radicals can be generated from triphenylphosphonium salts through cleavage of the carbon-phosphorus bond. By using visible light as an energy source instead of heat or UV light these reactions proceed in a more sustainable manner. A series of experiments were conducted testing the reactivity of the phosphonium salts under photoredox conditions. Initial experiments indicated that dimerization of the benzyl substrate was the major reaction pathway. Different aspects of the reaction were optimized such as light, catalyst, atmosphere, etc. Once optimal conditions were set, the substrate scope was explored. Preliminary experiments have demonstrated that substrates with electron-donating groups prefer to dimerize and substrates with electron-withdrawing groups undergo reduction. A natural product, brittonin A, was also synthesized using this method.

Presenter(s): Conor Broderick, Macalester College

Session: Poster P2.06

Title: Organic Electronic Materials Synthesis: Progress Toward n-Cationic Naphthalene Diimides

Advisor(s): Dennis Cao, Chemistry, Macalester College

Co-Author(s): Dennis Cao, Grace Eder

Abstract: Organic electronic materials are an important area of exploration in an attempt to create greener and more renewable electronics. Naphthalene diimides (NDIs) are particularly interesting due to their excellent reduction/oxidation chemistry and functionalization possibilities. This poster explores the synthesis of cationically functionalized NDIs for the creation of n-type electron accepting compounds. Successful substitution of diphenyl(phosphino)ethane nucleophiles onto the NDI scaffold has been completed, resulting in a diradical, dicationic NDI. Work continues on structural and electronic characterization of the synthesised NDI compounds, in addition to expansion of the synthetic techniques to other phosphorus and sulfur-based nucleophiles.

Presenter(s): Caroline Burkhardt, Hope College

Session: Poster P1.06

Title: Iterative Learning Techniques for Improved Performance of Bio-Inspired Control Law

Advisor(s): Courtney Peckens, Engineering, Hope College

Co-Author(s): Courtney Peckens

Abstract: Earthquakes and environmental loads produce risk of failure for civil infrastructure. Through inspiration from the biological nervous system, an active feedback control system can be implemented into infrastructure to mitigate risk. The control system comes from the derivation of a simplified control law through application of Particle Swarm Optimization (PSO), an iterative learning technique, that uses position and velocity of particles (i.e. potential weighting matrices) to converge to an optimal weighting matrix based on cost functions. Combined average cost functions, a ratio of the structure's controlled and uncontrolled responses on each floor, were optimized in simulation on a 4-story small-scale shear structure with two actuator carts. To increase the effectiveness of PSO, modifications to the algorithm were considered for the particles to converge more strategically. The inertia weighting method based off position resulted in an improvement by reducing the average cost function and increasing control effectiveness by 7.3%. Additionally, combination of the weighting method with neighborhood generation increased control effectiveness by 5.6%. Such improvements demonstrate that PSO is an effective method for developing weighting matrices that can improve performance in bio-inspired control architecture and increase the safety of infrastructure.

Presenter(s): Mesut Caliskan, University of Chicago

Session: Oral II.E.1 (2:15)

Title: The Hubble Constant from the Lensed Gravitational Waves

Advisor(s): Tjonnie Li, Department of Physics, The Chinese University of Hong Kong

Abstract: The Hubble Constant tells us the current rate of expansion of the universe. This allows us to learn about the size, age, and the density of the universe. There are several calculations of the Hubble. However, these differ significantly. Therefore, new methods of calculation, which are independent and accurate, are needed. Gravitational waves, like photons, can be lensed, possibly leading to multiple images detected as repeated events. Once detected, the time-delay induced by lensing could allow us to locate the gravitational wave source's host galaxy via sky localization, allowing us to determine the redshift of the source and the lens. By obtaining the redshift of the source and the lens, and measuring the lens' Fermat potential, we can measure the Hubble Constant without requiring an electromagnetic counterpart for the event as traditional methodologies do. This measurement has been done using mock data consisting of: source redshift $z_s = 2.00 \pm 0.05$, lens redshift $z_l = 0.50 \pm 0.05$, time difference with 0.01% uncertainty, and Fermat potential with ~0.6% uncertainty. The Hubble has been measured to be 70.8 ± 0.9 km/s/Mpc.

Presenter(s): Shauna Capron, Gustavus Adolphus College

Session: Poster P3.01

Title: Measuring the Success of Sustainable Land Use Practices in Seven Mile Creek Watershed

Advisor(s): Laura D. Triplett, Geology, Gustavus Adolphus College

Co-Author(s): Shauna R. Capron and Laura D. Triplett

Abstract: Seven Mile Creek watershed is located in south-central Minnesota. Historically, this watershed consisted of a variety of prairie and wetland landscapes, but in the wake of European-style agriculture coming to dominate the region, erosion rates accelerated and higher levels of pollutants (specifically nitrate, phosphorus, suspended solids, and E. coli) are found in Seven Mile Creek's water. In an attempt to offset the negative effects agriculture has had on this stream, some local farmers have

voluntarily implemented best management practices (BMPs) on their land. Others, however, remain skeptical of the effectiveness of BMPs. The purpose of this study was to monitor the water quality in Seven Mile Creek to determine how nutrient and sediment pollution has responded to changing agricultural practices at the sub-watershed level. In addition, it sought to uncover which BMPs are most effective in reducing sediment pollution through the use of LiDAR and GIS technology. This was accomplished by analyzing the rate of ravine erosion in which runoff flows primarily from farmlands dominated by a given BMP. Preliminary results indicate that these BMPs can reduce sediment levels, and that nitrate levels have decreased slightly since BMP implementation.

Presenter(s): Logan Caraco, Macalester College

Session: Poster P3.15

Title: Making the Blockly library accessible via touchscreen

Advisor(s): Lauren Milne, Mathematics, Statistics, and Computer Science, Macalester

Co-Author(s): Sebastian Deibel, Yufan Ma, Lauren Milne

Abstract: Block-based programming environments are a popular way to learn programming. Many of these libraries, including Scratch and MIT's App Inventor, are built on the Blockly library from Google. Unfortunately, programs built with the Blockly library are currently not accessible for people with visual impairments. We describe two designs to make the Blockly library accessible using a screen reader on a touchscreen device.

Presenter(s): Nicole Chavarria, Colorado College

Session: Poster P1.19

Title: Geospatial and Temporal Mapping of per-Fluorinated Alkyl Substances in Colorado Springs Via EPA Method 537.1

Advisor(s): Eli Fahrenkrug, Tyler Cornelius, Chemistry, Colorado College

Co-Author(s): Karina Grande

Abstract: Per- and poly-fluorinated alkyl substances (PFAS) are an unregulated class of human-made chemicals. PFAS has been used heavily in Aqueous Film Forming Foams (AFFFs) to suppress fuel fires at military installations and commercial airports. However, recent studies have connected PFAS exposure to several health conditions including three different types of cancers. This work is a joint academic/citizen science initiative aimed at investigating the fate and transport of ten individual PFAS compounds through the surface water and groundwater as it continues to infiltrate the aquifer. Groundwater samples are collected directly by citizens and organized for analysis in-house using a modified version of the EPA 537, a method employing a combination of solid phase extraction (SPE) and high-performance liquid chromatography tandem mass spectrometry (HPLC-MS/MS). Chemical data is analyzed using both geospatial and temporal models. Our initial work indicates differential diffusion/adsorption of PFAS compounds correlated with chain length and equilibrium partition coefficient. Further, surface water analyses confirm the point source of contamination as the Northwest boundary of the Peterson Air Force Base.

Presenter(s): Jerrell Cockerham, Colorado College

Session: Oral I.C.1 (9:50)

Title: Polynomial Conversion Involved in Describing Weight q -Multiplicities for Representations of the Exceptional Lie Algebra g_2

Advisor(s): Pamela Harris, Mathematics, Williams College

Co-Author(s): Melissa Gutierrez-Gonzalez and Amaury Minino

Abstract: In combinatorial representation theory, Kostant's partition function counts the number of ways a given weight of a Lie algebra g can be written as a non-negative integral linear combination of the positive roots of g . In this talk, we will learn a closed formula for Kostant's partition function for the

exceptional Lie algebra \mathfrak{g}_2 and the methods used for obtaining this formula. We will then learn a closed formula for the q -multiplicity of a weight in a highest weight representation of \mathfrak{g}_2 .

Presenter(s): Alexander Cohen, University of Chicago

Session: Oral II.H.4 (3:15)

Title: Coarse-grained simulations of conjugated polymers and graph-theoretic measures for exciton transport

Advisor(s): Juan de Pablo, Pritzker School of Molecular Engineering, University of Chicago

Co-Author(s): Nicholas Jackson, Alec Bowen, Juan de Pablo

Abstract: Conjugated polymers are well known to self-assemble into single-chain π -stacked configurations. Many groups have reported dramatically increased exciton diffusion lengths and charge mobilities in these polymeric structures, both of which are necessary for a variety of high-performance optoelectronic devices. Previously, simulations have been limited to either atomistic simulations or coarse-grained models using isotropic potentials; the former is too computationally costly to simulate mesoscopic length scales, whereas the latter does not capture the important anisotropic physics of π -stacking. In this work, we develop and apply an anisotropic coarse-grained polymer model utilizing ellipsoidal monomers and the Gay-Berne potential. We analyze how the coil-globule transition changes as a function of molecular design parameters, notably interaction strength, semiflexibility, and dihedral stiffness. In addition, we present computationally efficient graph-theoretic analysis of exciton transport properties within these polymeric structures, with explicit correlations to quantum-mechanically computed exciton mobilities. This work opens the door for computationally cost-effective models for the description of quantum-mechanical transport phenomena at mesoscopic scales.

Presenter(s): Maia Cohen, Washington University in St. Louis

Session: Poster P3.03

Title: Methods for finding supernova grains

Advisor(s): Ryan Ogliore, Physics, Washington University in St. Louis

Abstract: Supernova events are happening continuously, even before our solar system existed. One way that we can learn about the environment around our solar system is by comparing supernova events from before our solar system existed to contemporary ones. This can be done by comparing the dust that these supernovae create. We have developed a method that will efficiently search deep-sea sediment samples in order to find these contemporary supernova grains. After using a series of acid dissolutions to get rid of the organic matter in the sediment, we deposited a small amount of the sediment sample onto a stub and used a scanning electron microscope to image it in backscatter electrons. We used energy dispersive x-ray spectroscopy to determine the composition of each grain on the stub and identify potential supernova grains. We have found 6 potential supernova grains that are entirely composed of carbon, indicating that they could be contemporary graphite grains. Analyses of stable and unstable isotopes of these grains using nano-scale secondary ion mass-spectrometry will unambiguously identify them as presolar circumstellar grains, contemporary supernova grains, or terrestrial grains. Now that we have developed a method to search for these grains, we can search large amounts of sediment until we find the contemporary supernova grains we are looking for.

Presenter(s): Bryce Cook, Grinnell College

Session: Poster P1.05

Title: Synthesis and Biological Evaluation of Lugdunin Analogues

Advisor(s): Erick K. Leggans, Chemistry, Grinnell College

Abstract: Lugdunin, isolated from *Staphylococcus lugdunensis* found in the human nasal microbiome, has demonstrated promising results as a powerful antibiotic against many resistant strains of bacteria. One such bacteria that lugdunin has shown to be an effective antibiotic against is *S. aureus*, which demonstrates resistance to common antibiotics such as methicillin. In hopes of increasing lugdunin's ability as an antibiotic, we envision two synthetic approaches to derive different analogues at the heterocyclic position of lugdunin.

Presenter(s): Amy Crawford, Gustavus Adolphus College

Session: Oral II.H.2 (2:35)

Title: 2D-LC/HRMS for direct structure characterization of small molecule drugs

Advisor(s): Dwight Stoll, Chemistry, Gustavus Adolphus

Co-Author(s): Weijuan Tang, Yu He

Abstract: Many methods in use across the pharmaceutical industry for the purpose of certifying quality of drug product are based on high performance liquid chromatography and use non-volatile mobile phases that are incompatible with mass spectrometry (MS). This makes the direct analysis of active pharmaceutical ingredients and their related impurities difficult as it requires tedious fractionation and isolation prior to offline analysis by MS. An online alternative that allows for direct impurity analysis is adding a second dimension to desalt the sample before sending it to the MS. Effluent containing salt from the first dimension is diverted to waste while the remaining effluent is sent to the MS. This allows for both improved separation as well as the removal of any non-MS friendly components, making the online analysis of impurities by MS and MS/MS possible. 2D-LC-MS/MS methods were developed for three small molecule drugs: MK-8616; MK-8408; and MK-8742. Existing release methods in use for these products contain MS-incompatible salts. MS1 and MS/MS data were collected for the active pharmaceutical ingredient and related impurities for structural elucidation.

Presenter(s): Emma Daggett, Jonathan Rustad, St. Olaf College

Session: Poster P2.08

Title: Temperature dependence of the optical properties of cesium lead halide perovskite nanocrystals

Advisor(s): Rodrigo Sanchez-Gonzalez, Chemistry, St. Olaf College

Co-Author(s): Jonathan Rustad

Abstract: The use of laser diagnostics, such as Laser Induced Fluorescence (LIF), allows the measurement of a number of variables such as pressure, temperature, and velocity of flow fields relevant to numerous applications that include combustion, materials synthesis, energy and transportation, and high-speed aerodynamics. The use of lasers as measurement tools offers unique advantages such as minimum intrusiveness, selectivity, and high time and space resolution. Nanocrystal structures of various semiconductor materials, such as quantum dots, are known to exhibit notable optical properties in terms of their strong luminescence, wide excitation wavelength range, and narrow emission spectrum. A remarkable characteristic of these materials is the size-dependence of the absorption and emission properties that can be tuned by changing the size of the nanocrystals. While the optical characteristics of quantum dots have been thoroughly studied, other types of nanocrystals with similar properties remain generally optically uncharacterized. One such example is perovskite nanocrystals. These nanocrystals are notably easier to synthesize and show higher emission quantum yields. In this work, we study the optical properties of lead halide perovskite nanocrystals, specifically the relationship between their fluorescence spectrum and temperature. We propose how this relationship can be experimentally determined to employ these materials as temperature sensors.

