The Midstates Consortium for Math and Science presents

Undergraduate Research Symposium

Physical Sciences, Mathematics, and Computer Science

November 3 & 4, 2017
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

(Revised 10/31/17)

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Program Schedule

Friday, November 3

12:00 pm – 5:00 pm	**Graduate School Exploration Seminar**	**Various locations**
12:00 pm – 4:45 pm	**Registration**	**Lobby Hyatt Hotel**
5:00 pm – 5:30 pm	**Reception – sponsored by Graduate School**	**Wiliam Eckhardt Research Center (ERC)**
5:00 pm – 5:30 pm	**Registration**	**ERC 161**
5:30 pm – 5:40 pm	**WELCOME (MS^2)** Michael Stein, Symposium Organizer; University of Chicago Michael Seymour, Director – Midstates Consortium for Math and Sciences; Hope College	**ERC 161**
5:40 pm – 6:30 pm	**Keynote Lecture** Yamuna Krishnan, Professor, Department of Chemistry – The University of Chicago *DNA Nanobots probe Inner Space*	**ERC 161**
6:30 pm – 7:30 pm	**Dinner Buffet**	**Gordon Center for Integrative Science (GCIS)**
7:30 pm – 8:20 pm	**Janet Anderson Lecture** Dr. Thomas Varberg Dewitt Wallace Professor of Chemistry Macalester College *Chemical bonding in transition metal free radicals: Tantalizing and golden results from electronic spectroscopy*	**GCIS**
Following lecture	**Group Picture** **University shuttles to the Hyatt after group picture**	

Saturday, Nov 4

Begins at 7:00 am	**Breakfast**	**Hyatt Hotel**
	Depart for University of Chicago Campus Those with vans or cars will drive to campus. Others will walk or take Hyatt Shuttle. **NOTE: There will be a locked room for storage of luggage and posters at the meeting site**	**Hyatt Lobby**
8:00 am – 8:30am	Set-up for poster session 1 Check computer set-up for oral presentations	
8:45 am – 9:45 am	**Poster Presentations** Session 1	**GCIS Atrium**
9:45 am - 10:00 am	**Break, remove posters, check set-up for oral presentations in respective rooms**	**GCIS Atrium**
10:00 am -11:15 pm	**Oral Presentations of Student Papers**	**Kersten**
	Session A: Physics (4)	Room 101
	~~Session B: Biochemistry (3)~~ *see sessions E and G*	Room 103
	Session C: Astronomy and Physics (5)	Room 105
	Session D: Mathematics (5)	Room 120
11:20 – 12:15 pm	**Careers at Liberal Arts Colleges** **Set-up posters for session 2, check set-up for oral presentations in respective rooms**	**GCIS 301-303**
11:30 pm – 1:00 pm	**Lunch Buffet** **Set-up posters for session 2**	**Baker Dining Hall**
1:15 pm – 2:15 pm	**Poster Presentations** Session 2	**GCIS Atrium**
2:15 pm – 2:30 pm	**Break, remove posters, check set-up for oral presentations in respective rooms**	
2:30 pm – 3:30 pm	**Oral Presentations of Student Papers**	**Kersten**
	Session E: Biochemistry (4)	Room 101
	Session F: Physics (3)	Room 103
	Session G: Chemistry (4)	Room 105
3:30 pm -3:45 pm	**Break, set-up for poster session 3**	**GCIS Atrium**
3:45 pm – 4:45 pm	**Poster Presentations** Session 3	**GCIS Atrium**
4:45 pm	Remove posters	
4:45 pm – 5:00 pm	**Meeting Concludes** Complete evaluations – available online Boxed dinners to go Shuttle pick up and return to the Hyatt	**GCIS Atrium**

2017 Keynote Lecture: *DNA Nanobots probe Inner Space*

Professor Yamuna Krishnan

Department of Chemistry
The University of Chicago

Bionanotechnology aims to learn from nature - to understand the structure and function of biological devices and to utilize nature's solutions in advancing science and engineering. Evolution has produced an overwhelming number and variety of biological devices that function at the nanoscale or molecular level. My lab's central theme is one of synthetic biology, which involves taking a biological device, component or concept out of its natural cellular context and harnessing its function in a completely new setting so as to probe or reprogram the cell. Our research involves understanding the structure and dynamics of unusual forms of nucleic acids and translating this knowledge to create nucleic acid-based nanodevices for applications in biology.

An example of this type of device results from using DNA like wool on the nanoscale. We knit it into shapes to create little nanobots that respond to the presence of specific chemicals by glowing in different colors. We graft molecular information onto these nanobots that allows them to sail into the nooks and crannies of living cells to report on how healthy or diseased the cell is. This is exciting because we can now not only detect, but quantify protein activity inside cells while they are inside a living organism. This is important because we can identify small molecules that can have drug like activity with much greater ease inside whole organisms or whole cells without having to puree them into a soup. The overall goal of this work is to create a molecular framework for small molecule imaging, which can serve as a universal molecular imaging platform. If successful, I see this being the life science researcher's first go-to imaging solution, where they can get powerful clues as to which molecules, organelles, cells, or tissues they would want to probe, and how.

Yamuna Krishnan is a Professor of Chemistry and a Research Fellow with The Grossman Institute of Neuroscience, Quantiative Biology and Human Behavior at the University of Chicago. She received a PhD from the Indian Institute of Science, Bangalore and pursued her postdoctoral studies as an 1851 Research Fellow at the University of Cambridge, UK. She set up her research group at the National Center for Biological Sciences (NCBS), Bangalore, India, in 2005 with a focus on intelligent DNA-based molecular devices to interrogate cellular processes. She moved to the University of Chicago in 2014.

Yamuna is the youngest woman recipient of India’s highest scientific prize, the Shanti Swarup Bhatnagar Award. The journal Cell included her on their list of “40 under 40” young scientists who are shaping current and future trends in biology. She has also received the Wellcome Trust Senior Fellowship, the AVRA Young Scientist Award, the Innovative Young Biotechnologist Award, the Indian National Science Academy’s Young Scientist Medal, the YIM Boston Young Scientist Award and was named the Chemical Sciences Emerging Investigator by the Royal Society of Chemistry for 2015. Yamuna also serves as an editor for the journal Nanoscale.

2017 Janet Andersen Lecture: *Chemical bonding in transition metal free radicals: Tantalizing and golden results from electronic spectroscopy*

Professor Thomas Varberg
DeWitt Wallace Professor of Chemistry
Macalester College

Abstract: Transition metals play important roles in such diverse areas as chemical catalysis, metallurgy, stained glass, and nanoelectronics. More recently, physicists have begun studies of diatomic transition metal compounds with the goal of determining the electric dipole moment of the electron. My interest in transition metals and the spectroscopy of their compounds springs from the presence of unpaired electrons, which not only produce the distinctive chemistry of the transition metals but also give rise to interesting and challenging spectra to be unraveled and deciphered. I will describe our recent work involving the metals tantalum and gold. With visible and near---infrared lasers, we have recorded spectra of several different diatomic fluorides, oxides, sulfides and hydrides containing one of these two metals. Our analyses of their complex spectra have revealed interesting insights into the chemical bonding of these molecules.

About Professor Varberg: While physical chemistry is often viewed as one of the more challenging areas of chemistry, the nomination letter for Dr. Thomas Varberg describes him as an enthusiastic teacher whose "passion for pchem is clear and effusive; Tom enjoys stimulating student interest in physical chemistry and making the material accessible." This passion is evident in both his teaching and mentoring of undergraduate research at Macalester College. Chemistry majors regularly identify his quantum chemistry course as one of their favorite chemistry classes, while his teaching in the Accelerated and General Chemistry courses encourages many first-year students to continue with a chemistry major. Tom has obtained over $1 million in NSF-RUI funding to support students, both chemistry and physics majors, in molecular spectroscopy research projects at Macalester. Of the approximately 40 students he has mentored in the laboratory, 21 have been included as co-authors for peer reviewed publications. Tom is seen as a strong advocate of the liberal arts and his global perspective obtained from multiple sabbaticals in international venues supports Macalester's emphasis on internationalism and multiculturalism.

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 of Award	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 Lisenksy, 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

Oral Sessions Schedule

SESSION A: 10:00 – 11:15 a.m. Room: Kersten 101
Physics

Session #	Presenter Name	Institution	Title of Presentation
A.1 (10:00)	Soma Beleznay	St. Olaf College	Two Color Chiral Perturbation Theory at Finite Density
A.2 (10:15)	Willa Dworschack	Lawrence University	Determination of the Landé $g_J(2p_9)$ and $g_J(2p_8)$ factors in ^{20}Ne
A.3 (10:30)	Theo Jacobson	Macalester College	Gravitational leptogenesis in Chern-Simons modified gravity
A.4 (10:45)	Kelly Neubauer	Gustavus Adolphus College	Inverse magneto-caloric effect at the spin reorientation of Fe_2B alloys doped with Co
~~A.5 (11:00)~~ **See F.1 (2:30)**	Lucas Myers	Lawrence University	Method for tracking microtubules in gliding assays

SESSION B: 10:00 – 11:15 a.m. Room: Kersten 103
~~Biochemistry~~ Cancelled – see new times for talks in E.4 and G.4

Session #	Presenter Name	Institution	Title of Presentation
~~B.1 (10:00)~~ withdrawn	Garrett Arosemena Ott	Washington University in St. Louis	Apparent Diffusion Co-efficient and Cerebral Blood Volume as MR biomarkers of Genetic Subtypes of Glioblastoma Multiforme
~~B.2 (10:18)~~ **See E.4 (3:15)**	Shriram Chennakesavalu	University of Chicago	A Stochastic Model of SgrS-Mediated Translational Repression of the ptsG mRNA
~~B.3 (10:36)~~ **See G.4 (3:15)**	Andrej Corkovic	Grinnell College	Synthesis and Biological Evaluation of Teixobactin Derivatives

SESSION C: 10:00 – 11:15 a.m. Room: Kersten 105
Astronomy and Environmental Science

Session #	Presenter Name	Institution	Title of Presentation
C.1 (10:00)	James Grammich	Beloit College	Modelling the Magnetic Field of the Solar Corona Using Dynamo Theory
C.2 (10:15)	Xiaoqi Yu	Gustavus Adolphus College	Decomposed Velocity Field in $f(R)$ Cosmology
C.3 (10:30)	John Pavek	Gustavus Adolphus College	Mercury and Methylmercury Dynamics in the Surface Water of the Saint Louis River Estuary
C.4 (10:45)	Jonathan Pekarek	University of Chicago	Feasibility of wood chip permeable reactive barriers for large scale in-stream denitrification
C.5 (11:00)	Nicolette Puskar	Lawrence University	Tropospheric Ozone Production in Rural Wisconsin: An Air Quality Study on Adams Farm

SESSION D: 10:00 – 11:15 a.m. Room: Kersten 120 Mathematics			
Session #	**Presenter Name**	**Institution**	**Title of Presentation**
D.1 (10:00)	Ethan Holland	Colorado College	Generating new probability distributions using Applpy and Maple
D.2 (10:15)	Shane Kosieradzki	St. Olaf College	Invariantization of Finite Difference Approximations on Differential Equations
D.3 (10:30)	Samuel Kottler, Malcolm Gabbard	Colorado College	A Study of Metrics on Visual Boundaries
D.4 (10:45)	Bob Kuo	Colorado College	On Factor Pair Latin Squares
D.5 (11:00)	Lauren Stierman	Colorado College	Harmonic mappings from generalizations of hypocycloids

SESSION E: 2:30 - 3:30 p.m. Room: Kersten 101 Biochemistry			
Session #	**Presenter Name**	**Institution**	**Title of Presentation**
E.1 (2:30)	Alessandra Leong	University of Chicago	Probing the Binding of α-Synuclein to Lipid Membranes as a Function of Composition and Curvature
E.2 (2:45)	Andrew Molina	University of Chicago	Molecular mechanism of CNS myelinogenesis: in vitro self-assembly of myelin membrane lipid and protein structures
E.3 (3:00)	Jue Wang	Grinnell College	Conformational analysis of MTHFR mutants with substrate binding utilizing hydrogen-deuterium exchange and mass spectrometry
E.4 (3:15)	Shriram Chennakesavalu	University of Chicago	A Stochastic Model of SgrS-Mediated Translational Repression of the ptsG mRNA

SESSION F: 2:30 - 3:30 p.m. Room: Kersten 105
Physics

Session #	Presenter Name	Institution	Title of Presentation
F.1 (2:30)	Lucas Myers	Lawrence University	Method for tracking microtubules in gliding assays
~~F.1 (2:30)~~ **See P2.26 (1:15)**	Lindsay Berkhout	University of Chicago	Designing, Fabricating, and Testing an Optical Coupler for Use in the South Pole IceTop Array
F.2 (2:48)	Elise Le Boulicaut	Gustavus Adolphus College	Performance studies of the Transition Radiation Tracker at the Large Hadron Collider ATLAS experiment
F.3 (3:06)	Tatiana Proksch, Zachary Martin, Joshua Jackson	Luther College	Charm meson production from bottomonium decays

SESSION G: 2:30 - 3:30 p.m. Room: Kersten 120
Chemistry

Session #	Presenter Name	Institution	Title of Presentation
G.1 (2:30)	Brandon Derstine	Hope College	Ethynyl-substituted longer wavelength azo dyes for photomechanical applications
G.2 (2:15)	Andrew Hill	Lawrence University	Synthesis and Electrochemical Study of a Ditopic β-Diketiminate Ligand
G.3 (3:00)	Rebecca Katz	Knox College	Axial Adducts to Copper Dimers
G.4 (3:15)	Andrej Corkovic	Grinnell College	Synthesis and Biological Evaluation of Teixobactin Derivatives

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	Brook Anderson	Luther College	Analysis of a mathematical model for the cellular dynamics of CTL019 therapy in B-CLL patients
P1.02	Gabriela Basel	University of Chicago	Coarse-grained molecular simulations of PMPC brush-salt interactions
P1.03	Grant Benthin	Luther College	Synthesis of sulfonamide alcohol ligands for use as organocatalysts in ring-opening polymerization reactions
P1.04	Peter Cipriano	Grinnell College	Structural and Magnetization Report of $RCrSb_3$(R= Dy, Cr)
P1.05	Brittany Courteau	Gustavus Adolphus College	Determination of the kinetic expression of the photodegradation of the herbicide dicamba in aqueous solutions
P1.06	Patrick A. Fisher	Hope College	Diaminoacenapthylene.
P1.07	Kevin Honz	Luther College	Interlayer exciton lifetimes in two-dimensional semiconductors
P1.08	Aimee Iradukunda	Knox College	Synthesis and Analysis of Liquid Crystals based on Copper(II) Tetramers
P1.09	Michael Jones	Carthage College	Micelle-Catalyzed Metathesis Reactions in Flow
P1.10	Alexander Knapp	Beloit College	Superhydrophobic coatings on galvanized steel
P1.11	Khia Kurtenbach	University of Chicago	An Investigation on Biaxial and Uniaxial Strain-Induced Effects in Smectic and Nematic Liquid Crystals
P1.12	Caroline Loe	St. Olaf College	The use of structured imaging for the instantaneous measurement of temperature using two-line thermometry
P1.13	Matthew Mehrkens	Gustavus Adolphus College	Ultrasonic Imaging Using Refracto-Vibrometry
P1.14	Emma C. Olson	Grinnell College	Synthesis of water soluble rylene derivatives for sensor applications
P1.15	E. V. Ohstrom	Washington University in St. Louis	Nucleosynthesis and Reaction Rates in Core-Collapse Supernovae
P1.16	Anthony Ortiz	Lawrence University	Synthesis and Trapping Studies of Thienonaphthalene Biradicals
P1.17	Mark Powers	Hope College	Graph pebbling algorithms and Lemke graph construction

P1.18	Alexander Reiter, Jack Haggett	Carthage College	Synthesis of an Alkene-Terminating Steroidal Surfactant Designed for Micelle-Catalyzed Organic Synthesis
P1.19	Nivedina Sarma	University of Chicago	Silicon Nanowire Scaffold for Active Support of Cardiac Muscle
P1.20	Kaung Shein	Beloit College	Simple superhydrophobic coating process on copper
P1.21	Austin Szczodrowski	Carthage College	Synthesizing PSLA-mPEG-550 a designer surfactant for optimizing micellar catalysis through an immobilized Proline-derivative catalyst
P1.22	Victoria Vivtcharenko	Luther College	Dopamine Quantification in Caenorhabditis elegans with High-Performance Liquid Chromatography
P1.23	Yuan Wang	Grinnell College	New ASTRAL-III: scalable distance-based species tree estimation method
P1.24	Qifan Xiao	Macalester College	Toward Carboxylic Acid-Functionalized Naphthalene Diimides
P1.25	Lyujiangnan Ye, Hanbo Shao	Colorado College	On Computing Slice Genus of Non-alternating Prime Knots
P1.26	Junmian Zhu	Grinnell College	NMR Measurements of Ion Transport for Organosilicon Nitrile Electrolytes

Poster Session 2: 1:15 p.m. - 2:15 p.m. Room: GCIS Atrium

Poster #	Presenter Name	Institution	Title of Presentation
P2.01	Linh Chu	Gustavus Adolphus College	Steps Toward a Framework for the Determination of Solute Parameters using the Hydrophobic Subtraction Model of Selectivity in Liquid Chromatography
P2.02	Benjamin Constable	Lawrence University	Growth, structure and potential applications of bismuth doped zinc oxide films
P2.03	Evan Cunningham	Grinnell College	NMR Diffusion Studies of LiTFSI/Organosilyl Electrolytes
P2.04	Theo Gibbs	University of Chicago	The effect of population abundances on the stability of large random ecosystems
P2.05	Elyssa Glenn	Knox College	Synthesis and Analysis of Cobalt Carboxylates with Potential Mesophases
P2.06	Jacob Jansen	Hope College	Heterocycle-directed decarbonylation of diaryl ketones
P2.07	Scott Joffre	Hope College	Comparing Electrochemical Calculations and Particle Induced X-Ray Emission Measurements of Prussian Blue Analogue Deposits

P2.08	Dalir Kellett, Samuel Gleason	Macalester College	Rotational Structure of Electronic States of TaH in the Visible Region
P2.09	Matthew Koviekis	Carthage College	Formation and Strengthening of Silica Nanoparticle Crystals
P2.10	Nora Madrigal	Grinnell College	Detection of triazine herbicides through SPE/LC/MS and ELISA analysis
P2.11	Parveen Narula	Beloit College	Clumps in Saturns F ring
P2.12	Lydia Narum, Sydney Grossman	St. Olaf College	Stable Maximal Subgroups of Automorphism Groups
P2.13	Derrick Obiri-Yeboah	Hope College	Synthesis of an EDOT-substituted iron porphyrin for utilization as a redox mediator for glucose sensing
P2.14	Dona Pantova	Macalester College	UV Photoluminescence Measurements on GaN
P2.15	Benjamin Pederson	Hope College	A Model of Reproductive Success for Neotropical Pioneer Plants
P2.16	Hoang Anh Phan	Macalester College	Interactions of Copper (I) with Zinc-finger Domains of Transcription Factor Sp1
P2.17	Megan Roozeboom, Emily Fuller	Luther College	Using UV-vis spectrophotometry and fluorescence spectroscopy to analyze the binding relationship of Curcuminoids and HSA.
P2.18	Erik Schoonover	Hope College	Development of rhodium-catalyzed carbon-carbon single bond activation via in situ generated imine directing groups.
P2.19	Jacob Schulz	Luther College	Non-invasive Characterization of Mixed Renal Kidney Stones using Dual Energy CT and Photon Counting CT
P2.20	Andrew Smith	University of Chicago	Grain Growth in Sintered Uranium Dioxide for Fuel Performance Code Validation
P2.21	Shining Sun	University of Chicago	Hierarchical Equations of Motion Approach to the Mechanism of Tyrosine Oxidation in Photosynthesis
P2.22	Peter Timperman	Hope College	PyScan: Interfacing Laboratory Instruments using Python
P2.23	Anne Wampler	Washington University in St. Louis	Exploring the antimicrobial activity of beta-lactones to combat antibiotic resistance
P2.24	Benjamin Wollant	St. Olaf College	Characterization of SU-8 Spin Coating over High Aspect Ratio Substrate Topography
P2.25	Haoru Yang	Washington University in St. Louis	Synthetic Scheme of Graphite Oxide Using Hummers' Method
P2.26	Lindsay Berkhout	University of Chicago	Designing, Fabricating, and Testing an Optical Coupler for Use in the South Pole IceTop Array