Presenter(s): Fabian Dauzvardis, Beloit College

Session: Oral II.F.2 (2:35)

Title: Emulsion Polymerization, Size Determination and Self-Assembly of Monodispersed Poly (methyl methacrylate) Nanospheres for Photonics

Advisor(s): George Lisensky, Department of Chemistry, Beloit College

Co-Author(s): George Lisensky, Jiaqi Luo, Jacob Horger, Emma Koenig

Abstract: Monodispersed poly(methyl methacrylate) nanospheres are synthesized through addition or chain polymerization of a rapidly stirred aqueous mini-emulsion of methyl methacrylate. 2,2-Azobis(2-methylpropionamide) dihydrochloride serves as a heat activated, water soluble, free radical initiator to polymerize the emulsion droplets starting from their outer edge. The uniform small diameter particles after self-assembly appear iridescent since they are close-packed and their size is similar to the wavelength of visible light. The size of the poly(methyl methacrylate) spheres is characterized by five methods: the terminal velocity and Stoke's Law, evaporative self-assembly of a photonic material and visible spectroscopy, direct measurement using scanning electron microscopy (SEM), SEM measurement of the silica inverse opal, and atomic force microscopy.

Presenter(s): Anway De, St. Olaf College

Session: Poster P3.04

Title: Improving the Usability of Two-Parameter Persistence Software

Advisor(s): Matthew Wright, Mathematics, St. Olaf College

Co-Author(s): Jason Jung

Abstract: Topological Data Analysis (TDA) is the study of data and its shape. The field of TDA is useful for understanding features, not easily observable, of data in relatively high dimensions. The Rank Invariant Visualization and Exploration Tool, a.k.a RIVET, is a tool for visualizing two-parameter persistent homology, which is a type of TDA. RIVET computes and visualizes two-parameter persistence modules from various kinds of datasets, such as point clouds or distance matrices. Since this entire area is complicated, the aim of our research is to make this software more accessible to users. Towards this end, we have created diagrams of several simplicial complexes to describe the topological structure that RIVET detects. To make the final output more accessible and understandable to the user, documentation has been added, explaining the process at each step. We are working to make the RIVET interface more user-friendly, by adding features like loading new data files without exiting the software, supporting csv input files, and streamlining the required data parameters. For the advanced user, support has been added to specify advanced parameters in the input file. We are also continuing to work on further improvements like supporting cubical data as input and improving mathematical algorithms.

Presenter(s): Jennifer DeJong, Yilin Chen, Macalester College

Session: Poster P2.13

Title: Signal Processing on the Permutahedron: New Analysis Tools for Ranked Choice Data

Advisor(s): Thomas Halverson, David Shuman, MSCS, Macalester College

Co-Author(s): Yilin Chen, Thomas Halverson, David Shuman

Abstract: In ranked choice voting, voters order their preferences for n candidates. In this project, we investigate new methods to analyze the overall structure of and find patterns within ranked choice voting data. Each ranking is a permutation, and the permutahedron is the graph whose vertices are permutations and for which two permutations are connected if they differ by an adjacent transposition. This graph is the Cayley graph of the symmetric group. By viewing the number of votes for each permutation as a signal on the permutahedron, we can analyze the data using tools from graph signal processing in combination with tools from group representation theory. Eigenvectors and eigenvalues of the permutahedron graph Laplacian are important for understanding the underlying structure of

ranking data, and group theory captures symmetry in the data. These symmetries are maintained as its eigenvectors are lifted from smaller graphs, constructed through quotients of the symmetry group. This allows for faster computation as well as analysis of the data that captures information from two different fields of mathematics.

Presenter(s): Kavya Devgun, St. Olaf College

Session: Poster P1.14

Title: Development of an optical system to determine impurity content & composition in a snowpack

Advisor(s): Alden Adolph, Physics, St. Olaf College

Abstract: Snow influences global temperatures due to its high reflectivity. This reflective property is called albedo, the fraction of solar radiation reflected off of a surface. Among other factors, light absorbing particles (LAPs) such as black carbon, organic carbon, and dust can decrease snow albedo, subsequently accelerating snowmelt. Referencing previous studies, we built an optical system to measure LAP concentration in a snow sample following filtration through a Nuclepore filter. To do this, we used a light source ranging from 230 nm to 2500 nm, two integrating spheres, and a spectrometer to record light transmitted through a filter to measure LAP concentration. Following design and development, we have continued to characterize and calibrate the system. Preliminary analysis of varying concentrations of black carbon show that this is a promising measurement technique for use on snow from the St. Olaf Natural Lands. These local measurements will be helpful in understanding the role of impurities in Midwestern snow albedo and the implications for timing of seasonal snow melt as global temperatures continue to increase.

Presenter(s): Leonardo Ferreira Guilhoto, University of Chicago

Session: Poster P1.17

Title: Numerically Solving the Generalized Dirichlet Problem Using Stochastic Calculus

Advisor(s): Peter May, Department of Mathematics, University of Chicago

Abstract: Some problems in the area of Partial Differential Equations require solutions to satisfy some condition inside an open domain and agree with some pre-established values in the boundary of this domain. We use techniques from Stochastic Calculus to numerically solve some of these boundary value problems related to semi-elliptic differential operators which can be framed as what is known as generalized Dirichlet problem. By joining numerical techniques from Stochastic Calculus and Monte Carlo methods we present an algorithm able to numerically approximate the solution of the generalized Dirichlet problem at any desired point in space. Since this technique uses the Monte Carlo method, it is especially useful when dealing with problems in higher dimensions.

Presenter(s): Alexandru Florea, Gustavus Adolphus College

Session: Poster P3.05

Title: In Situ Determination of pH Changes Inside HPLC Columns

Advisor(s): Dwight Stoll, Analytical Chemistry, Gustavus Adolphus College

Co-Author(s): Gabriel Leme, Tyler Brau, Thomas Lauer, and Dwight Stoll

Abstract: In most modes of liquid chromatography a significant fraction of the mobile phase is an aqueous solution. When the analytes of interest to a particular separation are ionogenic, the pH of the aqueous component of the mobile phase can have a significant effect on retention and separation.

In this work the pH levels at the inlet and outlet of HPLC columns of varying lengths were studied. Generally, a plug of pH 3 buffer was injected into a pH 7 mobile phase, where the volume of the injected plug was varied from 10 to 360 μL , and a mixture of colorimetric indicator dyes was used to determine the local pH, either at the column inlet or outlet. Other variables studied include the use of Active Solvent Modulation (ASM) and the compositions of the buffers used in the injected plug vs. the mobile phase. A methodology was developed to predict the pH levels at the column inlet and outlet. While the accuracy of this approach is good for several conditions, in other cases it is not, and work is ongoing to understand the observed discrepancies between predictions and experimental results.

Presenter(s): Dreycen Foiles, Runyao Yin, Grinnell College

Session: Poster P3.06

Title: Improving the Sensitivity of LSPR Biosensors for Microtubule Nucleation Detection

Advisor(s): Keisuke Hasegawa, Physics, Grinnell College

Abstract: Microtubules (MTs) are a type of protein filament found in eukaryotic cells that play important roles in cell division. The components of MTs, $\alpha\beta$ -tubulins are smaller than the diffraction limit of light, limiting our understanding of the initial formation of MTs, called nucleation. Recently, localized surface plasmon resonance (LSPR) biosensors using spherical nanoparticles were developed to detect MT nucleation. In this project, we aimed to improve the sensitivity of LSPR biosensors for the detection of MT nucleation using nonspherical nanoparticles. We began by searching for software that can numerically solve Maxwell's equations for simulating LSPR biosensors, and eventually decided on using the discrete dipole approximation (DDA) implemented in the DDSCAT software. We then used DDSCAT to test both the cylinder and shell models for MTs. We found that nanorods experience double the shift of peak wavelength at a given MT length as nanospheres.

Presenter(s): João Francisco Shida, Fangjian (Roy) Wu, University of Chicago

Session: Poster P1.12

Title: Design of a Cesium Vapor Pressure Gauge Based on Electronic Thermionic Emission

Advisor(s): Henry Frisch, Physics Department, Enrico Fermi Institute, The University of Chicago

Co-Author(s): Fangjian (Roy) Wu, Mesut Caliskan

Abstract: We describe the design and underlying principles of a tungsten-filament gauge for the partial vapor pressure of cesium. Operation is based on the temperature dependence of electronic thermionic emission from a tungsten filament with a thermally equilibrated partial coverage of cesium, which increases with vapor pressure and decreases with filament temperature. Due to the reduction of the work function of thermionic emission, the current from the filament is a measure of the coverage. By fitting the curve of emission versus filament temperature to a theoretical model, the cesium vapor pressure is obtained. We explain the physical principles behind the device, and describe the construction, operation, and calibration of a prototype built to test the performance of this concept. We document the construction, operation, and calibration of the gauge and analyze the differences between the predicted and experimentally measured data. Based on the analysis, we elaborate on how to design this gauge to obtain better data on desired thermionic emission.

Presenter(s): Allie Goldman, Lawrence University

Session: Poster P2.02

Title: Progress Toward a Pyrene-derived Redox-active Ligand for use in Coordination Polymers

Advisor(s): Graham Sazama, Chemistry (Inorganic), Lawrence University

Abstract: Coordination polymers, macromolecules with repeated patterns of multi-topic ligands and metal centers, possess unique electrical characteristics, as demonstrated by recent research. The creation of coordination polymers using redox-active ligands—organic linkers with multiple accessible,

stable redox states when bound to a transition metal—may be an important avenue for accessing conductive properties in coordination polymer materials. These materials are promising for energy storage, sensors, and other electronics applications. Progress has been made on the production of novel pyrene-derived redox-active linker ligands: the partially completed ligand has been produced through the complete oxidation of pyrene into pyrene-4,5,9,10-tetraone using sodium periodate and catalytic ruthenium chloride. Future work will involve reductive amination of the ketones, followed by complexation with various transition metals to form molecular and coordination polymers materials.

Presenter(s): Gabriella Griffen, University of Chicago

Session: Poster P2.10

Title: Optimizing the Reversible Phosphate-Binding of a New Micelle-Based Material

Advisor(s): Matthew Tirrell, Pritzker School for Molecular Engineering, University of Chicago

Co-Author(s): Whitney Fowler

Abstract: The current methods for removing phosphate from wastewater convert aqueous phosphate into insoluble salts. While these methods effectively remove phosphate, the phosphate in these insoluble salts cannot be recovered for use in fertilizers, depleting usable phosphate. Thus, this project seeks to incorporate a proteinaceous P-Loop amino acid sequence into the design of a new material which will reversibly and selectively bind phosphate in order to remove and recover usable phosphate from wastewater. As the P-Loop interacts with phosphate via hydrogen bonds, these interactions change as a function of pH, creating the possibility for capture and release. To achieve these goals, we designed and synthesized self-assembling peptide amphiphiles (PAs) with hydrophilic “headgroups” containing the P-Loop and hydrophobic alkyl “tails”. The PAs display the phosphate-binding sequence to the surrounding aqueous environment when they self-assemble into micelles. In my work on this project, I tested the material’s reversibility and effectiveness. Using the molybdenum reaction across a range of pH values, I determined that maximum binding occurred at pH 6, with potential release pH values of 2 and 11. Based on this data, I devised reversibility tests which showed that the material can reversibly bind and release phosphate as a function of pH.

Presenter(s): Elvis Haisa, St. Olaf College

Session: Poster P2.07

Title: Developing and implementing technology to investigate the effects of temperature gradients on snow grain growth

Advisor(s): Alden Adolph, Physics, St Olaf College

Abstract: Studying snow properties is critical because current changes in snow and ice cover are affecting air temperatures, sea levels, ocean currents, and storm patterns globally. Snow’s high albedo, the ratio of light reflected from a surface, keeps the surface cooler by reflecting radiative solar energy. Previous studies have shown an inverse relationship between albedo and snow grain size. Our research addresses how snow grains grow under different temperature gradients. We designed and built a system to subject snow samples to different temperature gradients created by two plates that can be independently set to temperatures between 0 and -30°C. We tested and optimized the system to control temperature to within 0.5°C. Snow samples are placed between the plates over several days and are periodically removed for non-destructive analysis of snow grain size. To support these experiments, we have also worked to improve our optical grain size measurement techniques and have been implementing models to predict grain size change under temperature gradients. Model results will be compared to our measurements when we use our system to conduct temperature gradient experiments. Our findings will improve our ability to predict changes in snow structure under various conditions.

Presenter(s): Kathryn Hanggi, Luther College

Session: Poster P2.15

Title: Dopamine Quantification using HPLC for Biological Applications

Advisor(s): Molly Wilker, Chemistry, Luther College

Abstract: Dopamine is an important neurotransmitter in the body which has led to the desire to quantify levels in complex biological mixtures. One of the challenges of this is that dopamine is easily oxidized and common detection methods rely on it being in its reduced form. We are working to develop a method for dopamine detection and quantification using HPLC-FLD using sample conditions that prevent dopamine oxidation. In order to do this, we have identified a series of molecules with higher oxidation potentials than dopamine and investigated if these molecules prevent oxidation of dopamine in solutions. Three of the six molecules tested effectively slowed the rate of dopamine oxidation providing us with a window of time to detect the reduced form of DA using our methodology. This new method will provide us with a way to better quantify the amount and state of dopamine directly from complex biological samples by minimizing external sample oxidation.

Presenter(s): Kate Herman, Colorado College

Session: Oral I.C.3 (10:30)

Title: Numerical methods for Picard-Lefschetz solutions to the Path Integral

Advisor(s): Jonathan Brown, Physics, Colorado College

Abstract: The Path Integral provides a very general approach to analyzing quantum dynamics. However, computing closed form exact solutions to the Path Integral is usually impossible. Approximation schemes are then required to obtain useful results. Perturbative schemes (while very useful) cannot describe certain non-perturbative phenomena such as quantum tunneling. Traditionally the Euclidean time prescription is used to arrive at non-perturbative solutions to the Path Integral. However, a Picard-Lefschetz (PL) approach to the Path Integral may provide a schema more general than the Euclidean time prescription, which can also provide justification for Euclidean time instanton solutions. In this presentation we will introduce PL theory and cover our work numerically testing agreement between PL solutions and Euclidean solutions. To test such agreement, we are producing a program which will identify the complex saddles of the action which dominate dynamics. These saddles can then be compared to Euclidean solutions for verification. Further work is required to create such a program, however we have developed some techniques for identifying the contributing saddle which are reported here.