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

Poster #	Presenter Name	Institution	Title of Presentation
P3.01	Zachary Cole	Beloit College	In Silico Docking of Proposed Inhibitors of Antibiotic Resistance Enzyme AAC(6')-Ib
P3.02	Alexander DePillis	Beloit College	Spatial Calibration of Cassini Images
P3.03	Claire Doody	University of Chicago	Effects of Thermal Variability on Broadband Seismometers: Controlled Experiments, Observations, and Implications
P3.04	Li Fan	Macalester College	Computational Studies of Intramolecular Spiroether Synthesis from Peroxy Enolates
P3.05	Robert Grace	Macalester College	Detrital Zircon Dating and Paleo-geographic Reconstruction in the San Lucia Mountain Range in Coastal California
P3.06	Marlyne Hakizimana	St. Olaf College	Mathematical Modeling of Oncolytic Virotherapy
P3.07	Fry Intia	Lawrence University	Hydraulic Fracture Sand Mining
P3.08	Diamond Jelani	Knox College	Toward using Ar-BIAN Copper Precatalysts for the Hydrosilylation of Styrene
P3.09	Daniel King	St. Olaf College	Synthesis of New Glyoxime-Based Electrocatalysts for Small-Molecule Activation
P3.10	Allyson Leicht	Grinnell College	Exploration of Mechanisms of Hydrogen Deuterium Exchange (HDX) of Arginine containing Peptides
P3.11	Sophie Macfarland, Morgan Reik	University of Chicago	The Effects of Thiol Concentration on the Young's Modulus of Self-Assembled Nanoparticle Films
P3.12	Leah Mellett	Beloit College	Synthesis of AAC(6')-Ib Inhibitors to Combat Bacterial Resistance to Aminoglycosides
P3.13	Alec Nelson	Hope College	MeV Ion Beam Channeling in Strontium Titanate Crystals by Rutherford Backscattering (RBS)
P3.14	Benjamin November	University of Chicago	Effect of co-catalysts and thermal deposition on efficiency of silicon photoelectrodes for water splitting
P3.15	Emily Reasoner, Nathan Campbell	Luther College	Effects of ligand substitution on CdSe nanocrystal optical properties
P3.16	Leah Sanford	Carthage College	Size-matched nanoparticles for the detection of small organic compounds

P3.17	Shuruthi Senthil	Macalester College	An Investigation of Distant Inductive Effects on Donation into Group VI Metals in Tris(diphenylphosphinomethyl)phenylborate Complexes
P3.18	Madison Stamos	University of Chicago	HCV Screening and Linkage-to-Care Best Practices
P3.19	Ian Sutherland	St. Olaf College	Boltzmann Analysis of Gadolinium II Spectra
P3.20	Aileen Szczepanski	Carthage College	Organic Synthesis of O-acylated Amino Acid Surfactants to Examine Antibacterial Properties
P3.21	Judith Tong	Grinnell College	Analysis of organic pigments within art works using surface enhanced Raman spectroscopy
P3.22	Collin Wassilak	Hope College	Functionalization of electrode surfaces using iron-based redox mediating films for glucose detection
P3.23	Junze Yao	Grinnell College	Growth and analysis of single crystal TbCuAl alloy
P3.24	Kaiyuan Zhang	Beloit College	Characterization of ω-3 Fatty Acids in Fish Oil Dietary Supplements with FTIR Spectroscopy and 2D Correlation Analysis
P3.25	Gabe McAndrews, Raymond Wieser	St. Olaf College	Frictional properties of molybdenum disulfide: a combined indenter probe and quartz crystal microbalance investigation
P3.26	Logan Engberg	Carthage College	Teaching the Reactivity of Carboxylic Acid Derivatives through a Discovery-Format Laboratory

Abstracts for all Sessions

Physical Sciences, Math and Computer Science
MCMS Undergraduate Research Symposium, University of Chicago
November 3-4, 2017

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): Brook Anderson, Luther College
Session: Poster P1.01
Title: Analysis of a mathematical model for the cellular dynamics of CTL019 therapy in B-CLL patients
Advisor(s): Kyle Fey, Mathematics, Luther College
Co-Author(s): Kyle Fey

Abstract: We analyze a system of ordinary differential equations developed in 2013 used to model the cellular dynamics of CTL019 therapy in B-CLL patients. We find the qualitatively different phase portraits that are possible and prove the stability of the equilibria that exist in each. We then find the basin of attraction for each equilibria and determine what initial conditions are necessary in order to approach a healthy, stable equilibrium solution. The importance of pretreatment chemotherapy is re-emphasized. Next, we perform a Latin hypercube sampling to determine which parameters are most influential in determining a healthy equilibrium solution value before expanding the model to more accurately express the characteristics of the treatment.

Presenter(s): Garrett Arosemena Ott, Washington University in St. Louis
Session: Oral B.1 (10:00) *Withdrawn*
Title: Apparent Diffusion Co-efficient and Cerebral Blood Volume as MR biomarkers of Genetic Subtypes of Glioblastoma Multiforme
Advisor(s): Benjamin M. Ellingson, Radiology, UCLA
Co-Author(s): Kevin Leu, Albert Lai, Phioanh L. Nghiemphu, Whitney B. Pope, William H. Yong, Linda M. Liau, Timothy F. Cloughesy, Benjamin M. Ellingson

Abstract: Purpose: The value of perfusion and diffusion-weighted MRI in differentiating glioblastoma multiforme (GBM) according to 2016 WHO glioma reclassification guidelines (e.g. 1p/19q co-deletion and IDH1 mutation status) remains controversial. In the current study, we propose unique perfusion and diffusion MR signatures as biomarkers of genetic subtypes in GBM.

Materials and Methods: Sixty-five patients with 2016 genetic designations (e.g. 1p/19q status (+ = intact/- = codeleted), and IDH1 mutation status (MUT/WT)) were included in this study. In all patients, median relative cerebral blood volume (rCBV) and apparent diffusion coefficient (ADC) were estimated within T2 hyperintense lesions. Non-parametric statistical tests were used to compare GBM subpopulations, separated according to 2016 WHO genetic subtype.

Results: rCBV and ADC were significantly different between molecular subtypes, particularly between IDHWT and IDHMUT/1p19q+. IDHMUT/1p19q+ grade III gliomas had higher median ADC; IDHWT grade III gliomas had higher rCBV with lower ADC; and IDHMUT/1p19q- had intermediate rCBV and ADC values, similar to their grade II counterparts.

Conclusion: rCBV and ADC successfully differentiated between genetic subtypes of GBM according to the 2016 WHO classification. Results implicate rCBV and ADC as non-invasive biomarkers of genetic subtypes of GBM, as well as in early identification of malignant transformation.

Presenter(s): Gabriela Basel, University of Chicago
Session: Poster P1.02
Title: Coarse-grained molecular simulations of PMPC brush-salt interactions
Advisor(s): Juan de Pablo, Institute for Molecular Engineering, University of Chicago
Co-Author(s): Wei Chen, Nicholas Jackson

Abstract: Zwitterionic polymer brushes, i.e. zwitterionic polymer-chains end-grafted to a surface, exhibit high potential as stimuli-responsive and lubricative materials in applications ranging from marine coatings to drug delivery and various medical devices. Critical to these applications is how the presence of salt ions in solution influence brush morphology and functionality, though significant contradictions exist in the current literature pertaining to this topic. To elucidate these effects, coarse-grained molecular simulations of a common zwitterionic polymer, poly-2-methacryloyloxyethyl pyhosphorylcholine (PMPC), were performed to study the impact of varying the concentrations of NaCl and $CaCl_2$ on the height, density, and morphology of PMPC brushes. The results show that PMPC exhibits an increase in brush height as salt concentration increases as a result of electrostatic screening – the so-called "anti-polyelectrolyte effect". Unexpectedly, preliminary results indicate that increasing the valency of salt ions results in a decrease in PMPC brush height – an effect which is hypothesized to be the result of weak charge-dipole bridging interactions between PMPC chains.

Presenter(s): Soma Beleznay, St. Olaf College
Session: Oral A.1 (10:00)
Title: Two Color Chiral Perturbation Theory at Finite Density
Advisor(s): Prabal Adhikari, Physics, St Olaf College
Co-Author(s): Prabal Adhikari, Massimo Mannarelli

Abstract: We examine the phase diagram of two color Quantum Chromodynamics (QCD) in the presence of isospin and baryon chemical potentials in the regime of QCD where chiral-perturbation-theory is valid. We first investigate the phase diagram of the theory, which is known to possess a second order transition when the chemical potential is equal to the diquark or pion mass. Furthermore, it also contains a first order transition when the two chemical potentials are equal and greater than the diquark or pion mass. We show that the origin of this first order transition is not explained by a standard Ginzburg-Landau expansion, but is due to the change in order parameter of the theory. When the chemical potentials are unequal, the order parameter is a U(1) complex field; however, when the two chemical potentials are equal the order parameter is remarkably an SU(2) doublet. As such, the ground state at equal chemical potentials is neither in a diquark state or a pionic state but a degenerate mixture of the two.