Presenter(s): Runqi Huang, University of Chicago

Session: Oral II.F.1 (2:15)

Title: Stretchable Organic Electrochemical Transistor for Implantable Bioelectronics

Advisor(s): Sihong Wang, Pritzker School of Molecular Engineering, University of Chicago

Abstract: The emergence of flexible and stretchable bioelectronics that conform to human tissues holds great promises for healthcare applications and biomedical research. However, physiological signals are particularly challenging to record and thus require sensitive devices for signal detection and amplification. The high transconductance of organic electrochemical transistor (OECT) makes it a suitable candidate for implantable bioelectronics, as it makes use of ions in the human body to modulate the conductivity of the transistor at low voltage. Nevertheless, the state-of-the-art OECT operates in depletion mode and its semiconducting polymer does not possess intrinsic stretchability, thereby failing two crucial criteria for implantability. I here report the routes to the synthesis of a p-type semiconducting polymer that operates in accumulation mode and a strategy to render the polymer stretchable. Through sidechain engineering, a diketopyrrolopyrrole (DPP) based polymer with OECT

response is obtained. The path toward stretchability involves blending the polymer with elastomer and redox-active small molecules. Demonstrations include surface morphology characterization with atomic force microscopy and output curves of the device under different stretching ratios. The results confirm the proposed DPP-based polymer for OECT application and the blending strategy as a viable future direction to achieve a stretchable organic electrochemical transistor.

Presenter(s): Zuofu Huang, Kieu-Giang Nguyen, Macalester College

Session: Poster P1.16

Title: Clustering Longitudinal Categorical Data

Advisor(s): Brianna Heggeseth, Math, Statistics and Computer Science, Macalester College

Co-Author(s): Brianna Heggeseth, Kieu-Giang Nguyen, Ellen Graham

Abstract: Why do we wake up some mornings feeling refreshed and others feeling tired? Sleep stages (Awake, Light, Deep, and REM) play an important role in determining whether we have a good night's sleep. Similarly, since diagnosis, cancer patients repeatedly go through four stages: Hospital, Home, Hospice and Skilled Nursing Facility. Motivated by the application of health utilization, our project developed statistical methods to discover patterns over time among repeated measurements over time of a categorical variable, observed for many units or individuals, called longitudinal categorical data.

We first reviewed the cluster analysis literature to create a list of candidate statistical methods that account for temporal ordering and would be appropriate for the data context. We then designed and implemented a tool for comparing methods for clustering longitudinal categorical data. It supports cluster analysis on such data using a variety of appropriate clustering methods. For each method, it produces visualizations and statistics to help interpret the clustering assignments. We also allow for comparing different clusterings and producing clustering comparison statistics such as the adjusted Rand index. We include two data sets within our Shiny App, while users could upload and analyze datasets of their choosing.

Presenter(s): Max Huang, Washington University in St. Louis

Session: Poster P2.17

Title: Low voltage Muon telescope based on plastic Scintillators and wavelength shifting fibers

Advisor(s): Jim Buckley, Physics, University of Chicago

Abstract: The work focuses on building a compact, cost-effective, and low voltage portable Muon telescope. Instead of utilizing previous muon telescope setups that depend on photomultiplier tubes (PMT) and modulus designs in lab settings, one uses silicon photomultipliers (SiPM) which require a relatively lower voltage (~40V). However, signals are less obvious, and noises are more pronounced, so a coincidence check with two scintillators are stacked in parallel positions is placed in to act as a filter. A custom-built PCB is designed to be compact while merging the detection, amplification, filtering, and direct digital/analog outputs. With a two-stage operational amplifier, comparator, and one-shots to set the window time for coincidence (typically set to 40ns), the device is capable of picking up direct signals from Muons and then be further demonstrated through +5V digital signal or light pulses out from an LED. Accuracy of the electronics for each channel can reach sub 20ns. This project serves as an outreach and a prototype for the larger gamma-ray telescope as a possible anti-coincidence scope to "alert" false particles. Its application also extends to other educational purposes due to its less demanding and compact design.

Presenter(s): Amy Imdieke, St. Olaf College

Session: Poster P3.07

Title: Quantifying the Effects of Cosolutes on the Stability of Bulged RNA Duplexes

Advisor(s): Jeff Schweinefus, Chemistry, St. Olaf College

Co-Author(s): Jeff Schweinefus, Liban Jama

Abstract: Aqueous environments influence the stability of the three-dimensional structure of biopolymers. Past research has characterized the cosolutes urea, glycine betaine, and proline as denaturants of nucleic acid secondary and tertiary structure due to favorable interactions with functional groups exposed in the single stranded state. In this study, thermal denaturation experiments were performed in aqueous urea, glycine betaine, and proline solutions using four trinucleotide bulged RNA duplexes, in the context of HIV-1 TAR RNA. The trinucleotide bulges were constructed to determine the effect of cytosine and uracil-based codons on nucleic acid stability and their interactions with specific cosolutes. Our results showed that urea served as an effective denaturant for the CCU and CCC trinucleotide bulges, glycine betaine for the CCU bulge, and proline for the CCU and UUU bulges all relative to an RNA duplex lacking a trinucleotide bulge. Our work suggests that these three cosolutes are sensitive enough to chemically probe solvent-accessible surface area changes as small as those from trinucleotide bulges.

Presenter(s): Uriya Jankurazova, Lawrence University

Session: Oral II.H.3 (2:55)

Title: De-noising Data for Topological Data Analysis

Advisor(s): Deanna Donohue, Chemistry, Lawrence University

Abstract: Currently, most methods of analyzing data involve a statistical approach. While these methods are powerful, many of these methods share similar assumptions and limitations. This work focuses on using a different approach, Topological Data Analysis (TDA). TDA is a suite of methods which focus on analyzing and retrieving the shape of a dataset and then using that shape to obtain valuable information. One TDA technique is Persistent Homology, where the dataset is evaluated for shape under a series of conditions. Shapes which persist over a large range of conditions are identified as key features. One limitation of this technique is that if the data is noisy, retrieving the underlying shape is difficult. As we evaluate the TDA methods for use in geoscience applications, the issue of noise is significant. Therefore, here we have focused on incorporating a pre-processing or de-noising step before analysis of the persistent homology.

Presenter(s): Sydney Jenkins, University of Chicago

Session: Oral I.A.5 (11:10)

Title: Cloud Characterization with Deep Learning

Advisor(s): Elisabeth Moyer, Department of Geophysical Sciences, University of Chicago

Co-Author(s): Takuya Kurihana, Ian Foster, Elisabeth Moyer, Rebecca Willett, Michael Maire, Kathryn Koenig, Ruby Werman

Abstract: Clouds play a critical role in the global climate, serving to both reflect sunlight and trap infrared radiation. However, they represent the largest source of uncertainty in projections of future climate change. Improving predictions of cloud behavior requires a refined method of cloud classification. While supervised learning methods have been used to characterize clouds, this approach requires costly label assignment by domain experts and restricts the model to artificial categories. An unsupervised learning framework, however, negates the need for human guidance and is unbiased by conventional cloud categorization techniques. In our study, we train an unsupervised Convolutional

Autoencoder to extract meaningful features from MODIS satellite data. A hierarchical clustering algorithm is then applied to the latent space at the bottleneck layer to identify novel cloud classifications. We examine the distribution of five relevant cloud optical and top features among clusters, and find preliminary verification that our model can successfully extract physically relevant features. In addition, a comparison of cluster results with labeled data demonstrates that our model can differentiate between open and closed stratocumulus clouds. Our results show that unsupervised learning can produce novel cloud classifications that capture relevant features from unlabeled satellite data.

Presenter(s): Xiaohe Jia, University of Chicago

Session: Poster P1.23

Title: Isolation of Displaced Leptons from Long-lived Slepton Decays

Advisor(s): Young-Kee Kim, Department of Physics, The University of Chicago

Abstract: In the proton-proton collisions from the Large Hadron Collider, we search for long-lived sleptons predicted by a GMSB SUSY model which decay after traveling some distance in the ATLAS detector. This decay process leaves a signal of displaced leptons, which are electrons and muons produced away from the vertex of the main event. However, heavy flavor quark decays produce jets that could also contain displaced leptons. These events are a background to our search because they could be mistaken as our signal. In this paper, I try to distinguish our signal from the heavy flavor background by considering how the background should be less isolated due to the higher energy density in the jet surrounding the leptons.

Presenter(s): Chankyung Jung, St. Olaf College

Session: Poster P2.05

Title: Improving the Usability of Two-Parameter Persistence Software

Advisor(s): Matthew Wright, Mathematics, St. Olaf College

Co-Author(s): Anway De

Abstract: Topological Data Analysis (TDA) is the study of data and its shape. The Rank Invariant Visualization and Exploration Tool, popularly known as RIVET, is a tool for visualizing two-parameter persistent homology, which is a type of TDA. RIVET computes and visualizes two-parameter persistence modules from various kinds of datasets, such as a point cloud or a distance matrix. Since this entire area is complicated, the aim of our research is to make this software more accessible to users. We have created diagrams of several simplicial complexes to describe the topological structure that RIVET detects. To make the final output more accessible and understandable to the user, we added documentation, explaining the process at each step. We developed several new features for the software, including a feature to load new data and a simplified input file format.

Presenter(s): Asa Kalish, Washington University in St. Louis

Session: Poster P1.04

Title: Robust organelle size control in *Saccharomyces cerevisiae*

Advisor(s): Shankar Mukherji, Department of Physics; Department of Cell Biology and Physiology; Center for the Science and Engineering of Living Systems, McKelvey School of Engineering, Washington University in St. Louis

Co-Author(s): Kiandokht Panjtan-Amiri, Shankar Mukherji

Abstract: Among the most important processes in the self-assembly of the eukaryotic cell is the synthesis of its organelles, specialized biochemical compartments that house processes crucial to cellular physiology. A critical property that governs organelle function is its size. Numerous molecular factors that regulate the sizes of a diverse array of organelles, including the Golgi, mitochondria, peroxisomes, and lipid droplets, have been identified. However, our understanding of the quantitative

principles governing organelle size control remains incomplete. Here, we combine organelle size data from the single-celled eukaryote *Saccharomyces cerevisiae* and mathematical theory to show that cells can robustly control organelle size fluctuations across a range of organelle sizes. In particular, our framework suggests that organelle size increases in random bursts from a limited pool of building blocks. Bursty organelle growth allows the cell to decouple the average magnitude of organelle size fluctuations from mean organelle size, provided the bursts do not deplete the pool of building blocks from which organelles grow. Bursty growth thus provides a potentially general mechanism by which cells can regulate the noise of the sizes of its sub-cellular structures.

Presenter(s): Sonja Katt, Carthage College

Session: Poster P2.22

Title: Synthesis of ZIF-8 Metal Organic Framework to Improve Water Quality

Advisor(s): Megan Moyer, Chemistry, Carthage College

Co-Author(s): Grace Tews and Megan Moyer

Abstract: Metal organic frameworks (MOFs) are a class of materials that exhibit an open framework with permanent porosity, high surface area, and crystallinity. They are constructed by joining metal-containing units with organic linkers through self-assembly. Using MOFs for filtration applications is a new and upcoming approach to improve water quality. ZIF-8 is a MOF that is part of the zeolitic imidazolate framework family, formed by the bonding of the zinc metal and nitrogen atom in the organic linker. Its small pore size allows the MOF to filter out smaller heavy metal ions from water sources compared to the standard water filtration with activate porous carbon. After successful synthesis of ZIF-8, the future steps are to test the ability of ZIF-8 to filter out heavy metal ion from water sources. The end aims are to engineer a layer fabrication of porous carbon with MOF layers under to better filter smaller molecules from contaminated water.

Presenter(s): Emmet Katzer, Carthage College

Session: Poster P3.08

Title: Correlations Between Different UV Environments and DIB Strengths

Advisor(s): Julie Dahlstrom, Physics, Carthage College

Abstract: We analyzed correlations between equivalent widths of 12 selected diffuse interstellar bands (DIBs), color excess and select column densities of known atoms and molecules. Scatterplots between DIB equivalent widths and other relevant measurements were fit with a linear model to separate points into two groups: high points and low points. High point and low point groups were selected based on sufficient deviation above or below the fitting line. Analysis of the differences of average UV extinction curves of the high and low points allowed for a comparison of preferred UV extinction environments between DIBs. Weaker DIB strengths at a fixed color excess were associated with lower average 2175 Angstrom bump strength in the UV extinction curve as well as other overall shape and level variations. By comparing differences in preferred UV extinction environments between DIBs, we established a relative order of UV tolerance among the 12 selected DIBs.

Presenter(s): Shelby Klomp, Gustavus Adolphus College

Session: Oral I.C.4 (10:50)

Title: Simulation for radio detection of dark matter photons

Advisor(s): J Anthony Tyson, Physics, University of California, Davis

Co-Author(s): Joseph Levine

Abstract: An experiment for the detection of dark photons is currently in progress at the University of California Davis, making use of coupling of dark photons to electromagnetism. In support of this project, Python code was written to explore possible analysis techniques to find small signals in noisy data. Additionally, simulations of the experimental setup containing an antenna in a room with conducting

walls were constructed in COMSOL to characterize the antenna response. Agreement between the COMSOL model and manufacturer data for the biconnical antenna model in free space give confidence to the accuracy of later models of the antenna in the room. The antenna factor determined from simulation for the model of the biconical antenna in the room will ultimately be useful for analysis of a dark photon signal to determine electric field and therefore the coupling constant of dark photons to electromagnetism, and the dark photon mass will be determined from the frequency of the signal.