Sound modes in the mixture state are still under investigation. Thermodynamic considerations suggest that at least one of the three modes is the same as in the U(1) case.

Presenter(s): Grant Benthin, Luther College
Session: Poster P1.03
Title: Synthesis of sulfonamide alcohol ligands for use as organocatalysts in ring-opening polymerization reactions
Advisor(s): Bradley M. Chamberlain, Chemistry, Luther College
Co-Author(s): Jordan Keeton

Abstract: Biodegradable polymers made from renewable resources are a fundamental part of sustainable commercial technologies. One of the most successful advancements in biodegradable polymer development, polylactide (PLA), is a polyester with substantial potential to replace some traditional petroleum based plastics; it is synthesized by a ring-opening polymerization (ROP) of D,L-lactide.

In recent years, considerable effort has been made to develop catalysts for PLA synthesis that control the rates of polymerization and the three-dimensional orientation of substituents along the polymer chain. Most catalysts currently used in PLA synthesis are metal-based and are often associated with levels of conductivity and/or toxicity that are undesirable in electrical or biological systems. Hoping to avoid these undesirable properties, a library of metal-free sulfonamide catalysts was prepared. Herein, we report the synthesis of characterization of this library containing a broader range of electronic and steric properties.

Presenter(s): Lindsay Berkhout, University of Chicago
Session: Poster 2.26
Title: Designing, Fabricating, and Testing an Optical Coupler for Use in the South Pole IceTop Array
Advisor(s): Lowell McCann, Physics, University of Wisconsin-River Falls
Co-Author(s):

Abstract: The IceCube Neutrino Observatory detects astrophysical neutrinos via light produced when the neutrino interacts with the Antarctic ice. IceCube includes the IceTop array, which is used as a veto system to detect muons originating in the atmosphere. IceTop is slated for an expansion that will increase its size and fiber optic detectors are being investigated to provide a cheap, lightweight method for expansion. The sensors used in this kind of setup are incredibly small and can only fit a few fibers onto the sensor area. To remedy this, this project designed and investigated an optical coupler for use in the expansion that could funnel light from a large number of fibers onto a small aperture sensor, allowing the detector to be expanded without changing the small sensor. The design was modeled off the compound parabolic concentrator. A number of CPC's were printed on a Formlabs resin printer, polished smooth, and subjected to a number of tests to determine their feasibility as optical couplers. In conclusion, we found that optical coupler design did not behave exactly as expected, but results seem promising. Upon further testing, we expect this optical coupler will provide a neat and cost-effective solution for expanding IceTop.

Presenter(s): Shriram Chennakesavalu, University of Chicago
Session: Oral E.4 (3:15)
Title: A Stochastic Model of SgrS-Mediated Translational Repression of the ptsG mRNA
Advisor(s): Jingyi Fei, Department of Biochemistry and Molecular Biology, The University of Chicago
Co-Author(s): Matt Reyer, Emily Heideman, Jingyi Fei

Abstract: Bacterial small RNAs (sRNAs) are highly structured RNAs that play important roles in regulating genes involved in many cellular processes. In *E. Coli*, the sRNA SgrS regulates the translation of the *ptsG* mRNA in response to glucose phosphate stress. SgrS-mediated regulation is understood qualitatively; however, a quantitative understanding of the pathway—such as the kinetics of translational regulation—is limited. Using only fluorescent imaging, we are unable to quantify the regulation. To overcome this limitation, we have successfully developed a mathematical simulation of SgrS-meditated translational regulation using the Gillespie Algorithm. Our stochastic simulation allows for a more robust investigation of the kinetics of regulation. With this simulation completed, we will carry out fluorescent imaging experiments to validate our simulation with data in order to accurately and successfully determine the kinetic parameters of SgrS regulation.

Presenter(s): Linh Chu, Gustavus Adolphus College
Session: Poster P2.01
Title: Steps Toward a Framework for the Determination of Solute Parameters using the Hydrophobic Subtraction Model of Selectivity in Liquid Chromatography
Advisor(s): Dwight Stoll, Chemistry Department, Gustavus Adolphus College
Co-Author(s): Kelson Oram

Abstract: Hydrophobic Subtraction (HS) model was formulated in the early 2000s to understand and characterize the selectivity of reversed-phase columns used in liquid chromatography. The model describes column selectivity as the sum of five solute – column interactions: 1) hydrophobic interaction; 2) steric resistance; 3,4) hydrogen bonding; and 5) cation exchange. With a given column, the HS model yields quantitative values of five column parameters that relate to the chemistry of this particular stationary phase.

In this project we focused on determining solute parameters for the HS Model. The ultimate goal is to find an effective tool to limit the guesswork involved in column selection, enable predictions of retention time as a means optimizing separations. In order to determine solute parameters, a UV absorbance spectral library of test compounds was created to serve as the database for compounds when analyzed as mixtures. Then, retention data (about 4000 measurements) were obtained using different mixtures of acetonitrile/water mobile phases. Future work will involve analysis of the resulting solute retention factors for many different columns having different stationary phases to determine how accurately retention time can be predicted using the solute parameters determined in this way.

Presenter(s): Peter Cipriano, Grinnell College
Session: Poster P1.04
Title: Structural and Magnetization Report of $RCrSb_3$(R= Dy, Cr)
Advisor(s): Charles Cunningham, Physics, Grinnell College
Co-Author(s):

Abstract: Single crystals of $RCrSb_3$(R=Tb, Dy) were grown via the flux method. X-ray diffraction measurements have determined that they crystallize in an orthorhombic bravais lattice with a space group of Pbcm. $DyCrSb_3$ has parameters of a=12.6292, b=6.15390, c=5.9837, and has ferromagnetic ordering at curie temperature of 80K and antiferromagnetic ordering transitions at a Neél temperature of 15K and 20K. $TbCrSb_3$ were found to have parameters of a=12.6647, b=6.14027, c=5.98837, and to undergo antiferromagnetic ordering and ferromagnetic ordering at a Neél temperature of 37K and a Curie Temperature of 72K, respectively.

Presenter(s): Zachary Cole, Beloit College
Session: Poster P3.01
Title: In Silico Docking of Proposed Inhibitors of Antibiotic Resistance Enzyme AAC(6')-Ib
Advisor(s): Kristin Labby, Chemistry, Beloit College
Co-Author(s): Zachary Cole

Abstract: The use of computational resources for drug design and discovery represents a significant component of the current medicinal chemistry process. A low cost, primarily open source method was used to characterize the binding affinity and active site interactions of a series of ligands, as well as compounds from the ZINC database, to identify potential inhibitors of the antibiotic resistance enzyme AAC(6')-Ib. Methods include the use of AutoDock Vina, Pyrex, PyMol, and LigPlot+. Characterization of ligand-receptor interactions aids the synthesis of AAC(6')-Ib inhibitors by informing the researcher of potentially useful inhibitor structure.

Presenter(s): Benjamin Constable, Lawrence University
Session: Poster P2.02
Title: Growth, structure and potential applications of bismuth doped zinc oxide films
Advisor(s): Sara Chamberlin, Physics, Lawrence University
Co-Author(s): Sara Chamberlin

Abstract: There is a constant search for more efficient materials for use in electronics. Zinc Oxide (ZnO) is a well-known semiconductor used in numerous applications. However, the effects of doping ZnO with bismuth (Bi) are less documented. Using spray pyrolysis—a robust and industrially relevant technique—a solution of Zn and Bi nitrates is sprayed onto a heated substrate to grow thin films of polycrystalline $ZnBi_xO_{1-x}$ with various Bi concentrations below x=0.05. X-ray diffraction (XRD) is used to verify the retention of ZnO's structure, verifying that Bi substitutes for O in the crystal lattice. Scanning electron microscopy (SEM) is used to investigate how our growth parameters impact density and uniformity of the films. Understanding the structure of these films is a crucial step in creating applications of $ZnBi_xO_{1-x}$ with various Bi concentrations below x=0.05. X-ray diffraction (XRD) is used to verify the retention of Zn, and we will next analyze electrical properties in the hope of producing stable, P-type doped ZnO for use in 100% ZnO semiconductor devices.

Presenter(s): Andrej Corkovic, Grinnell College
Session: Oral G.4 (3:15)
Title: Synthesis and Biological Evaluation of Teixobactin Derivatives
Advisor(s): Erick Leggans, Chemistry, Grinnell College
Co-Author(s):

Abstract: Antimicrobial-resistant infectious strains of bacteria have risen over the past 20 years limiting the lifespans of existing antibiotics. Natural products have been at the forefront of this research since the golden era of antibiotic drug discovery. Advances in technology have led to the possibility of isolating and growing previously remote natural products. Many of the peptide natural products' precursors are commercially available amino acids, leading to a higher desirability for structure-activity relationship (SAR) studies. One such natural product is teixobactin. The goal of conducting SAR studies on teixobactin is to synthesize, characterize, and biologically evaluate derivatives of the biologically active molecule. As opposed to previous attempts to synthesize the compound through solid phase chemistry, this research focuses on a fragment-based synthetic approach, allowing us to biologically evaluate the intermediary compounds in addition to the final product.

Presenter(s): Brittany Courteau, Gustavus Adolphus College
Session: Poster P1.05
Title: Determination of the kinetic expression of the photodegradation of the herbicide dicamba in aqueous solutions
Advisor(s): Amanda Nienow, Chemistry, Gustavus Adolphus College
Co-Author(s):

Abstract: Dicamba, 3,6-dichloro-2-methoxybenzoic acid, is a post emergent herbicide, typically sprayed on corn and soybean crops across the U.S under the commercial name Diablo. This research project explored the kinetics of the photodegradation of dicamba in aqueous solutions of different water quality, including differences in pH, natural organic matter (NOM concentrations), and dissolved oxygen concentrations. The overall rate was determined to be first order. Addition of the NOM had the largest impact on the rate of the reaction, showing decreasing rates with increasing NOM concentrations. The pH only had a moderate impact, with a higher rate at neutral pH, while the concentration of dissolved oxygen did not have an impact on the rate. Photoproducts were analyzed using UV-VIS and GC-MS. Through UV-VIS analysis two products may be present in solution after irradiation due to the presence of an isosbestic point. GC-MS data supports the theory of two photoproducts present in solution, dichlorophenol and dichloromethoxybenzene.