Presenter(s): Madeline Kroeger, Jam Hamza, Michaela Lindemann, Noah Mayer, Luther College

Session: Poster P3.09

Title: Synthesis and characterization of new unsymmetrical diglycolamide ligands for rare earth metal extraction

Advisor(s): Benjamin G. Tokheim, Chemistry, Luther College

Co-Author(s): Jam R. Hamza, Michaela S. Lindemann, Noah H. Mayer

Abstract: Unsymmetrical diglycolamide (UDGA) ligands extract rare earth metals by coordinating with them through an anhydride pocket. UDGA ligands are designed to improve the kinetics of metal partitioning from the aqueous phase to the organic phase in the solvent extraction process. Our research was comprised of the synthesis and purification of the new ligands and the determination of the metal-ligand complex ratios. Synthesis reactions were monitored using infrared (IR) spectroscopy and product identity was confirmed with proton and carbon nuclear magnetic resonance (NMR) spectroscopy. Column chromatography was used as the purification method for removing impurities from crude UDGA ligands. Ultraviolet-visible (UV-vis) spectrophotometry was used to determine that the UDGA ligand-neodymium complex ratio is 3:1. A fitting method was also used to solve for conditional stability constants for the three metal-ligand complexes for comparison between the UDGA ligands. Inductively coupled plasma-optical emission spectrometry (ICP-OES) was used to determine distribution ratios for some of the UDGA ligands to understand their equilibration tendencies. UDGA ligands have potential application in removing rare earth metals from consumer electronics for recycling.

Presenter(s): Hope Lee, University of Chicago

Session: Oral I.D.4 (10:50)

Title: High Quality Factor SiGe Optical Ring Resonators for Microwave to Optical Quantum Transduction

Advisor: Chi Xiong, Silicon Photonics for Quantum Scalability Group, IBM TJ Watson Research Center

Co-Author(s): Chi Xiong, Ryan Schilling, Jason Orcutt

Abstract: Despite the promise of quantum computation, a serious technical obstacle—the susceptibility of lower energy, microwave photons to decoherence—restricts large-scale implementation. Therefore, efficient single-photon level transduction between microwave and optical photons is desired. My work at IBM Research was involved with the development and characterization of two-port optical SiGe/Si ring resonators intended for a microwave-to-optical transducer.

The resonator properties of interest are the quality factor (Q) and free spectral range (FSR). To characterize these, I measured the transmission signal at two outputs (through and drop) which demonstrate periodic dips (through) and peaks (drop). The FSR is determined from the distance between adjacent features. By fitting the outputs with simultaneous models, physical parameters are obtained, including the cross-coupling coefficient and the round-trip attenuation, from which the intrinsic Q can be calculated. The maximum measured intrinsic Q for a device was 2.072 million.

To determine additional causes limiting the current Q, I investigated loss induced from the bus-waveguide-to-ring coupler by running FDTD simulations. The lowest coupling loss was found for larger coupling gaps, suggesting that larger gaps may improve intrinsic Q. Planned work include reduction of defect density, exploration of additional device designs, and more precise data background analysis.

Presenter(s): Frederick Lehman, Knox College

Session: Poster P2.23

Title: Synthesis and characterization of Mn(II) carboxylate caprolactam adducts

Advisor(s): Thomas Clayton, Chemistry, Knox College

Abstract: Previous work has shown that $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ will form polymers in combination with carboxylate salts in water. In methanol and ethanol, $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ undergoes a similar process that yields oligomers. Further reducing the polarity of the solvent, the same reactions proceed in THF to yield brown solids soluble in toluene. In the same vein $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ reacts with short-chain carboxylates in the presence of caprolactam, the resulting products are soluble in toluene. Additionally, a colorless toluene soluble caprolactam adduct is produced by direct stoichiometric replacement of water from $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ by caprolactam. The colorless caprolactam adduct reacts directly with both short and long chain carboxylates yielding brown products. Significantly, all species have low melting and clearing point; current efforts seek to identify liquid crystalline mesophases for these materials through polarized optical microscopy. The colorless caprolactam adducts of $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ also have low melting points, which persist through several cycles of melting and crystallization. All products have been characterized by IR spectroscopy, polarized optical microscopy, and DSC. Characterization by elemental analysis has been undertaken for selected samples.

Presenter(s): Maya Lengvenis, Gustavus Adolphus College

Session: Poster P2.18

Title: Midrange wireless power transfer using strongly coupled resonant printed circuit boards

Advisor(s): Jessie Petricka, Physics, Gustavus Adolphus

Abstract: Power can be transferred wirelessly across distances from centimeters to meters using strongly coupled magnetic resonance. The resonant RLC circuits required for this power transfer are traditionally made of large coils of wire, which while efficient, are neither practical for daily use nor easily integrated into current technology. To make strongly coupled RLC circuits more cost effective and practical, a printed circuit board (PCB)-based design was utilized. The design of resonant PCBs was tested computationally and experimentally with the goal of creating strongly coupled circuits with high Q factors. Computational testing revealed that PCBs with very high Q-factors can be manufactured using a non-traditional PCB substrate. Experimental testing demonstrated that an automated impedance matching system is required to continue this experiment.

Presenter(s): Hanqing Li, Colorado College

Session: Poster P2.12

Title: Stochastic Models of Feed Forward Loops in Gene Regulatory Networks

Advisor(s): David Brown, Department of Mathematics and Computer Science, Colorado College

Abstract: Mathematical models help us generate a better understanding of gene regulatory networks. The incoherent feedforward loop (I-FFL) is a prominent motif in gene regulatory networks and plays an important role in the self-regulation of the cell. In this paper, we focus on the behavior of IFFL under conditions of molecular noise using stochastic models. We use the Gibson-Bruck algorithm to model all four types of I-FFL and compare the results with the predictions of deterministic models. We also examine I-FFL under different conditions of dimerization, transcription, and translation. Our results show that in the stochastic model, I-FFL manifests significant variation and lacks certain features that are demonstrated by the deterministic model. Moreover, this study sheds light on how networks perform certain functions in the presence of high levels of noise.

Presenter(s): Alexander Liebl, Gustavus Adolphus College

Session: Poster P1.01

Title: Synthesizing peptides for identifying PfGCN5 bromodomain recognition for specific acetyl-modified histone tail marks

Advisor(s): Scott Bur, Chemistry, Gustavus Adolphus College

Abstract: Designing peptides as a facile approach for determining various Plasmodium falciparum histone tail acetylation marks specificity for Plasmodium f. GCN5 bromodomain (PfGCN5). Titrations using various acetylated marks in tandem with Protein-Observed Fluorine (ProF) NMR to determine the dissociation constants for each acetyl-modified histone tail marks using a non-linear regress analysis of the dose-dependent changes using chemical shifts of the incorporated fluorine residue of the PfGCN5 bromodomain.

Presenter(s): Lisa Lin, University of Chicago

Session: Poster P3.11

Title: Chemical Consequences of Giant Impacts on Proto-Uranus

Advisor(s): Chris Fryer, Astrophysics, Los Alamos National Laboratory

Co-Author(s): Sahil Hegde

Abstract: In this study, we perform a series of Smooth Particle Hydrodynamics (SPH) simulations to model a giant impact between a large planetesimal and proto-Uranus by varying the initial velocity and impact parameter of impactors between $1 - 3 M_{\oplus}$. The 98° obliquity in Uranus' orbit is attributed to the impact, which has also been used to account for observational abnormalities such as the orbits of the Uranian satellites, the planet's low thermal flux rate, and the tilt of its magnetic field. Previous studies primarily focus on analyzing dynamics of the system and do not comment on the effects of the impact on Uranus' long-term chemical configuration. Using more refined EOS schemes and a variety of chemically motivated approaches, we build on the results of the SPH simulations to better inform our understanding of the composition of Uranus and its satellites. In particular, we compare the results of a broad equilibrium chemistry framework to those obtained from species conversion within a thermochemical kinetics network to construct a holistic image of chemical developments surrounding proto-Uranus. Globally, we see a large loss of molecular hydrogen H_2 and loss in HCN and C_2H_2 . Hydrocarbon abundances fluctuate slightly in both regions, though atmospheric trajectories saw CH_4 , C_2H_6 , and C_2H_4 production while chemical analyses of mantle particles resulted in the disappearance of some of these hydrocarbons that serve as precursors to organic molecule synthesis. The results we observe offer prospects for broadening the scope of such a study to understanding the long term, large scale chemical effects of the impact. The results of this study provide us with further evidence that can be used to validate the giant impact hypothesis, and a purely chemical signature that could observationally constrain the parameters of such an impact.

Presenter(s): Tianle Liu, University of Chicago

Session: Oral I.D.5 (11:10)

Title: ProtoDUNE: measuring electric field in the drift direction using cathode-anode crossing muons

Advisor(s): Edward Blucher, Department of Physics, The University of Chicago,

Abstract: The Deep Underground Neutrino Experiment (DUNE) aims to measure unknown parameters of the Standard Model of particle physics and search for new phenomena. The prototype single-phase DUNE detector consists of a liquid argon time projection chamber (TPC). The TPC performs three-dimensional particle trajectory reconstruction using electrons ionized along particle trajectories. Understanding the electric field inside the TPC is crucial to performing accurate track reconstruction. Although the electric field is applied uniformly, accumulated positive argon ions distorts the field (space

charge effect), resulting in non-uniform electron drift velocity across the TPC. In this study, we first use cathode-anode crossing muons to determine local drift velocity along the drift direction of the TPC. Then we convert the drift velocity to the electric field. This is a good method for cross checking against other analysis of the electric field in the drift direction.

Presenter(s): Lily Liu, University of Chicago

Session: Oral II.F.4 (3:15)

Title: Modeling Systems of Drop Carrier Particles Using Energy Minimization

Advisor(s): Andrea Bertozzi, Department of Mathematics, University of California, Los Angeles

Co-Author(s): Bernardo Hernandez Adame, Ryan Shijie Du, Simon Ng, Hansell Perez, Sneha Sambandam, Kyung Ha, Claudia Falcon, Dino Di Carlo, and Andrea Bertozzi

Abstract: Drop Carrier Particles (DCPs) are microparticles designed to capture uniform microliter drops of water in water-oil emulsions without using costly microfluidic equipment. DCPs are extremely useful for automated, high-throughput biological reactions, assays, and single-cell analyses. However, since the behavior of DCPs in multi-particle systems is not well understood, researchers have had difficulty achieving uniform volume across the particles. Here we present a method for modeling these systems using energy minimization techniques. We first determined the energy-minimizing surface configurations of water captured inside DCPs submerged in oil; we modeled two-particle interactions as energy-minimizing redistributions of water. Macro-scale experiments demonstrated that physical systems exhibit the same water-splitting patterns as simulated systems. The multi-particle systems were modeled with successive pairwise interactions; we developed an algorithm to predict the mixing time necessary to achieve volume uniformity. We then used probability theory to determine the mixing time probability density functions, which informed our parametric study of particle geometries. Our collaborating bioengineering group is currently employing these simulations, as they develop methods for fabricating DCPs with optimized geometries. These models provide a foundation for "lab-on-a-particle" research: DCPs have unique properties unavailable with conventional research technologies, including the ability to conduct solid phase reactions and prevent solution exchange.

Presenter(s): YiLi Luo, Tanvi Jindal, Grinnell College

Session: Poster P1.21

Title: A latent variable approach for evaluating collision scenarios with application to driving simulator time-series data

Advisor(s): Ryan Miller, Mathematics and Statistics, Grinnell College

Co-Author(s): Tanvi Jindal, Ryan Miller

Abstract: Vehicular collisions are a major cause of death in the U.S. Therefore, it is essential to measure the proximity to collision that two vehicles face in two-dimensional scenarios. We approach this task by modeling the position of two vehicles using equations based upon each vehicle's initial position, velocity, acceleration, and steering. By augmenting each equation with a latent variable, and forcing the adjusted positions to coincide, we are able to measure the distance (in time) by which the vehicles avoided collision. Since there are many combinations that satisfy these augmented equations, we summarize them by developing a metric called "Standardized Degree of Collision Avoidance" (SDCA), which measures the expected distance by which the pair of vehicles avoided collision. We apply SDCA to time-series driving simulator data from a vehicle-to-vehicle alert experiment conducted at the National Advanced Driving Simulator (NADS). Our analysis of the NADS data supports the use of SDCA as a classifier of collision. Our analysis also demonstrates that using SDCA as an endpoint offers improved statistical power relative to using a binary collision outcome variable.

Presenter(s): Vennela Mannava, University of Chicago

Session: Oral I.B.5 (11:10)

Title: Nickel-mediated dehydrogenative aryl-aryl homocoupling of a bulky phosphino-pyridine

Advisor(s): John S. Anderson, Chemistry, University of Chicago

Co-Author(s): Kate A. Jesse

Abstract: Transition metal-catalyzed reactions are widely used for the construction of C–C bonds. Coupling aromatic carbons is essential for many synthetic pathways toward pharmaceuticals and other useful compounds. Aryl-aryl bond formation through dehydrogenative coupling is an attractive transformation due to the atom- and step-economy of working with unfunctionalized C–H bonds. Pd catalysts are common for this application, but Ni complexes have been targeted as less expensive alternatives. Here we show the ability of Ni(0) to activate a bulky phosphino-pyridine ligand (PNPh) with resulting dehydrogenative aryl-aryl homocoupling. The net H₂ equivalent is transferred to the co-ligand, resulting in hydrogenation of a C–C double bond. From the reaction of PNPh with Ni(1,5-COD)₂, an intermediate Ni(II) complex (1) can be isolated. Characterization of 1 shows a PNPh ligand activated at a pyridine carbon. The co-ligand is an activated allylic cyclooctene resulting from partial hydrogenation of 1,5-COD. 1 decomposes bimolecularly to form a bi-PNPh compound coupled through the activated pyridyl position. 1 displays low reactivity toward other representative carbon substrates, possibly suggesting a preference for PNPh homocoupling over cross couplings. Although stoichiometric, this system demonstrates a potential pathway for Ni(0)-mediated aromatic C–H activation and homocoupling toward synthetic applications.

Presenter(s): Innes Maxwell, Lawrence University

Session: Poster P1.11

Title: Developing an Integrated Light Source in Band Gap Photonic Crystals

Advisor(s): Willem Vos, Complex Photonic Systems, University of Twente

Abstract: Photonic band gap structures can be used to control and study the propagation of light in cavities. However, current methods of illumination using suspended quantum dots suffer from broad band emission. This motivates the development of an integrated light source within the material of the crystal to create a significant contrast between the crystal and the air that fills its cavities. In this project we explore silicon chips doped with bismuth as a potential light source within a photonic crystal. As a group V donor bismuth is able to fluoresce within silicon under excitation, the rate of which is explored within this experiment. In doped samples held at cryogenic temperatures under incidence from a 688nm laser we observe unique emission near the theoretically predicted wavelength of 1082nm. With these findings we hope to support further developments and improvements in the field of photonic crystal research, allowing for improved control of photons in crystal structures.