Presenter(s): Evan Cunningham, Grinnell College
Session: Poster P2.03
Title: NMR Diffusion Studies of LiTFSI/Organosilyl Electrolytes
Advisor(s): Leslie Lyons, Chemistry, Grinnell College
Co-Author(s):

Abstract: The temperature dependent self-diffusion coefficients of lithium cations (DLi) and fluorine anions (DTFSI) were measured by $^{7}Li^{+}$ and $^{19}F^{-}$ pulsed-field gradient (PFG) NMR spectroscopy for six electrolytes, using three silyl solvents doped with the lithium salt LiTFSI at two different salt concentrations. The silyl solvents, prepared and patented by Silatronix (Madison, WI) vary in the degree of fluorination of the solvent. The effects of salt concentration, solvent composition, and temperature on the self-diffusion coefficients, transference numbers, molar conductivities, and α (salt dissociation) values are discussed. Diffusion is faster for both ions in the dilute electrolytes compared to the concentrated salt electrolytes for all temperatures. Lithium transference numbers ranged from 0.42 to 0.52 at 295 K. These values are considerably higher than conventional ethylene carbonate electrolytes and quite promising for lithium ion battery applications. As fluorination of the samples increased, α values at 300 K increased from 0.20 to 0.37 in the dilute samples, and from 0.18 to 0.31 in the concentrated samples.

Presenter(s): Alexander DePillis, Beloit College
Session: Poster P3.02
Title: Spatial Calibration of Cassini Images
Advisor(s): Britt Scharringhausen, Physics & Astronomy, Beloit College
Co-Author(s):

Abstract: In 2005 the Cassini spacecraft passed through Saturn's ring plane while taking pictures of the ring. A novel approach to the measurement of the ring was developed based on the fitting of gaussian curves to columns of pixels. Measurement of the position of the ring within these images in combination with previous work enables the use of trigonometry to perform spatial calibration with increased accuracy. The parameters generated by the gaussian fits have the potential to provide information on the vertical size of clumps in Saturn's F ring.

Presenter(s): Brandon Derstine, Hope College
Session: Oral G.1 (2:30)
Title: Ethynyl-substituted longer wavelength azo dyes for photomechanical applications
Advisor(s): Jason Gillmore, Department of Chemistry, Hope College
Co-Author(s): Sean Gitter, Jason Gillmore, Matt Smith

Abstract: Azo dyes are a class of compounds that undergo reversible trans- to cis- isomerization upon irradiation with specific wavelengths of light. Typically, azo dyes isomerize by absorbing ultraviolet to blue-green light. In this region of the electromagnetic spectrum, competitive absorption by other organic molecules is at a maximum, and these higher energy wavelengths provide a greater likelihood of photodegradation of the material. Aprahamian and coworkers have reported a class of BF_2-coordinated azo dyes that absorb red-orange to near infrared light. These lower energy wavelengths mitigate competitive absorption and photodegradation. Efforts in the Gillmore group have been made to install a polymerizable substituent on the azo dye for pendant incorporation into a polymeric system for photomechanical applications in the Smith group. Thus, an ethynyl-substituted BF_2-coordinated azo dye was synthesized for incorporation into a polymer by Sonogashira coupling, direct alkynyl polymerization, or partial reduction to a vinyl-substituted dye for vinyl free radical polymerization. Current and future syntheses and polymerization efforts are reported.

Presenter(s): Claire Doody, University of Chicago
Session: Poster P3.03
Title: Effects of Thermal Variability on Broadband Seismometers: Controlled Experiments, Observations, and Implications
Advisor(s): Andrew Campbell, Department of Geophysical Sciences, University of Chicago
Co-Author(s): Adam T. Ringler, Robert E. Anthony, David C. Wilson, Austin A. Holland, Charles R. Hutt, Leo D. Sandoval

Abstract: Isolating seismic instruments from temperature fluctuations is routine practice within the seismological community. However, the necessary degree of thermal stability to avoid generating noise or compromising the fidelity in the seismic records is largely unknown and likely application dependent. To quantify the temperature sensitivity of seismometers over a broad range of frequencies, we artificially induced local temperature changes to measure the effect of thermal variations on seismometer output. We found that diurnal temperature changes above 0.002˚C Root-Mean-Square (RMS) showed significant changes in velocity and acceleration output in comparison to thermally stable reference measurements. We also found that sensor incoherent self-noise increased with temperature variation; these increases in noise can be modeled as 1/f noise (pink noise) and are unlikely to be easily corrected for. These results are compared to data from Incorporated Research Institutions for Seismology (IRIS) U. S. Geological Survey (USGS) Global Seismographic Network (GSN) station TUC (Tucson, Arizona). We show that the water bricks and borehole installations at this station give ample temperature attenuation to isolate seismometers from diurnal thermal variability. We find seismometer installations that provide thermal stability below 0.002˚C RMS could help to improve long-period vertical seismic data across the GSN by decreasing temperature-driven 1/f noise.

Presenter(s): Willa Dworschack, Lawrence University
Session: Oral A.2 (10:15)
Title: Determination of the Landé $g_J(2p_9)$ and $g_J(2p_8)$ factors in ^{20}Ne
Advisor(s): John Brandenberger, Physics, Lawrence University
Co-Author(s):

Abstract: New measurements of the Landé g_J factors for the $2p_9$ and $2p_8$ states in ^{20}Ne have been determined. We employ the technique of saturated absorption laser spectroscopy to measure ratios of $g_J(2p_9)/g_J(1s_5)$ and $g_J(2p_8)/g_J(1s_5)$. We combine these ratios with the well-known g_J factor for the $1s_5$ state for a result of $g_J(2p_9)$ and $g_J(2p_8)$. This method allows us to bypass supplemental measurements. Additionally, saturated absorption spectroscopy provides Doppler-free and redundant spectra which yield multiple determinations of the g_J factor. We have arrived at new experimental values for $g_J(2p_9)$ and $g_J(2p_8)$ with uncertainties that are substantially less than previously published values. It is our hope that these new measurements will prompt further refinement of calculations concerning the Landé g_J factor. Supported by Lawrence University.

Presenter(s): Logan Engberg, Carthage College
Session: Poster P3.26
Title: Teaching the Reactivity of Carboxylic Acid Derivatives through a Discovery-Format Laboratory
Advisor(s): David Brownholland, Chemistry, Carthage College
Co-Author(s):

Abstract: Discovery-based labs, in which students learn a chemical concept through collecting data in an experiment, instead of through lecture, have been heavily adopted in the general chemistry curriculum. These labs have been shown to enhance student's understanding of the material, improve engagement in the learning process, and increase student responsibility for learning the material. Unfortunately, data collection in organic chemistry is slow and students rarely collect significant amounts of data. As such, few examples exist of these types of discovery-based experiments in the undergraduate curriculum. We aim to design a discovery-based laboratory demonstrating the relative reactivity of electrophiles and nucleophiles in carboxylic acid derivatives for inclusion into the Carthage College organic chemistry curriculum. Our initial goal was to evaluate the relative effectiveness of synthesizing aspirin from salicylic acid using a variety of carboxylic acid derivatives via microwave irradiation. Unfortunately, we ran into problems with polymerization, toxicity of materials, and cost. Due to these issues, we altered the experiment to evaluate the effectiveness of treating acetic anhydride or ethyl acetate with either phenol or aniline. Each student will attempt their own nucleophilic acyl substitution and the class will combine their data at the end of the class to evaluate the trends. Our preliminary results indicate this new discovery-based lab will provide appropriate results for students to determine the relative reactivity of ethyl acetate and acetic anhydride as well as the relative nucleophilicity of phenol and aniline.

Presenter(s): Li Fan, Macalester College
Session: Poster P3.04
Title: Intramolecular Spiroether Synthesis from Peroxy Enolates
Advisor(s): Keith Kuwata, Chemistry, Macalester College
Co-Author(s): Keith Kuwata

Abstract: Intramolecular synthetic mechanisms of spiroethers from peroxy enolates were studied with density functional theory methods. The mechanisms consist of an enolate formation step followed by the cleavage of peroxy O-O bond with the attack of the enolate carbon on a peroxy oxygen. The reactions of 2-(methylperoxypropyl)-hexanone with M-diisopropylamine (M = no metal, Li) and M-tert-butoxide (M = no metal, Na, K) were explored under conditions of both without solvent and in THF. B3LYP/6-31G(d) geometry optimization and vibrational frequencies calculations and B3LYP/6-31+G(d,p) molecular energy calculations were performed in order to locate transition state structures and evaluate reaction enthalpies, activation energies, equilibrium constants, and relative rates of reactions. The proposed mechanisms were validated with all related transition state structures located. Furthermore, diisopropylamine reagents were predicted to undergo more exothermic reactions than tert-butoxide reagents. The presence of alkali metals added to the exothermicity of reactions, which effect weakened with increasing atom size. THF showed a stronger stabilizing effect on starting materials and products than on transition state structures. Minor reactions had lower reaction barriers and thus were preferred kinetically, leading to the observed lower yield for reactions mediated with alkali metals of small size.

Presenter(s): Patrick A. Fisher, Hope College
Session: Poster P1.06
Title: Diaminoacenapthylene.
Advisor(s): Jason G. Gillmore, Chemistry, Hope College
Co-Author(s): Amber J. Prins, and Jason G. Gillmore

Abstract: The Gillmore research group's former photochromic photooxidants project was based on the perimidinespirohexadienone (PSHD) family of photochromes. In the course of this work it was desired to prepare carbonyl-substituted PSHDs. The title compound, diaminoacenaphthylene (DAAnl), was a necessary intermediate. Although it appears to be a simple molecule to synthesize, the unusually reactive alkene and unusually unreactive aryl nitro groups of dinitroacenaphthylene caused several normally selective reductions to DAAnl to fail. Years later, we now report the successful synthesis of DAAnl for others for whom it may be a valuable intermediate.