Presenter(s): Hannah McCall, Washington University in St. Louis

Session: Poster P1.10

Title: Supernova Cosmology without Spectroscopy

Advisor(s): Dan Scolnic, Department of Physics, Duke University

Abstract: Upcoming type Ia supernova analyses must overcome several challenges to improve their measurements of dark energy. Without the resources for spectroscopic follow-up of every transient, it is necessary to find alternative methods of determining supernova type, obtaining supernova redshift, and navigating systematic uncertainties due to correlations with host galaxy properties. We present here a new approach that addresses these obstacles. From the 3,000 supernovae discovered by the Dark Energy Survey, we take the sample of supernovae hosted in luminous red galaxies (LRGs). These galaxies exclusively host type Ia supernovae, so no spectroscopy is required for classification.

Furthermore, we are able to measure precise photometric redshifts for these types of galaxies ($\sigma_z / (1 + z) \sim 0.02$), eliminating the need of spectroscopy for determination of redshift. In addition, as SNe can be found in LRGs from low to high redshift, use of supernovae located in this galaxy subset ensures a consistent host galaxy demographic. We use the redshifts of the host galaxies to ascertain distances of supernovae and combine this information to create a Hubble diagram. In the future, we can utilize measure cosmological parameters and continue to refine our method for use in upcoming surveys like LSST.

Presenter(s): Elijah McMahon, Gustavus Adolphus College

Session: Oral I.A.1 (9:50)

Title: The Environmental Fate of Dicamba

Advisor(s): Dr. Amanda Nienow, Chemistry, Gustavus Adolphus College

Abstract: Dicamba, a post-emergent herbicide, has seen an increase in use as weeds become resistant to other herbicides. After application, dicamba can be distributed to different components of the environment. We are examining the photodegradation of dicamba as it adsorbs to corn leaves, runs off into rivers, and volatilizes into the atmosphere. By using HPLC, we have determined the kinetic rate constants for the photodegradation of dicamba in aqueous solutions (modeling river run-off) and on the surface of corn epicuticular waxes (modeling the surface of corn plants). In the aqueous phase, solutions containing Natural Organic Matter (NOM) were found to have a slower rate of reaction, while no perceivable trends have yet been found in the solid-phase data. Using LC-MS, we have preliminary results on the identity of photoproducts of both phases. Finally, we have begun to formulate methods for testing the photodegradation of dicamba in a quartz reaction chamber, received at the end of the summer. This chamber will allow us to study the photodegradation of dicamba in the gas-phase, modeling atmospheric photoreactions.

Presenter(s): Mattias McMullin, Lawrence University

Session: Oral I.D.1 (9:50)

Title: Tuning of Photonic Band Gap Superconducting RF Cavities

Advisor(s): Thomas Oseroff, Physics (CLASSE), Cornell University

Abstract: The use of photonic band gap structures (PBGs) in superconducting RF cavities promises improved damping of higher order modes in accelerator applications. The tuning of PBG cavities differs from the tuning of traditional RF cavities due to their different geometries, but remains a vital part of smooth operation. This tuning must be accomplished through predictable deformation of the PBG cavity by mechanical means, altering its electromagnetic properties. A possible tuning system for PBG structures is discussed, accompanied by results of both mechanical and electromagnetic simulations using ANSYS. A numerical computation of an approximate sensitivity for the proposed tuning system is presented, confirming its viability.

Presenter(s): Sarah Mersch, Gustavus Adolphus College

Session: Oral I.A.2 (10:10)

Title: DeepCHALLA sediment core: Atmospheric mercury and lead in Equatorial East Africa over the last 250,000 yrs

Advisor(s): Jeffery Jeremiason, Chemistry, Gustavus Adolphus College

Abstract: Lake Challa is a crater lake in Tanzania, located less than five miles from Mt. Kilimanjaro. Lake Challa has several properties that make it ideal for paleoclimate analysis: varved sediments, a small watershed, and an anoxic hypolimnion. Lead and mercury are primarily atmospheric pollutants and complimentary climate proxies, with deposition related to dust production and origin, wind

trajectories, and precipitation patterns. This project aims to show how mercury and lead deposition change over time and compare the Lake Challa record to other global climate and regional climate records. The results show that lead and mercury concentrations in sediments have varied approximately in line with glacial and interglacial cycles over the past 225,000 years, and that increases in lead correlate with increases in mercury.

Presenter(s): Makenzie Mullan, Gunnar Goetz, Carthage College

Session: Oral II.F.3 (2:55)

Title: Micellar-Facilitated Peptide Coupling Reactions in Continuous-Flow Conditions

Advisor(s): David Brownholland, Chemistry, Carthage College

Abstract: Micelle-facilitated reactions are receiving significant attention due to their potential to remove toxic organic solvents from organic reactions in favor of water. These reactions often produce equivalent or superior results compared to their analogous reactions in organic solvent. Furthermore, micelle-facilitated reactions can often be conducted at room temperature with shorter reaction times, offering significant environmental and practical advantages. Despite growing interest, micelle-facilitated organic synthesis has yet to be adapted for flow conditions. Continuous-flow synthetic processes offer advantages over batch reactions, such as improved heat transfer and the ability to increase pressure and temperature safely above the boiling point of the solvent, thus enabling faster reactions. These benefits enable quick screening of reaction conditions. Further, flow chemistry is easily scalable, either through collecting a sample for longer periods of time or through running reactions in parallel. In addition to the benefits to traditional research, flow chemistry is recognized as necessary to conduct extraterrestrial chemical research. We report our progress on a peptide coupling reaction in aqueous flow conditions using micellar catalysts.

Presenter(s): Arsalan Bin Najeeb, Knox College

Session: Poster P2.04

Title: Facial Recognition Assignment on the Raspberry Pi

Advisor(s): Prof. David Bunde, Computer Science, Knox College

Co-Author(s): Prof. David Bunde, Annie Song, Shebaz Chowdhury

Abstract: Heterogeneous computing is the idea of using different types of processors together to solve complex problems. With heterogeneity, processes can be faster and more efficient, setting the foundation for future technologies to be run smoothly. There are examples of these types of systems around us everywhere, both smartphones and supercomputers typically use heterogeneous processors now. Processors are the building blocks of computing systems and, as a Computer Science student, it is essential to be able to understand and learn more about them. In this project, we developed an assignment in which students implement the Local Binary Patterns facial recognition algorithm on a Raspberry Pi, a small single-board heterogeneous computer. At the end of the assignment students will be able to compare running times of their image recognition algorithm before and after parallelization.

Presenter(s): Alexandra Nisenoff, University of Chicago

Session: Poster P1.02

Title: Study of UChicago affiliates' vulnerability to password-guessing attacks

Advisor(s): Blase Ur, Computer Science, University of Chicago

Co-Author(s): Maximilian Golla, Miranda Wei, Juliette Hainline, Lydia Filipe, Annika Hildebrandt

Abstract: Digital users have an increasing number of password protected accounts, many containing sensitive information, but it is unrealistic to expect users to remember strong unique passwords for each of them. To reduce cognitive demands, users tend to recycle passwords across accounts. In addition to directly reusing passwords, users may modify their login credentials with simple and predictable

transformations, such as appending numbers or symbols. This widespread phenomenon can be utilized, in combination with available data breaches, to guess users' passwords across multiple sites.

UChicago accounts can be linked to sensitive information such as grades, payroll, and emails, this study uses these accounts to examine research questions related to password reuse, modification, and user attitudes. We leverage publicly available data breaches and password modification strategies to generate password guesses for UChicago accounts. We then provide these generated guesses to UChicago IT Services to run against their password database in a simulated attack to assess the vulnerability of UChicago accounts to password guessing attacks. Information is obtained from users who are identified as vulnerable in this simulated attack using anonymous online surveys. Attitudes, intentions, and planned behavior change are surveyed in an effort to design interventions that promote better password security habits.

Presenter(s): Alain Brilliant Nishimwe, Luther College

Session: Poster P3.12

Title: Quantifying atomic scale wear with an atomic force microscope

Advisor(s): Dr. Erin Flater, Physics, Luther College

Co-Author(s): Grace Seiler

Abstract: Wear occurs when two surfaces rub against one another and volume is lost over time. It is important for scientists to quantify wear in order to develop materials that are more resistant to wear. We used an atomic force microscope (AFM) to quantify how much a silicon AFM tip wears when slid against an amorphous aluminum oxide surface. In previous work we developed an AFM tip wear method that allows us to quantify wear if we assume that the tip is a simple pyramid with a constant cone angle that gets flattened as the wear occurs. Over the course of our research this last summer, we found that rather than being worn down flat, the tip developed bumps that made it difficult to quantify the volume loss. This led to the use of a transmission electron microscope (TEM) to examine what was happening to the tips. From the TEM images, we could conclude that the bumps were not from the tip itself but that these bumps were due to a dirty sample. This led us to change the sample so that this contamination did not occur in future experiments.

Presenter(s): Yu Nishio, Grinnell College

Session: Poster P3.13

Title: Synthesis of Lugdunin and Lugdunin Derivatives

Advisor(s): Erick Leggans, Chemistry, Grinnell College

Co-Author(s): Erick Leggans

Abstract: Antibiotic resistance has been an increasing problem due to the overuse of antibiotics such as penicillin. It is estimated that 33,000 people die annually due to infections by antibiotic resistant bacteria. One common antibiotic resistant bacteria is *S. aureus*, with strains such as MRSA and GISA, and VISA being the most known kinds with resistance. Approximately 120,000 *S. aureus* infections and 20,000 deaths occurred in the United States in 2017. Due to the number of antibiotic resistant bacteria increasing, there is a high demand for new antibiotics to improve previously used antibiotics.

Lugdunin is a cyclic polypeptide molecule discovered from *Staphylococcus lugdunensis*, a nasal bacteria. Lugdunin has been found effective against various gram-positive bacteria as well as *S. aureus* and resistant forms of it. Due to the unique structure of lugdunin and its activity against *S. aureus*, lugdunin is an attractive molecule to synthesize. Here, the synthesis of lugdunin and its derivatives using peptide coupling is described. This strategy gives an extremely efficient route of synthesizing various lugdunin derivatives through the change of the heterocycle. This methodology appears to be applicable for the synthesis of cyclic polypeptide amino acids with heterocycles for the purpose of drug discovery.

Presenter(s): Jonny Norwine, Colorado College

Session: Oral I.A.3 (10:30)

Title: Mechanisms of Land Subsidence in Colorado Springs Related to Abandoned Coal Mine Tunnels

Advisor(s): Solomon Seyum, Geology, Colorado College

Co-Author(s): Solomon Seyum

Abstract: Sinkholes and land subsidence in Colorado Springs are coincident with the distribution of abandoned coal mine tunnels. Property damage due to sinkholes has been reported continuously since the 1960s during early urban development, shortly after coal mine abandonment. Correlations between sinkholes and soil saturation due to rainfall or pipe leaks have been observed, but sinkholes are not occurring in all places where there are subsurface tunnels and wet soil. This suggests a need for a robust physical description of ground failure where tunnel geometry and material properties are considered as potential controlling factors. We developed conceptual and mechanical models of tunnels in the subsurface to reproduce surface displacement measurements of sinkholes and subsidence features. We constrain model geometries, material properties, body forces, and stress boundary conditions using field and published data, such as tunnel maps, geologic maps, stress maps, petrographic data, and rock mechanics data. Model results and intuition from rock mechanics experiments suggest that specific ranges of values for tunnel depth, tunnel height/width ratio, and failure mechanisms of rock and soil types contribute to sinkhole and subsidence development. We compare model results to field measurements and discuss the potential for predictive capabilities.

Presenter(s): Sami Pathak, Washington University in St. Louis

Session: Poster P3.14

Title: Mathematical modeling of thin-filament regulation and its application to understanding modulators of cardiac contraction

Advisor(s): Michael Greenberg, Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis School of Medicine

Co-Author(s): Sami Pathak, Samantha Barrick, Lina Greenberg, Michael Greenberg

Abstract: Cardiac contraction occurs when myosin pulls on the thin filament. This process must be regulated to meet the changing needs of the body. The thin filament is composed of actin, tropomyosin and the troponin complex. During beta-adrenergic stimulation of the heart, troponin I (TnI) becomes phosphorylated. This increases the rate of calcium dissociation from troponin C, decreasing the calcium-sensitivity of the thin filament and increasing muscle relaxation. Certain mutations in cardiac troponin uncouple calcium sensitivity from TnI phosphorylation and are associated with familial cardiomyopathies. The drug epigallocatechin-3-gallate (EGCG) can restore this coupling, suggesting therapeutic potential. However, the biophysical mechanisms of TnI phosphorylation and its modulation by EGCG are not well understood. To better understand the relationship between TnI phosphorylation and calcium sensitivity, we performed stopped-flow assays and fluorescence titrations using reconstituted thin filaments in the presence and absence of TnI phosphorylation and EGCG. We found that phosphorylation likely increases activation of the thin filament and that EGCG is able to reverse these effects. We developed mathematical models to represent these changes, and we found that an early step in thin-filament regulation is likely slower in the presence of EGCG. Our results have implications for understanding cardiac physiology and heart failure.

Presenter(s): Aldo Portillo, Knox College

Session: Poster P1.24

Title: Ligand Exchange in Copper Tetramer Complexes with Axial Caprolactam: Synthesis and Characterization of Novel Copper Tetramers with Bridging Carboxylate Ligands

Advisor(s): Thomas Clayton, Chemistry, Knox College

Co-Author(s): Thomas Clayton

Abstract: Previous work at Knox has focused on the synthesis and characterization of tetramers of copper with bridging carboxylate ligands. Many of these compounds have low melting points and exhibit birefringence by polarized optical microscopy. A typical synthesis entails replacement of bridging chloride ligands in $\text{Cu}_4\text{OCl}_6 \cdot 4\text{solv}$. The present work reports the reactions of the related $\text{Cu}_4\text{OCl}_6 \cdot 4\text{caprolactam}$ complex with sodium carboxylates with carbon chain lengths of 4-16. The resulting compounds are soluble in non-polar solvents (toluene) and exhibit low melting points. Observation of birefringence by plane polarized microscopy confirms the existence of liquid crystalline mesophases for these materials. Further characterization by differential scanning calorimetry and elemental analysis will also be reported.