Presenter(s): Theo Gibbs, University of Chicago
Session: Poster P2.04
Title: The effect of population abundances on the stability of large random ecosystems
Advisor(s): Stefano Allesina, Ecology and Evolution, University of Chicago
Co-Author(s): Jacopo Grilli, Tim Rogers, Stefano Allesina

Abstract: Random matrix theory successfully connects the structure of interactions of large ecological communities to their ability to respond to perturbations. One of the most debated aspects of this approach is the missing role of population abundances. Despite being one of the most studied patterns in ecology, and one of the most empirically accessible quantities, population abundances are always neglected in random matrix approaches and their role in determining stability is still not understood. Here, we tackle this question by explicitly including population abundances in a random matrix framework. We obtain an analytical formula that describes the spectrum of a large community matrix for arbitrary feasible species abundance distributions. The emerging picture is remarkably simple: while population abundances affect the rate to return to equilibrium after a perturbation, the stability of large ecosystems is uniquely determined by the interaction matrix. We confirm this result by showing that the likelihood of having a feasible and unstable solution in the Lotka-Volterra system of equations decreases exponentially with the number of species for stable interaction matrices.

Presenter(s): Elyssa Glenn, Knox College
Session: Poster P2.05
Title: Synthesis and Analysis of Cobalt Carboxylates with Potential Mesophases
Advisor(s): Thomas Clayton, Chemistry, Knox College
Co-Author(s): Thomas Clayton

Abstract: Metal soaps have long been known to be liquid crystalline. This includes common soaps (like sodium carboxylates), and carboxylate soaps of transition metals, which often take on a paddlewheel shape with the carboxylate ligands bridging two metal atoms. In contrast to the copper (II) octanoate dimer, cobalt (II) octanoate has been previously reported as a non-birefringent pink polymer formed through hydrogen bonding between water ligands. Still, cobalt analogues of the paddlewheel transition metal carboxylates have been reported with additional nitrogen-donating ligands at the axial sites. We report the synthesis of a series of cobalt carboxylates with systematically varied chain length by two methods. In the first, pink polymers were precipitated from water. These polymers were subsequently dissolved in THF forming deep green products readily soluble in toluene. The second method yielded deep green toluene soluble products directly from the reaction of $CoCl_{26}H_2O$ and the appropriate sodium carboxylate salt in THF. The ligands varied from four carbon to sixteen carbon aliphatic chains. Products were characterized using polarized optical microscopy (POM), infrared spectroscopy (IR), elemental analysis, and differential scanning calorimetry (DSC).

Presenter(s): Robert Grace, Macalester College
Session: Poster P3.05
Title: Detrital Zircon Dating and Paleo-geographic Reconstruction in the San Lucia Mountain Range in Coastal California
Advisor(s): Alan D. Chapman, Geology, Macalester College
Co-Author(s):

Abstract: The San Lucia Mountains in central coastal California are a unique mountain range because they are composed of arc rocks adjacent to trench rocks. They are on the western side of the San Andreas fault and have thus been displaced north by the San Andreas fault system. The prevailing theory is that the San Lucia Mountains are a surviving block that faulted off of the North American plate as the Shatsky Rise Conjugate subducted under the continental plate. U/Pb dating of detrital zircons from rocks in the center of the San Lucia mountain range (Salinian Block) revealed several ages in support of a Mojave origin of the range. Several age peaks match previously dated sites in the Mojave, which indicates that the rocks we sampled may have come from the Mojave region. This research provides new data in consistent with the current theory.

Presenter(s): James Grammich, Beloit College
Session: Oral C.1 (10:00)
Title: Modelling the Magnetic Field of the Solar Corona Using Dynamo Theory
Advisor(s): Britt Scharringhausen, Physics, Beloit College
Co-Author(s):

Abstract: In this project, we aim to model the magnetic field generated by the rotation of the solar corona using dynamo theory. In order to do this, we first construct a model of a hollow sphere made of plasma, and then model how the sphere generates a magnetic field when rotating rigidly. After that, we introduce differential rotation into the sphere, and examine how this changes to magnetic field that is generated. Finally, we introduce complicating factors, such as sunspots and solar wind, and examine how those affect the generation of the solar corona’s dynamo.

Presenter(s): Marlyne Hakizimana, St. Olaf College
Session: Poster P3.06
Title: Mathematical Modeling of Oncolytic Virotherapy
Advisor(s): Bruce Pell, Mathematics, Statistics and Computer Science, St Olaf College
Co-Author(s): Sawyer Jacobson

Abstract: An oncolytic virus is designed to specifically target and kill cancer cells while leaving normal cells alone. Oncolytic Virotherapy uses oncolytic viruses as a form of therapy to treat cancer. Previous models have used ordinary differential equations in their modeling process. Our model implements a system of delay differential equations to incorporate the time delay in the adaptive immune system. The model assumes that the adaptive immune system is completely dependent on infected tumor cells created by timed injections of an oncolytic adenovirus. The model was fit to data obtained from Zhang et al. (2011) using the statistical program R-studio. Numerical simulations were implemented in order to find key parameters that could control the extinction of Cancer. A univariate local sensitivity analysis was performed to see which parameters were most sensitive to a slight perturbation. It is hoped that the model can be used in clinical trials to help determine the best course of treatment for individual patients.

Presenter(s): Andrew Hill, Lawrence University
Session: Oral G.2 (2:15)
Title: Synthesis and Electrochemical Study of a Ditopic β-Diketiminate Ligand
Advisor(s): Graham T. Sazama, Chemistry, Lawrence University
Co-Author(s): Graham T. Sazama

Abstract: Molecular electronic materials promise to have the potential to make next-generation devices significantly smaller and thinner. Before building the bulk material, we may establish its desirable properties in a model dimer through electrochemical experiments. Here we propose a coordination complex bridging two first-row transition metal centers, a step towards a coordination polymer. Starting from the complex 1 [M(L)$_x$(nacnac-I)] (nacnac-I= N,N'-diphenyl-3-iodo-2,4-pentanediketiminate ion), the complex 2 [M(L)$_x$(nacnac-DEB-nacnac)] (DEB = 1,4-diethynylbenzene) will be obtained through a Sonogashira cross coupling reaction. This complex 2 will be characterized by elemental analysis, IR, 1H NMR, 13C NMR, UV−vis, cyclic voltammetry, mass spectroscopy and X-ray single-crystal diffraction. The SOMO DFT plot of the oxidized complex predicts that electron transfer between the two metal centers of the proposed complex is possible.

Presenter(s): Ethan Holland, Colorado College
Session: Oral D.1 (10:00)
Title: Generating new probability distributions using Applpy and Maple
Advisor(s): Andrew Glen, Mathematics, Colorado College
Co-Author(s): Marketa Harastova

Abstract: The goal of our research project was to write a code in Maple using Applpy that could generate new probability distributions. Basing our research in theory, we used integration to get marginal distributions, and minima and maxima of existing probability density functions (PDFs) to generate new PDFs that were then tested using Maple. Additionally, we wrote a code to automatically transfer our results into LaTeX to enable more efficient classification of the newly generated distributions. Moreover, we substituted values for our parameters in the new probability density functions which allowed us to observe various characteristics of the distributions such as cumulative density function, survivor function, and hazard function. Some of the interesting examples are observed through the plots of the hazard functions. Finally, this research's outcome is presented in a form of LaTeX charts and documents.

Presenter(s): Kevin Honz, Luther College
Session: Poster P1.07
Title: Interlayer exciton lifetimes in two-dimensional semiconductors
Advisor(s): Kin Fai Mak, Physics, Pennsylvania State University
Co-Author(s): Yi-Hsin Chiu, Zefang Wang, Kin Fai Mak, Jie Shan

Abstract: Two-dimensional semiconductors, specifically transition metal dichalcogenides, have strong excitonic effects. These excitonic effects arise from the low dimensionality, which reduces screening of the Coulomb interactions between charge carriers. The ensuing excitons, bound electron-hole pairs, have the potential to exhibit exotic quantum states like Bose-Einstein condensation. However, intralayer excitons, with lifetimes of 1-10 ps, recombine too quickly to reach thermal equilibrium and achieve such exotic states. To increase lifetimes, the electrons and holes can be spatially separated into different layers using an external electric field, forming interlayer excitons. In this study, we applied an external electric field to a dual-gated bilayer WSe_2 device. Excitons were generated by optically pumping the device with a femtosecond pulsed laser. Excitons then recombined radiatively, and the resulting photoluminescence was measured by an avalanche photodiode using time-correlated single photon counting techniques. Exciton lifetimes were extracted from measurements with an iterative reconvolution script. Exciton lifetimes were observed to remain at less than 0.1 ns for electric fields less than a critical value. Above the critical electric field value, lifetimes dramatically increased, up to 22 ns. Our results demonstrate that interlayer excitons in bilayer WSe_2 exhibit significantly longer lifetimes, opening new possibilities for exotic quantum states.

Presenter(s): Fry Intia, Lawrence University
Session: Poster P3.07
Title: Hydraulic Fracture Sand Mining
Advisor(s): Deanna Donohoue, Chemistry, Lawrence University
Co-Author(s): Deanna Donohoue and Nicolette Puskar

Abstract: Recent investment in mining hydraulic fracturing crystalline silica sand increased the concern of air quality for residents near the mines in rural Wisconsin. Mining this sand releases crystalline silica dust into the air which causes long term damage to the lungs. This sort of pollutant is known as particulate matter (PM). To investigate the amount of PM coming off one quarry, we used TSI's Optical Particle Sizer at Adam's farm near a newly active Hydraulic Fracturing Sand quarry. We included the Kestrel 4500 to monitor the relative weather and used a Raman Spectroscopy microscope to examine the PM that collected on the Optical Particle Sizer's filter. Through the data, we observed that there are no high counts of PM coming from the direction of the quarry. There are high counts of PM coming from the direction of a nearby granary. This could be due to the wind-carrying particulate matter from the mines in other directions possibly containing the crystalline silica dust, which is worth investigating. The data from the Raman Spectroscopy Microscope is currently inconclusive with possible interference from the filter. The current data shows, there is not an alarming amount of PM coming from the quarry to the farm.

Presenter(s): Aimee Iradukunda, Knox College
Session: Poster P1.08
Title: Synthesis and Analysis of Liquid Crystals based on Copper(II) Tetramers
Advisor(s): Thomas Clayton, Chemistry, Knox College
Co-Author(s): Thomas Clayton

Abstract: Homoleptic copper (II) dimers with long chain bridging carboxylates have long been known to form liquid crystalline mesophases. Previous work at Knox has shown that heteroleptic (mixed ligand) copper (II) carboxylate dimers have liquid crystalline phases with lower melting points than related homoleptic copper (II) dimers. Both homoleptic and heteroleptic dimers are blue; however, an interesting orange intermediate is observed during the synthesis of the heteroleptic copper (II) dimers. Crystals grown from the orange intermediate were analyzed by X-ray diffraction revealing a copper (II) oxo cluster with four copper atoms surrounding a central oxygen with six chlorides bridging the edge of a copper tetrahedron. In the present work, we report that the sodium salts of long chain carboxylates (chain length varies from 4 to 12) replace the bridging chlorides of oxo centered copper (II) tetramer. The resulting blue products were characterized by IR, POM, DSC and Elemental Analysis. The isolated products exhibited birefringence above room temperature and are liquid crystals. The melting points and mesophase textures of these new products are distinct from the parent homoleptic copper (II) carboxylate dimers.

Presenter(s): Theo Jacobson, Macalester College
Session: Oral A.3 (10:30)
Title: Gravitational leptogenesis in Chern-Simons modified gravity
Advisor(s): Tonnis ter Veldhuis, Physics and Astronomy, Macalester College
Co-Author(s):

Abstract: We investigate a leptogenesis mechanism that relies on the gravitational anomaly in the lepton number current. In this model, the inflaton is an axion, a real pseudoscalar field that couples to a gravitational Chern-Simons term. The slow-roll of the axion drives inflation, and the CP-violation results in helicity-asymmetric gravitational waves, a sign of inflationary birefringence. The gravitational anomaly is dominated by sub-horizon quantum modes, and the net lepton number density is computed from the vacuum expectation value of the Chern-Simons invariant. We find that the resulting lepton number is very sensitive to the UV cut-off scale of the effective theory. The parameter space of the model is large enough to explain the observed matter asymmetry.

Presenter(s): Jacob Jansen, Hope College
Session: Poster P.06
Title: Heterocycle-directed decarbonylation of diaryl ketones
Advisor(s): Jeffrey B. Johnson, Chemistry, Hope College
Co-Author(s): Katherine Reed, Cole Wagner

Abstract: A mechanistic study of carbon monoxide extrusion from aryl ketones has been performed. The reaction uses a nitrogen-containing directing group to selectively cleave a carbon-carbon bond adjacent to an aryl ketone. A rhodium catalyst then removes the carbonyl and gives a coupled, diaryl product. It has been found that varying the directing group allows for probing of the relative rates of the mechanistic steps and varying the substituents on the aryl ring gives insight into the likely intermediates formed.

Presenter(s): Diamond Jelani, Knox College
Session: Poster P3.08
Title: Toward using Ar-BIAN Copper Precatalysts for the Hydrosilylation of Styrene
Advisor(s): Helen M Hoyt, Chemistry, Knox College
Co-Author(s):

Abstract: Copper (II) halide precatalysts bearing ArBIAN ligands (BIAN = bis(imino)acenaphthene; Ar = dpp or mes; dpp = diisopropylphenyl and mes = 2,4,6-trimethylphenyl) were prepared following published procedures and were preliminarily evaluated for the copper-catalyzed hydrosilylation of styrene with phenylsilane. After activation of $dppBIANCuCl_2$ with sodium triethylborohydride, copper-catalyzed hydrosilylation of styrene with phenylsilane initially produced a product in low yield (7%). An ongoing focus of this project is to improve product yield by optimization of reaction conditions, including catalyst activation methods, along with evaluation of variations in precatalyst structure.

Presenter(s): Scott Joffre, Hope College
Session: Poster P2.07
Title: Comparing Electrochemical Calculations and Particle Induced X-Ray Emission Measurements of Prussian Blue Analogue Deposits
Advisor(s): Jennifer Hampton, Physics, Hope College
Co-Author(s): Jennifer Hampton

Abstract: Prussian Blue Analogues (PBAs) have become a popular area of study due to their low cost and ability to store charge. Producing Nickel Hexacyanoferrate (a PBA) can be time consuming and expensive. In order to reduce time and streamline the production, one can use electrochemistry to plate a PBA film onto a metallic surface. Although this provides a more efficient and faster method for production, one major disadvantage is that the amount of PBA formed by this process is not precisely known. The purpose of this research is to develop a method to compare this electrochemical process of creation with other methods which allow one to know the amount of PBA formed.
The Nickel Hexacyanoferrate (a PBA) was analyzed with Particle Induced X-ray Emission (PIXE) to determine the amount of Fe and Ni deposited. These values were then compared to the amounts determined during electrochemical production. Early measurements of the amount of PBA show that the electrochemical calculations always report a greater value than the PIXE values measured. One explanation for this discrepancy is possibly unaccounted side reactions adding to the electrochemical measurement.

Presenter(s): Michael Jones, Carthage College
Session: Poster P1.09
Title: Micelle-Catalyzed Metathesis Reactions in Flow
Advisor(s): David Brownholland, Chemistry, Carthage College
Co-Author(s):

Abstract: Water is in many ways the ideal “green” solvent – it is non-toxic, abundant, and renewable. Unfortunately, the water insolubility of organic compounds limits its ability to facilitate organic reactions. Recent work on using aqueous micellar solutions have helped remove the insolubility challenge. Non-polar organic compounds are entropically driven into the interior of the micelle and react. Flow chemistry has generated increased interest for organic synthesis, especially in the pharmaceutical industry. Compared to traditional batch chemistry, reactions conducted in flow occur faster, have greater temperature homogeneity, enable rapid changes to conditions for rapid condition screening, and allow for safe high-pressure conditions. We report the results of micelle-catalyzed metathesis reactions, in-flow. We successfully completed a ring-closing metathesis reaction under these conditions of diethyl diallylmalonate in yields compatible to those obtained in batch conditions of either dichloromethane or through micelle-catalyzed reactions. The progress of micelle-catalyzed cross-metathesis reactions, in-flow, is also reported.

Presenter(s): Rebecca Katz, Knox College
Session: Oral G.3 (3:00)
Title: Axial Adducts to Copper Dimers
Advisor(s): Thomas Clayton, Chemistry, Knox College
Co-Author(s):

Abstract: This research involves following up on an interesting observation on the effects of adding caprolactam in differing stoichiometric ratios to copper II dimers. It has been demonstrated that at a 2:1 ratio caprolactam binds to either side of the molecule and then interacts by hydrogen bonding to create columnar structures. However, adding caprolactam in smaller ratios decreases the order of the structure and promotes the formation of a mesophase at lower temperatures. Comparing a ratio of 2 to 0.5 caprolactam has shown an increase in the temperature of the clearing point, when the mesophase becomes isotropic.

Presenter(s): Dalir Kellett, Samuel Gleason, Macalester College
Session: Poster P2.08
Title: Rotational Structure of Electronic States of TaH in the Visible Region
Advisor(s): Thomas Varberg, Chemistry, Macalester College
Co-Author(s): Samuel Gleason, Thomas Varberg

Abstract: The interest in studying the bond between tantalum and hydrogen and deuterium stems from the use of tantalum as a catalyst. This research was done with the intention of providing more insight into the fundamental properties of tantalum and the bonds it forms. There has also been computational and theoretical work done on the TaH molecule and another goal was to compare experimental results with the predicted works of theoretical chemists.

The focus of this research was to record Doppler limited spectra of both TaH and TaD molecules, as well as study the rotational structure of various electronic states. Doppler limited spectra for these molecules were recorded in the visible region by a continuous-wave ring dye laser. Through a least squares fitting routine the rotational constants, the centrifugal distortion constants, and the term energies (the electronic energy) of seven electronic states for TaH were determined. Furthermore, using the rotational constants the bond lengths for each of these electronic states were also determined.

Presenter(s): Daniel King, St. Olaf College
Session: Poster P3.09
Title: Synthesis of New Glyoxime-Based Electrocatalysts for Small-Molecule Activation
Advisor(s): James D. Blakemore, Department of Chemistry, Kansas University
Co-Author(s): Amit Kumar, Victor W. Day, and James D. Blakemore

Abstract: Combustion of fuels liberates CO_2 and H_2O. The thermodynamic stability and kinetic inertness of these molecules makes their conversion into useful chemicals quite challenging. However, the ability to convert these molecules to useful materials and fuels would be advantageous to modern day society both because they are quite abundant on earth, and because CO_2 is a known pollutant. Under proper electrochemical conditions, water can be oxidized to O_2, protons, and electrons, and CO_2 can be converted to CO using the liberated protons and electrons. CO is a feedstock for many chemical processes, and is thus an attractive target molecule for generation from CO_2. Here, we will discuss the synthesis and characterization of monometallic and bimetallic compounds that could potentially serve as catalysts for CO_2 reduction, proton reduction, or water oxidation. The compounds are supported in part by the ligand dimethylglyoxime and its derivatives, as these are cheap and can support a variety of redox-active metal complexes. The latest results will be discussed, including solid-state structural data obtained from X-ray diffraction studies on novel heterobimetallic complexes.