Presenter(s): Keegan Proctor, Knox College

Session: Poster P1.15

Title: Synthesis of Heteroleptic Copper Dimers of Various Alkoxybenzoates and 8-Carbon Carboxylates

Advisor(s): Thomas Clayton, Chemistry, Knox College

Co-Author(s): Thomas Clayton

Abstract: Previous studies at Knox College have investigated the liquid crystal properties of copper dimers, initially with straight chain carboxylate ligands such as butanoate, and later substituting in multiple different carboxylates to form mono- and disubstituted species with altered thermal behavior. In this project, novel copper dimers were synthesized using the novel ligands 4-butoxybenzoate and 4-isopropoxybenzoate, and further heteroleptic dimers were constructed by substituting various 8-carbon carboxylates into the original two dimers. Each dimer was also axially ligated with caprolactam or TPPO to alter thermal properties. Successful creation of these compounds was verified through the use of IR, and when possible, elemental analysis or X-ray diffraction. Additionally, the liquid crystal properties of created dimers were tested through polarized optical microscopy and DSC. Several of the generated dimers exhibited liquid crystallinity, including unexpected liquid crystals incorporating TPPO.

Presenter(s): Jonathan Rebelsky, Grinnell College

Session: Oral I.B.1 (9:50)

Title: $\text{La}_x\text{Sr}_{1-x}\text{Co}_y\text{Fe}_{1-y}\text{O}_3$ Thin-Film Oxygen Reduction and Evolution Catalysts Grown by Spray Pyrolysis

Advisor(s): Lee R. Sharpe, Chemistry, Grinnell College

Abstract: The reduction of oxygen and oxidation of water are key to efficient metal-air batteries and fundamental to many green energy technologies. The current catalysts for the reactions are precious-metal based, making them expensive and impractical for industrial use. Metal oxides of the form ABO_3 , with A a lanthanide and B a transition metal, both with +3 charges, have been shown as effective bi-functional catalysts. Substitutions within both sites has shown further improvements. This project explores the material $\text{La}_x\text{Sr}_{1-x}\text{Co}_y\text{Fe}_{1-y}\text{O}_3$ (LSCF). The optimal composition for these thin-film catalysts was determined through a two-dimensional series search, varying the A and B site compositions. The series of LSCF 64XY was run this summer, finding that 6455 was the best performing, showing improvements in oxygen reduction through 60 layers. Staggered annealing was also seen to improve catalytic effect. This fall we explore the XY55 series, hoping that the cross-sectional search will lead to the optimized LSCF compositional blend.

Presenter(s): Adam Rivkin, University of Chicago

Session: Poster P2.01

Title: Multidimensional Database Reconstruction from Range Query Access Patterns

Advisor(s): David Cash, Department of Computer Science, The University of Chicago

Co-Author(s): Akshima; David Cash; Francesca M. Falzon; Jesse Stern

Abstract: This work considers the security of searchable encrypted database systems that process multi-dimensional range queries with only access pattern leakage. The majority of practical encryption schemes which can be searched by querying a database for some range reveal access pattern information, where an adversary learns which encrypted records are returned by a query. Recent cryptographic work showed that in one dimension, an adversary could use the access patterns of several uniformly random range queries to reconstruct a plaintext column of numbers up to its reflection. We extend this attack to two dimensions and find that the situation is much more complicated: Information theoretically it is complex to describe even what is possible to recover for the adversary in general. We provide a classification of these limits under certain technical conditions. We also give a faster algorithm that works for "dense" databases that contain at least one record for each possible value. Finally, we explore the implications for our classification with real data sets.

Presenter(s): Pei Robins, Lawrence University

Session: Oral I.D.2 (10:10)

Title: Measuring the Frequency Response of a Harmonic Potential and Gaussian Potential

Advisor(s): Jeffrey Collett, Physics, Lawrence University

Abstract: Optical traps are used to trap atoms that become the quantum bits or qubits in quantum computers. We measure and compare the resonant frequencies of a harmonic trap and a Gaussian trap by shaking the atoms out. We shake the atoms out by applying a sinusoidal modulation that adds external energy to the system. This is a common technique to measure the resonant frequencies of optical traps, which is important for controlling the atoms in a quantum computer. When we compare the two traps, we find that the harmonic potential produces a sharp frequency response that is ideal for experiments. The frequency response is well-defined and has a sharp peak. However, a Gaussian potential, a type of anharmonic trap, is harder to measure. Instead, the frequency response is not as well-defined. Any traps used to control atoms in a quantum computer will have anharmonic shape.

Presenter(s): Serena Rolland, Luther College

Session: Poster P1.20

Title: Nanocrystal ligand substitution: a mechanistic study

Advisor(s): Molly Wilker, Chemistry, Luther College

Abstract: There has been an increased emphasis on understanding nanocrystal surface chemistry and the way that these surfaces interact with diverse solvent environments for broadening applications. A deeper understanding of the mechanism of ligand binding and the conditions that control the rate of ligand binding is necessary to control the surface chemistry of nanocrystals. In this study, long, native ligands were substituted for shorter ligands using a series of bifunctional molecules with consistent thiol anchoring groups and changing secondary functional groups. The optical properties of the nanocrystals were measured as the new ligands were added to the as-synthesized nanocrystal solutions to observe fluorescence quenching, which is a characteristic of thiol ligand binding. The ligand exchange was more quantitatively analyzed by using ¹H NMR. The ¹H NMR peaks of the free ligand and the nanocrystal-bound ligand were monitored and used to calculate the equilibrium constant of the ligand exchange. Further, the pH dependence of this mechanism was clarified by varying the pH of the ligand solutions before substitution. These data were used to gain insight into the ligand binding mechanisms and to understand how the strength of binding is influenced by ligand functionality.

Presenter(s): Emily Saari, Gustavus Adolphus College

Session: Poster P1.07

Title: Synthesis and optimization of drug-like molecules for inhibition of the PfGCN5 bromodomain

Advisor(s): Scott Bur, Chemistry, Gustavus Adolphus College

Abstract: The molecular structure indanone was identified through a Protein-Observed Fluorine (PrOF) NMR screen to have a high affinity for binding to the PfGCN5 bromodomain, found in the parasite *Plasmodium falciparum*. Additionally, the molecular structure 1,2,3,4-Tetrahydroquinoline was identified through a virtual screen using docking studies for selectivity towards the PfGCN5 bromodomain, relative to similar human bromodomains. The two identified molecular structures can be used as small molecular probes for further optimization through Fragment-Based Ligand Design (FBLD) to synthesize a small drug-like molecule that binds tightly and selectively towards the PfGCN5 bromodomain.

Presenter(s): Andrea Salazar, University of Chicago

Session: Oral I.A.4 (10:50)

Title: Modeling the role of volcanism in the last 20 million years of global cooling

Advisor(s): Timothy Herbert, Department of Earth, Environment, and Planetary Sciences, Brown University

Co-Author(s): Weimin Si, Timothy Herbert, Colleen Dalton, Alberto Sal

Abstract: The carbon-silicate cycle provides a negative feedback that facilitates the long-term stability of Earth's climate. The global cooling that occurred during the last 20 million years of the Cenozoic era can be examined through the lens of the carbon-silicate cycle and how it responds to perturbations on million-year time scales. Previous works have shown that the plate spreading rate at mid-ocean ridges is variable, which would directly impact the rate of CO₂ emission into the atmosphere. In this work, we construct a box model that couples atmospheric inputs and weathering to the oceanic calcium carbonate cycle. We can then compare our values of oceanic DIC, alkalinity, and the CCD to values interpreted from isotopic proxies. Better parameterizations of weathering and oceanic uptake of pCO₂ allows us to predict how Earth's climate will react to the current anthropogenic rise in CO₂ emissions.

Presenter(s): Eric Salisbury, Jacob P. Vander Roest, Erik J. Schoonover, Hope College

Session: Poster P2.09

Title: Carbon-Carbon Bond Activation: ortho-fluoro Pyridyl Ketones in Substitution-Decarbonylation Reactions with Boronic Acids

Advisor(s): Jeffrey B. Johnson, Chemistry, Hope College

Co-Author(s): Anne O. Armstrong, Erik J. Schoonover, Julia M. Loula, Jacob P. VanderRoest

Abstract: Ketones substituted with 2-pyridyl groups are known to undergo decarbonylation when treated with a rhodium catalyst. In contrast, it has been observed that ortho-fluoro and diortho-fluoro substituted ketones do not decarbonylate under the same conditions and may undergo substitution instead. This presentation explores the reactivity of these unusual substrates.

Presenter(s): Chris Seong, St. Olaf College

Session: Poster P3.16

Title: Synthesis of Novel PNNP Ligands and their First Row Transition Metal Complexes

Advisor(s): Elodie Marlier, Chemistry, St. Olaf

Co-Author(s): Anna Olson, Meg Swanson, Sam Brunclik, Melanie Nevins, Emily Nolan, Monica Osnaya, Andrew Reuter, Daron Janzen

Abstract: Most catalysts are comprised of second and third row transition metals which are expensive and less abundant. Research involving first row transition metals works to develop a cheaper, more

abundant, and more sustainable alternative to rare second and third row transition metals. Our approach focuses on the development of a family of tetradentate mixed donor ligands to stabilize the late first row transition metals. The unique binding environment of these PNNP ligands is formed by a β -diketiminato backbone and pendant phosphine donors. The synthesis of this new ligand family as well as the synthesis and characterization of its zinc(II) complexes will be discussed.

Presenter(s): William Setterberg, Macalester College

Session: Poster P3.17

Title: Diamond-Based Optical Magnetic Sensing of Superconductors

Advisor(s): Naufer Nusran, Ames National Laboratory

Abstract: Sensing the magnetic field around a superconducting sample is important to understand its properties. In this project, we use NV center magnetometry to sense these fields. An NV center is comprised of a nitrogen atom and an adjacent void (vacancy) in the diamond crystalline lattice. NV centers can sense magnetic fields with nanometer spatial resolution (about 1/1000 the width of a human hair) and have the sensitivity to detect magnetic fields thousands of times weaker than the Earth's. The measurements are performed optically in a confocal fluorescence microscope equipped with lasers, microwave electronics, and photon counters.

We use NV magnetometry to measure the lower critical field (H_{c1}) of an iron-based superconductor at four different temperatures near absolute zero. The lower critical field is the applied magnetic field strength at which small tube-like magnetic flux quanta known as Abrikosov vortices begin to penetrate the superconductor. Knowing H_{c1} allows us to calculate the absolute value of the London penetration depth (L) which is a measure of how deep the magnetic field penetrates into a superconductor. Knowledge of how L changes with temperature is essential to understand the mechanisms of superconductivity.

Presenter(s): Sanjeeda Shutrishna, Gustavus Adolphus College

Session: Oral II.G.2 (2:35)

Title: Modeling of altruistic suicide in E.Coli Bacteria

Advisor(s): Jeffery Ford, Mathematics, Computer Science and Statistics, Gustavus Adolphus College

Abstract: When exposed to pathogens, some E. Coli bacteria has a tendency to commit suicide in order to stop further spreading of the disease within the colony. We attempted to model this altruistic behavior, using graph theory instead of the usual differential equations model. We calculated the percentage of bacteria which need to show altruistic suicide behavior, in order for this to be of advantage to the colony. We represent the bacterial colony as a random graph and computed the number of vertex-disjoint paths between the two randomly chosen bacteria. We then computed the expected number of bacteria that would need to be removed in order to disconnect the graph, representing these bacteria as having altruistic suicidal behavior. This estimates the number of bacteria needing to evolve altruistic suicidal behavior in order to increase the probability of the colony surviving a virus attack.

Presenter(s): Jared Siegel, University of Chicago

Session: Poster P3.18

Title: Smoothed Particle Inference Studies of Supernova Remnant Abundances

Advisor(s): Vikram Dwarkadas, Astronomy and Astrophysics, University of Chicago

Co-Author(s): Vikram Dwarkadas, Kari Frank, David Burrows, Aldo Panfichi

Abstract: Supernova remnants (SNRs) are formed by the expanding shells of gas and dust expelled by supernova explosions. The progenitors of SNRs are divided between two explosion mechanisms:

Core Collapse, supernova caused by the implosion of massive stars, and Type Ia, supernova arising from the thermonuclear detonation of a white dwarf in a binary system. Here we apply Smoothed Particle Inference (SPI) to study the X-Ray emission from three SNRs and present the ability of elemental abundances within the SNR to discern the progenitor type. By analyzing the X-Ray spectra from SNRs, it is possible to characterize the traits of the emitting plasma, such as temperature, density, and chemical composition. The origins of the remnant can then be studied by comparing the observed elemental abundances with the ejecta yields predicted by a selection of models. However, as complex, three-dimensional objects, accurately interpreting the X-Rays presents a unique challenge. The SPI process captures this complexity, by modeling the gas as a collection of independent regions and fitting the regions' parameters to match the observed X-Ray spectrum. Here we present the abundances of three SNRs, compare the observed values with a selection of explosion models, and discuss the conclusions.

Presenter(s): Siddhant Singh, Macalester College

Session: Poster P2.21

Title: Laser Excitation Spectra of Niobium and Tantalum Hydride

Advisor(s): Thomas D. Varberg, Chemistry, Macalester College

Co-Author(s): Thomas D. Varberg, Zachary Fried

Abstract: Laser-excitation spectra were recorded for six bands of niobium hydride in the wavelength range 570-650 nm. Dispersed fluorescence experiments were used to confirm the identities of the observed states. Running non-linear fits to find the values of the constants in the Hamiltonian allowed for the determination of the term energies and rotational constants for each band. The data obtained for the identities of each of the states and their energies were in reasonable agreement with the multiconfiguration self-consistent field calculations of Koseki et al. (2004). It was found that the upper states in the bands did not fit the Hamiltonian well indicating local perturbations with dark states.

Presenter(s): Chase Snodgrass, Grinnell College

Session: Poster P3.10

Title: Analysis of Noise Enhanced Propagation in a Mechanical Array

Advisor(s): Barbara Breen, Physics, Grinnell College

Co-Author(s): ShengZhuo Wang

Abstract: We have successfully provided proof of principle regarding demonstrating noise enhanced propagation in a one-dimensional array of simple, nonlinear, mechanical, bistable elements. The noise source consisted flags for each element flapping in wind generated by fans. Our bistable elements consisted of inverted pendulums made out of an aluminum rods attached to a steel rods coupled by torsional springs. Only the first oscillator is driven sinusoidally, and without noise, that sinusoidal signal propagates a small distance through the array. However, when optimal noise is introduced, the signal propagation length is optimized as well, thus demonstrating noise enhance propagation.

Presenter(s): Terrell Solberg, Hope College

Session: Poster P3.19

Title: Preparation of a PEDOT-based redox mediator for the electrochemical detection of glucose

Advisor(s): Elizabeth Sanford, Chemistry, Hope College

Co-Author(s): Elizabeth M. Sanford

Abstract: An ethylenedioxythiophene (EDOT)-substituted iron porphyrin monomer and an aminomethyl-substituted EDOT monomer (AMEDOT) were synthesized and electropolymerized to form a redox-active mediation film on a glassy carbon electrode. The EDOT-substituted iron porphyrin was prepared via a four-step sequence from hydroxymethyl EDOT (HMEDOT). The HMEDOT was activated

with 4-toluenesulfonyl chloride and then reacted in a Williamson ether synthesis with 4-hydroxybenzaldehyde. The EDOT-functionalized benzaldehyde was condensed with pyrrole to form the substituted porphyrin and then metallated with iron. The AMEDOT was synthesized via formation of the azide from the tosylated HMEDOT followed by reduction. The two monomers were copolymerized electrochemically onto a glassy carbon electrode, functionalized with glucose oxidase, and tested for an electrochemical response to glucose.

Presenter(s): Amy Sorge, Carthage College

Session: Poster P2.03

Title: Development of Flow Chemistry Experiments for the Organic Chemistry Curriculum

Advisor(s): David Thompson, Chemistry, Purdue University; David Brownholland, Chemistry, Carthage College

Co-Author(s): Makenzie Mullan, Shruti Biyani, David Thompson, David Brownholland

Abstract: Organic reactions are typically conducted through a process known as batch chemistry, involving mixing reagents in glassware such as round bottom flasks. However, batch processes are often limited by the boiling point of the solvent, difficulty of conducting safe high-pressure experiments, high solvent use, and suffer from poor heat transfer, light penetration, and mixing. Flow chemistry, a process in which reagents are injected into either tubing or etched channels in solid supports, has been shown to address many of these limitations. The benefits of flow microreactors have led to the adoption of flow chemistry in many pharmaceutical companies and have promoted research of flow microreactors in space. In an effort to modernize our introductory organic chemistry laboratory courses, we have developed three continuous-flow reactions to be piloted at Carthage College and Purdue University: the synthesis of biodiesel, the acetylation of phenols, and the synthesis of phenacetin.

Presenter(s): Kathryn Stein, St. Olaf College

Session: Poster P1.13

Title: G-Quadruplex Stability in Aqueous Cosolute Solutions

Advisor(s): Jeff Schweinfus, Chemistry, St. Olaf College

Co-Author(s): Jeff Schweinfus

Abstract: A G-quadruplex is a strand of DNA containing G-quartets that are characterized by a coplanar arrangement of four guanines through Hoogsteen base-pairing. In this study, we characterized the stability of the G3 (d(G3T2G3TGTG3T2G3)) and G2 (d(G2T2G2TGTG2T2G2)) quadruplexes in aqueous potassium chloride solutions containing glycine betaine, L-proline, or urea using thermal denaturation monitored by uv-absorbance. Solutions of G3 contain two conformations, chair and basket, while only the chair conformation exists in G2 solutions. The basket conformation of G3 was destabilized in urea and proline, indicating favorable interactions between urea and proline and the solvent-accessible surface area exposed during unfolding. G3 stabilization in glycine betaine solutions indicated unfavorable interactions between glycine betaine and the surface area exposed during thermal unfolding, possibly with the sequestered potassium cations released upon unfolding. The behavior of G3 in glycine betaine, proline, and urea solutions is in marked contrast to the G2 G-quadruplex. G2 saw virtually no stabilization or destabilization in any of the three cosolute solutions. The differential interactions of glycine betaine, L-proline and urea with the G3 and G2 quadruplexes suggest these cosolutes may be used as probes of conformational and surface area changes during biochemical reactions.

Presenter(s): Austin Stover, Washington University in St. Louis

Session: Oral II.E.3 (2:55)

Title: Photonic Crystal Fibers Improve Light Collection in a Gamma-ray Telescope

Advisor(s): James H. Buckley, Physics, Washington University in St. Louis

Co-Author(s): James H. Buckley

Abstract: We investigate a novel type of optical fiber to improve light collection in particle detectors that use plastic wavelength-shifting or scintillating optical fibers to pipe scintillation light to a detector. Specifically, we explore how replacing the typical homogeneous dielectric cladding used in optical fibers with a two-dimensional photonic crystal cladding increases light-piping to detectors in the proposed Advanced Particle-physics Telescope (APT), thereby improving the telescope's energy and angular resolution. We characterize the light-piping characteristics of the proposed photonic crystal cladding by two methods: an analytical ray-tracing approximation for reflected plane waves in the large fiber core and the plane-wave expansion method to determine the dispersion relations for different angles of propagation in the photonic crystal cladding. We use these results to derive the fraction of light piped down the end of our scintillating photonic crystal fiber and compare this fraction to that of conventional fibers. Our proposed fiber outperforms classical fibers in light collection almost twofold, even with a conservative geometry.

Presenter(s): Tiffany Suwatthee, University of Chicago

Session: Poster P3.20

Title: Electrostatic Effects on the Binding of Milk Fat Globule EGF Factor 8 to Phospholipid Membranes

Advisor(s): Ka Yee C. Lee, Chemistry, University of Chicago

Co-Author(s): Daniel Kerr, Ka Yee C. Lee

Abstract: Milk fat globule EGF factor 8 (MFG-E8) belongs to a class of proteins that identify and bind phosphatidylserine (PS), the most abundant negatively charged lipid in cell membranes. These proteins detect membrane dysregulation, which is implicated in exposed PS in apoptosis and malignant cells. In addition to PS-binding, we have evidence that MFG-E8 also binds to phosphatidic acid (PA), another negatively charged lipid present in cell membranes. To better understand the factors affecting this binding, we used a model system of large unilamellar vesicles with varying amounts of PA and PS to identify the sensitivity of the binding affinity of MFG-E8 to changes in electrostatics using a tryptophan fluorescence spectral shift assay. We find that MFG-E8 has a stronger binding affinity for membranes containing both PS and PA as well as a weak binding affinity for membranes only containing PA. These results indicate that MFG-E8 may target other negatively charged lipids in addition to PS, and that electrostatics, rather than the exact identity of the lipid headgroup, have an influence on binding. The interactions of MFG-E8 with lipid membranes under different membrane conditions allows for better understanding of similar membrane binding proteins that target specific membrane fluidity and charge.

Presenter(s): Sophia Tajnai, Carthage College

Session: Poster P3.21

Title: Developing Light Sheet Microscopy at a Small Liberal-Arts College

Advisor(s): Steven Henle, Neuroscience, Carthage College

Abstract: Microscopy throughout its history has seen limited change. However, within the past decade, there have been many advancements in quality and speed. In particular, multidirectional Selective Plane Imaging Microscopy (mSPIM) is an emerging, imaging method that minimizes phototoxicity by transforming a cylindrical laser beam into a thin light sheet that acts as an excitation light. This light excites certain proteins in the specimen, and in turn, these proteins fluoresce. Then, the emitted light is captured by a camera. The images, which contain each layer excited by the light sheet, are combined to render a high-quality, 3D image of the specimen at high speeds. Many microscope setups require

large amounts of time and/or money to obtain and implement. We sought to make a cost-effective microscope with resources available at a small liberal arts college. This process entailed identifying and using appropriate software in order to devise an efficient and user-friendly interface; and identifying what components need to be created followed by deciding how to make these components. Our short-term goal is to finalize components and finish assembling the light path. In the future, we look forward to creating a fully operational system by the end of the year.

Presenter(s): Jason Tang, Washington University in St. Louis

Session: Oral II.E.4 (3:15)

Title: Optimization of small-pixel CZT detectors for hard X-ray astronomy

Advisor(s): Henric Krawczynski, Department of Physics, Washington University in St. Louis

Co-Author(s): Fabian Kislak, Shaorui Li, Henric Krawczynski

Abstract: Hard X-ray astronomy is used to study high-energy astrophysical objects such as neutron stars, black holes, and supernova remnants. We are currently developing Cadmium Zinc Telluride (CZT) detectors for a next-generation space-borne hard X-ray telescope working in the 2 keV - 160 keV energy range which can follow up on the highly successful NuSTAR (Nuclear Spectroscopic Telescope Array) mission launched by NASA in June 2012. Our work focuses on the development of Application Specific Integrated Circuits (ASICs) and matched CZT detectors with a small (150 μm) distance between adjacent pixel centers. The new ASIC/detector packages will be well matched to the recently developed hard X-ray mirrors made from monocrystalline Si shells which achieve $\sim 10''$ angular resolutions. I will present here the results from Monte Carlo simulations of the detectors and the charge transport inside the CZT detectors. Based on the simulations, I am developing algorithms to optimize the energy and spatial resolutions of the detectors. The simulation results are being used to guide the design of the ASIC circuitry and the detector contacts.

Presenter(s): Grace Tews, Carthage College

Session: Poster P1.09

Title: Synthesis of Gamma-Cyclodextrin Based Metal Organic Frameworks (MOFs) to Improve Water Quality

Advisor(s): Megan Moyer, Chemistry, Carthage College

Co-Author(s): Megan Moyer, Sonja Katt

Abstract: Metal organic frameworks (MOFs) are open crystalline, porous materials that are constructed by joining metal-containing units with organic linkers through strong bonds. Variation in the starting materials results in MOFs with diverse surface areas, pore volumes, and subsequent applications including gas adsorption, separation, molecular recognition, and drug delivery. An organic starch, gamma-cyclodextrin, has recently gained attention as an organic linker due to its environmentally friendly and cost-effective nature. Two simple methods to synthesize a gamma-cyclodextrin based MOF are reported here. Characterization and an application test were done with the two MOFs. The results showed that gamma-cyclodextrin based MOFs can successfully remove an organic dye from an organic solvent. The larger pore size and hydrophobic properties of these MOFs likely contribute to its capability to remove organic material. The removal of an organic dye with the MOF suggests that they would be applicable in water filtration. Further research will include the removal of other organic materials, the carbonization of each MOF, and the creation of an efficient filter.

Presenter(s): Ishaan Tibrewal, Grinnell College

Session: Oral II.G.1 (2:15)

Title: Driving Performance Under Influence of Cannabis and Alcohol During Secondary Task Engagement

Advisor(s): Ryan Miller, Statistics, Grinnell College

Co-Author(s): Seoyeon Lee

Abstract: Alcohol and marijuana are the most common legal and illegal drugs detected in drivers worldwide. While there is a general consensus regarding the effects of alcohol on driving performance, the effects of marijuana remain relatively unknown. This study examines the effects of cannabis and alcohol on performance during secondary tasks performed while driving using a within-subject, placebo-controlled experiment conducted in advanced driving simulator. For cognitively demanding secondary tasks, higher blood THC concentrations were associated with lower rates of task completion, and higher rates of incorrect responses. However, changes in driving performance were limited to differential decreases in speed during task periods. Additionally, some previously established effects of alcohol were detected, though alcohol was not found to interact with THC, with each drug being found to have separate effects on different aspects of driving performance.

Presenter(s): Linh Tran, St. Olaf College

Session: Poster P1.18

Title: CSinParallel Platform Benchmarking Project

Advisor(s): Richard Brown, Computer Science, St. Olaf College

Abstract: The CSinParallel Platform Benchmarking Project compares and analyzes the performance of multiple parallel and distributed computing platforms, namely physical machines, virtual machines, Google Cloud Platform systems, and Docker containers. For testing the performance of these platforms, we use the High-Performance Computing Challenge Benchmark (HPCC) and several more recent benchmarks. These benchmarks measure three main areas: CPU performance; memory bandwidth; and network communication performance. We ran these benchmark tests on dedicated hardware-based local multicore and eight-node Beowulf cluster systems constructed for this project, physical and virtual multicore machines, a four-node virtual cloud Beowulf cluster, and a Kubernetes configuration on the local cluster. Based on the collected data and details about the chosen platforms, we analyzed and compared the performance among these platforms.

Presenter(s): Evan Unruh-Friesen, Macalester College

Session: Poster P1.08

Title: Detrital Zircon Geochronology: The blueschist facies sequences of Baja California

Advisor(s): Alan Chapman, Geology, Macalester

Abstract: Blueschist facies sequences exist as fault-bounded blocks on Isla Santa Margarita, located on the western margin of central Baja California, Mexico. These sequences of blueschist facies metasediments and metabasites constitute the Western Baja terrane (WBt) and represent the exhumed products of tectonic underplating along the western North American plate margin. A serpentinite matrix mélangé containing exotic blocks of blueschist and serpentinite crop out along the WBt terrane contact zone and also separates the subterrane of the WBt. The WBt subterrane varies by protolith and degree of metamorphism, suggesting that they represent discrete packages of rock sequentially underplated beneath the accretionary prism. We present new detrital zircon geochronologic data from metasediments representing each subterrane in the WBt. Samples of metaturbidite from WBt

subterrane 4 were collected on Isla Santa Margarita This work places new constraints on the maximum depositional ages and detrital sources of WBT metaclastic rocks, thereby clarifying regional sediment dispersal pathways; constraining the time at which the WBT subducted; revealing patterns between degree of metamorphism, current spatial position, and time. Results are discussed in the context of forearc and intra-arc thrusting in the northern Peninsular Ranges.

Presenter(s): Nicholas Vaporciyan, Lawrence University

Session: Oral I.C.5 (11:10)

Title: What Makes A Rainbow?

Advisor(s): Megan Pickett, Physics, Lawrence University

Abstract: Why are the colours of the rainbow in the order they are? Why are the stars different colours? Why is the sky blue? Why are embers red? Why is the sunset pink? These are all basic questions about the world around us that we have all asked ourselves -- but people have been asking these same questions throughout all of human history. We now know that their answers lie in quantum physics, but does the story end there? By investigating who first asked these questions and how they attempted to answer them, we can discover new perspectives and narratives in the development of modern science. Approaching history in this way can lead us to exciting tales and fascinating people left out of today's textbooks. This methodology can help us uncover exciting connections between things as mundane as rainbows and fireflies to techniques as groundbreaking as spectroscopy and laser cooling.

Presenter(s): Kelly Vences, Lawrence University

Session: Oral I.B.3 (10:30)

Title: Investigating the Doublet State Photophysics of the Organic Luminescent Radical BAXPA

Advisor(s): Graham Sazama, Chemistry, Lawrence University

Abstract: We are synthesizing radical organic molecules to understand their luminescence at their doublet ground state. Radicals are found in organic light-emitting diodes (OLEDs), but they lack efficient fluorescence. BDPA is a known stable radical and my research is to alter the structure of BDPA to make a luminescent radical. Prior research has shown the addition of a pyridine ring increases a radical's photostability. Thus, the radical BAXPA was synthesized to test the pyridine ring's photophysics. The addition of 1-azaxanthone into the structure of the radical could potentially increase the radical's luminescence. 1-azaxanthone was synthesized via the ring closure of 2-phenoxy nicotinic acid by reacting it with polyphosphoric acid. 1-azaxanthone was fused with a Pudovik phosphene molecule via a Horner-Wadsworth-Emmons reaction. The resulting molecule fluoresced faintly under long wave ultraviolet light. The addition of 2,7-dibromofluorene led to BAXPAH, which was then reacted with t-BuOK, and oxidized with silver triflate. Electron resonance spectroscopy shows the presence of the radical. The future of this project is to test if BAXPA luminesces.

Presenter(s): Matthew Venzke, Gustavus Adolphus College

Session: Poster P2.16

Title: Electrochemical Reduction of Nitro Groups: From Bioanalysis to Lightweight High-Energy Density Cathodic Materials

Advisor(s): Miles Koppang, Chemistry, University of South Dakota

Co-Author(s): Brady Samuelson, Peyton Keller, Brock Goeden, Miththira Balasingam, Miles Koppang and Haoran Sun

Abstract: Derivatization of amino acids and aliphatic amines with suitable reagents enhances the separation and detection using liquid chromatography. Sanger's reagent (1-fluoro-2,4-dinitrobenzene, DNFB) makes amino acids and amines suitable for absorbance detection but little has been done using liquid chromatography with electrochemical detection (LC-EC). Electrochemical investigation of

nitrobenzene (NB) demonstrated that NB is reduced to phenylhydroxylamine (PHA) by addition of four electrons and four protons. PHA can be reversibly oxidized into nitrosobenzene by removal of two electrons and two protons. LC-EC analysis of derivatized amino acids with Sanger's Reagent was achieved via in-series dual electrode detection preceded by coulometric conversion. The coulometric cell converted the nitro groups to hydroxylamines and the dual electrode detection upstream and downstream electrodes oxidized the resultant hydroxylamines to nitroso groups and then back, respectively. The reduction of nitro-substituted aromatics has also been investigated as a route for new cathodic materials for lithium batteries. We are investigating a new type of Schiff Base polymeric material with a conductive backbone as cathodic materials for primary lithium batteries. The new conductive polymer with theoretical capacity of 4 times the energy density of LiCoO₂ cathodes is based on nitro group reduction. We have also investigated quinone reduction in the presence of lithium cations for the development of new cathodic materials for secondary batteries. This project explores the field of light-weight organic cathodic materials and has the potential to greatly increase the energy density for lithium batteries.

Presenter(s): Thong Vo, St. Olaf College

Session: Oral I.C.2 (10:10)

Title: The Delicate Details of Filling Space

Advisor(s): Paul Humke, Mathematics, St. Olaf College

Co-Author(s): Emily Olson, Sonya Flaten

Abstract: Space-filling curves, once thought impossible to define, were first discovered in 1879 by Italian mathematician Giuseppe Peano, who was inspired by Georg Cantor's discovery that the unit line and unit square have the same cardinality. In our research, we first investigate known constructions of space filling curves $f: [0,1] \rightarrow [0,1] \times [0,1]$ with the goal of understanding when two of them define the same function. We develop machinery to describe in detail the points at which a given space-filling curve is 1-1, 2-1, etc. Finally, we generalize these techniques to investigate space filling curves, $f: [0,1] \rightarrow [0,1]^n$, $n > 2$. We found N. Rose's "Adjacency" and "Nesting" Conditions to be particularly useful in accomplishing the first goals, and these conditions became a paradigm for dealing with later issues. Netto's Theorem shows that there is no one-to-one space filling curve, but in order to answer more delicate questions concerning n-to-1 points, we design and employ a unique version of symbolic dynamics. We then generalize this two-dimensional machinery to higher dimensions by first inductively employing an elementary combinatorial relation between vertices of the n-dimensional cube. This establishes the requisite nesting and adjacency conditions. We then use a generalized form of the two-dimensional symbolic dynamics to investigate specific behavior of higher dimensional space-filling curves.

Presenter(s): Tyler Walker, Colorado College

Session: Oral II.H.1 (2:15)

Title: Computational screening and optimization of small molecules for African sleeping sickness

Advisor(s): Amy Dounay, Department of Chemistry and Biochemistry, Colorado College

Co-Author(s): Amy Dounay, Ben Sokol, Don Backos

Abstract: Despite thousands of cases a year, African sleeping sickness (trypanosomiasis) receives limited investment from the pharmaceutical industry. In this research, synthetic and computational methods yielded two new series for development against the disease's late stage, central nervous system form. Through laboratory synthesis, four compounds were prepared and submitted for whole cell assay against *T. brucei*, the parasite that causes the disease. A homology model of GSK-3 β , an essential kinase for *T. brucei* proliferation, was prepared computationally based on the crystal structure of human GSK-3 β . Reagent libraries were compiled computationally, and compounds for screening were generated in directed "ligand growing." The screening results were filtered for likelihood of central

nervous system penetration. The best small molecules were docked into the homology model. High binding affinity compounds from each modification were visualized computationally using conformations from the docking simulation. The most compelling binding profiles included multiple interactions with the scaffold backbone, a generally uncommon mode in the "ligand growing" results. These experiments in silico led to our design of promising new molecular structures. Future work will involve laboratory preparation and evaluation of compounds with these new modifications. A continued avenue of inquiry will be structure-based computational prediction of optimal scaffold substituents.

Presenter(s): Ying Wang, Colorado College

Session: Poster P1.22

Title: The Inverse Problem for Rational Equivariant Cohomology

Advisor(s): Harrison Chen, Mathematics Department, Cornell University

Co-Author(s): Alexander Wang, Juntao Zhou

Abstract: In topology, it is a natural question to ask if we can recover a topological space from a given rational cohomology, a simplified version of homotopy theory which tells essential information of topological spaces. The non-equivariant case, where the topological spaces are not affected by group actions, was solved by Sullivan using the spatial realization functor. In our research, we produce a model-categorical construction for a topological space such that its equivariant cohomology is isomorphic to any given commutative differential graded algebra.

Presenter(s): Haocheng Wang, St. Olaf College

Session: Poster P3.22

Title: HiPerCiC: Custom Web Applications and Infrastructure

Advisor(s): Richard Brown, Computer Science, St. Olaf College

Co-Author(s): Lam Lo

Abstract: HiPerCiC (High Performance Computing in Context) is an interdisciplinary collaboration initiative for creating custom web applications for professors in other fields to support their research and teaching. This summer, we finished our training as HiPerCiC developers. We familiarized ourselves with Django and industry standard development methodologies such as test-driven development, separation of concerns, continuous integration, using an up-to-date container-based automated deployment system. We focused on two HiPerCiC apps: the QuizGame app with Professor Epstein and the Archeology app with Professor Howe. We added automated tests and updated the interface for end-users. We started user testing for the QuizGame app to prepare for its use in Fall music courses. We also implemented new features for the Archaeology app to show the dig process through sequential 3D-models. Overall, the apps became more integrated and easy-to-use. In the future, we will continue to support and improve the performance of existing applications and potentially build new ones.

Presenter(s): Nicholas Weigle, Elliott J. Berens, Hope College

Session: Poster P2.19

Title: Chemical defenses in the seeds of pioneer plants

Advisor(s): Elizabeth M. Sanford, Chemistry, Hope College

Co-Author(s): Elliott J. Berens, Elizabeth M. Sanford, Eleda V. Plouch, K. Greg Murray

Abstract: *Phytolacca americana*, pokeweed, is a pioneer species native to the United States. Pioneer species like *P. americana* remain dormant in the seed bank until an event that triggers high light conditions, such as a tree fall that causes a gap in the canopy. To enable longevity in the seed bank,

pioneer species have developed numerous chemical defenses to persist despite constant threats from the environment. Pioneer species are, therefore, a rich resource of biologically active compounds. This research seeks to identify and characterize the compounds in *P. americana* that protect the seeds of this pioneer species from fungal attack while dormant in the soil. To isolate possible anti-fungal components of *P. americana*, extracts of the crushed seeds were prepared, and the components separated using preparative TLC. A subset of components were identified using ¹H NMR. Anti-fungal properties were characterized by poisoned-medium bioassays with pathogenic fungi on the separated and identified fractions. Current efforts seek to better separate the components. The work will then be extended to identify the active antifungal components in *Phytolacca rivinoides*, a related species found in Costa Rica.

Presenter(s): Hannah Wilkins, Grinnell College

Session: Poster P2.11

Title: Semi-Synthesis and Biological Activity of Enoxolone Derivatives

Advisor(s): Erick Leggans, Chemistry, Grinnell College

Co-Author(s): Erick Leggans

Abstract: Terpenes are commonly found in plants and exhibit various biological activities, such as antibacterial, anti-inflammatory, and anticancer properties. In recent years, interest in terpenes has grown within the scientific community due to their various biological activities, especially with the rise of antibacterial resistance, which causes the deaths of at least 23,000 people in the U.S. every year.

Enoxolone is a triterpene isolated from the root of the licorice plant that has anti-inflammatory, anticancer, and antibacterial properties. However, it has also been demonstrated that enoxolone causes a decrease in potassium levels in the body, leading to complications when taken in high doses and making it a less effective treatment in its current state. On the other hand, lupeol is another triterpene that has a similar structure and activity to enoxolone but does not cause the same complications. The work presented here demonstrates progress toward the modification of enoxolone's structure, such as its cis-fused ring, to make it more similar to lupeol's and investigates the semi-synthesis of enoxolone derivatives with the goal of creating more potent antibiotics that do not affect the body's potassium levels.

Presenter(s): Yu Wu, Colorado College

Session: Poster P3.02

Title: Reactivity of Malonic Acid Half Thioester Derivative with Benzyne Precursor under Base Catalyst Conditions

Advisor(s): Jessica Kisunzu, Chemistry & Biochemistry, Colorado College

Abstract: Malonic acid half thioesters (MAHTs) are capable of forming C-C bonds through nucleophilic addition reactions without metal catalysts at room temperature. In nature, polyketide synthases use MAHTs for the biosynthesis of fatty acids and polyketides in all life. In previous studies, ketones and aldehydes have been tested and shown to work well in reacting with MAHTs. We propose that *o*-benzynes could also be considered as great electrophiles for the C-C bond formation, for their high reactivity from bond strains. Since MAHTs tend to decarboxylate spontaneously, thus preventing further reaction, conditions that use an amine base as a catalyst are considered to be favored to move the reaction forward. We herein introduce a new addition reaction between the MAHT derivative and the benzyne, and the optimized conditions for this reaction. ¹H NMR, ¹³C NMR and LC-MS were used to characterize the product, which might bring a mechanistic insight of such addition reaction.

Presenter(s): Salamong Xiong, Macalester College

Session: Oral I.D.3 (10:30)

Title: SuperCDMS: Energy Calibration of a Cryogenic Ge HV Particle Detector

Advisor(s): Vuk Mandic, Physics & Astronomy, University of Minnesota - Twin Cities

Co-Author(s): Jacob Nelson, Nicholas Mast, Matthew Fritts, Vuk Mandic

Abstract: The goal of the SuperCDMS collaboration is to directly detect dark matter. Potential candidates for dark matter are Weakly Interacting Massive Particles (WIMPs). To detect WIMPs, it is important to be able to predict how a Ge/Si particle detector will respond to a dark matter signal. In particular, it is necessary to calibrate the recoil energy measured by these detectors. This paper presents the energy calibration spectrum of a SuperCDMS-HV Ge particle detector using Am-241 and a PuBe neutron source. Due to high event rate, criteria were developed to remove low-quality data arising from particle interactions that occur too soon after a previous interaction. Peaks in histograms of pulse amplitudes were identified as energy peaks from the various radioactive sources, and fits of these peaks formed the basis for generating an energy calibration function. The calibration function was used to generate the calibrated energy spectrum.

Presenter(s): Hanjue Zhu, University of Chicago

Session: Oral II.E.2 (2:35)

Title: Galaxy-Halo Connection in the Cosmic Reionization on Computers Simulation

Advisor(s): Nickolay Y. Gnedin, Department of Astronomy, University of Chicago

Abstract: We examine the galaxy-halo connection in the Cosmic Reionization on Computers (CROC) project. CROC is a simulation suite of the epoch of reionization (EoR) that models relevant physical processes during the EoR, such as radiative transfer, gas dynamics, and star formation. The EoR is an extremely fascinating period in the evolution of the universe: it is when the first stars and galaxies were born, turning the dark cosmos into the one filled with luminous objects as we see today. Our goal is to answer the following question: how do galaxy properties at high redshifts depend on their host halos? We compare relationships that probe the galaxy-halo connection with observations that constrain theoretical models. With the upcoming James Webb Space Telescope data, which will probe the faint end of the galaxy luminosity function, we will be able to distinguish between models such as CROC.

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