Presenter(s): Alexander Knapp, Beloit College
Session: Poster P1.10
Title: Superhydrophobic coatings on galvanized steel
Advisor(s): George Lisensky, Chemistry, Beloit college
Co-Author(s): Kaung Shein

Abstract: Galvanized steel is a commonly used material such as car parts, light weight truss components, and pipes. Superhydrophobic coatings hold many promising applications from self-cleaning surfaces to anti-corrosion. There are numerous approaches to producing a superhydrophobic coating, having varying degrees of economic viability. Many of these coatings can be applied to galvanized steel. Finding a cheap means of producing a superhydrophobic coating on galvanized steel opens the door for the application of superhydrophobicity to a wide range areas

Presenter(s): Shane Kosieradzki, St. Olaf College
Session: Oral D.2 (10:15)
Title: Invariantization of Finite Difference Approximations on Differential Equations
Advisor(s): Joseph Benson, Math, Macalester
Co-Author(s): Spencer Eanes

Abstract: To increase accuracy of numerical solutions to differential equations, the equations' inherent geometric properties, called Lie symmetries, can be exploited. These symmetries encompass a change of variables that preserves solutions. They are an integral part of the equations that exhibit them, but are not considered by traditional finite difference approximations. We can parameterize these symmetries based on a set of normalization equations, the result of which is known as moving frame. Using this moving frame allows the finite difference scheme to inherit the differential equations' symmetries, thus constructing a corresponding invariant scheme. We will show that invariantization increases accuracy of multistep schemes on ordinary differential equations, as well as the Crank-Nicolson method applied to Burgers equation.

Presenter(s): Samuel Kottler, Malcolm Gabbard, Colorado College
Session: Oral D.3 (10:30)
Title: A Study of Metrics on Visual Boundaries
Advisor(s): Molly Moran, Mathematics and Computer Science, Colorado College
Co-Author(s): Malcolm Gabbard

Abstract: Certain metrics on the boundary of CAT(0) spaces have been well studied. However, these metrics are not easily extendable to the interior of the CAT(0) space. We propose a new family of metrics on the boundary of CAT(0) spaces which can be extended to metrics on the interior of the space. We explore whether changing the parameters for these metrics is a quasi-symmetric transformation. The advantage of this family of metrics is that it depends on the entire geodesic ray so it captures more of the geometry of the space. This will hopefully help with problems such as generalizing which boundaries of CAT(0) spaces have finite linearly controlled dimension.

Presenter(s): Matthew Koviekis, Carthage College
Session: Poster P2.09
Title: Formation and Strengthening of Silica Nanoparticle Crystals
Advisor(s): John Kirk, Chemistry, Carthage College
Co-Author(s): Alissa Fischer

Abstract: The use of crystals made from silica nanoparticles can be used as a stationary phase for chemical separations. Silica colloidal crystals are loosely held together and unless treated properly with high temperature sintering, they will disperse when exposed to aqueous solutions. The goal of this work is to form these crystals and increase their strength without the use of high temperatures. The silica nanoparticles were deposited via vertical evaporative deposition from an ethanol solution. One of the problems encountered was the formation of a well-ordered crystal. The issues included horizontal drying lines as well as vertical cracks in the crystals. To mitigate these problems, a miniature deposition table was fabricated from aluminum. Following the formation of the colloidal crystals, various treatments were applied to achieve higher strength.

Presenter(s): Bob Kuo, Colorado College
Session: Oral D.4 (10:45)
Title: On Factor Pair Latin Squares
Advisor(s): James Hammer, Math, Cedar Crest College
Co-Author(s): Leah Miller, Jordan Lenchitz, Boyang Su, Makkah Davis

Abstract: Latin Squares have been of interest to mathematicians for a while. One variation of Latin squares is the popular game of Sudoku, which we can be generalized to the concept of a factor pair Latin square. That is, we will label a n by n square array with n characters. Then, we call this square a factor pair Latin square if for any a and b such that n = ab, each a by b sub-array, tiled starting from the top left corner of the square, contains all n characters. This project is mainly concerned with when factor pair Latin squares cannot exist. In particular, we provide two different sets of conditions such that a factor pair Latin square of order n cannot exists if n fulfills either of the conditions.

Presenter(s): Khia Kurtenbach, University of Chicago
Session: Poster P1.11
Title: An Investigation on Biaxial and Uniaxial Strain-Induced Effects in Smectic and Nematic Liquid Crystals
Advisor(s): Juan De Pablo, Molecular Engineering, University of Chicago
Co-Author(s): Monirosadat Sadati

Abstract: In the DePablo lab, we study the behavior of liquid crystals (LC). LC displays Bragg's refraction, reflecting light in the visible range; thus, topological defects and LC ordering can be studied using a polarized microscope. Our recent work explores the effect of mechanical strain on LCs droplets. We induced geometric confinement by dispersing LCs in a polymer (Polydimethylsiloxane (PDMS)) film. In the PDMS film, LCs adopt homeotropic anchoring, meaning the rod-like LC molecules line up perpendicular to the substrate with a point defect at the droplet center. Upon uniaxial stretching, nematic LC retains radial configuration and defect position remains fixed. However, uniaxial strain on smectic LCs results in a change from a point topological defect to a line defect. Reordering can be attributed to misorientation and dilation of smectic layers in the LC droplet. When nematic LC droplets undergo biaxial stretching, the strain-induced topological defect competes with the homeotropic anchoring to result in a configurational director twist. At a critical strain level, dependent on draw ratio and droplet size, the LC molecules in the twisted oblate align normal to their respective stretch axis. For smectic LCs undergoing biaxial strain, the layers transition from radial alignment to parallel alignment.

Presenter(s): Elise Le Boulicaut, Gustavus Adolphus College
Session: Oral F.2 (2:48)
Title: Performance studies of the Transition Radiation Tracker at the Large Hadron Collider ATLAS experiment
Advisor(s): Mark Kruse, Physics, Duke University
Co-Author(s): Mark Kruse, Andrea Bocci

Abstract: The Large Hadron Collider, which straddles the border of France and Switzerland, is the largest particle accelerator in the world. With its high energy proton-proton collisions, it provides researchers with the opportunity to learn more about fundamental particles and forces. The ATLAS experiment is one of the detectors used for this purpose. The part of the ATLAS detector on which this research is focused, the Transition Radiation Tracker, provides tracking and particle identification information. Data monitoring during and immediately after a run is essential in order to avoid losses of possible physics results due to detector malfunctions. Our work consists in assisting monitoring by summarizing raw data plots to create a visual and intuitive representation of the performance of the detector. This procedure makes locating and identifying potential defects easier and generally agrees with existing monitoring systems.

Presenter(s): Allyson Leicht, Grinnell College
Session: Poster P3.10
Title: Exploration of Mechanisms of Hydrogen Deuterium Exchange (HDX) of Arginine containing Peptides
Advisor(s): Elaine Marzluff, Chemistry, Grinnell College
Co-Author(s):

Abstract: The mechanism of gas-phase hydrogen/deuterium exchange (HDX), where labile covalently bonded hydrogen are replaced by deuterium, is investigated for three arginine containing peptides; Bradykinin (RPPGFSPFR), RKRARKE (RA), and RKRSRAE (RS) has been previously studied. Bradykinin is an excellent reference due to the fact that it has been extensively studied, HDX data was gathered for $[RA+H]^+$ and $[RS+H]^+$ and compared to previous $[BK+H]^+$ data. [RA] rapidly exchanged nearly all labile protons and [RS] demonstrated slow exchange of few of its labile protons. [RA] and [RS] were simulated using Molecular modeling software with focus placed on the singly protonated $[M+H]^+$ ions. Macromodel was used to generate the lowest energy conformations of each species. Structures were grouped into families based on similarities in conformation and optimized in Gaussian09 to the DFT (BYL3P 6-311G) level. Both Charge Solvated (CS) and zwitterionic structures were modeled and energies were compared to determine the most energetically favorable conformations. Computational results of $[RA+H]^+$ demonstrated zwitterion formation while $[RS+H]^+$ showed minimal zwitterion formation due to localization of the charges on the guanidinium groups in the absence of water. The computational results allow reasoning behind the different exchange behavior between [RA] and [RS].

Presenter(s): Alessandra Leong, University of Chicago
Session: Oral E.1 (2:30)
Title: Probing the Binding of α-Synuclein to Lipid Membranes as a Function of Composition and Curvature
Advisor(s): Ka Yee Lee, Department of Chemistry, University of Chicago
Co-Author(s):

Abstract: α-Synuclein (α-Syn) has been implicated in many neurodegenerative disorders, most notably Parkinson's Disease. Despite the abundance of α-Syn present within the presynaptic terminal and its localization around synaptic vesicles, a great deal remains unknown about its physiological and pathological function. Here, we created a robust model system to accurately probe the binding of α-Syn to lipid membranes as a function of physiological compositions and curvatures. We developed a technique to construct monodisperse spherical-nanoparticle supported lipid bilayers (SSLBs) that act as biologically relevant mimics of the highly curved synaptic vesicles. Confirmed by cryo-electron microscopy, our novel technique for SSLB formation via osmotic stress allows for precise and rigorous experimental control. Using isothermal titration calorimetry, we extrapolate thermodynamic parameters to investigate the binding affinity of α-Syn as a function of electrostatics and membrane surface defects modulated by lipid composition and SSLB curvature, respectively. We find significantly stronger binding affinities ($K_d < 1$ μM) to SSLBs with higher anionic lipid content and increased curvatures, suggesting that α-Syn is a curvature probing protein. By understanding the precise parameters that control α-Syn binding to biological membranes, we hope to deduce the physiological function of α-Syn and its transition to the diseased states.

Presenter(s): Caroline Loe, St. Olaf College
Session: Poster P1.12
Title: The use of structured imaging for the instantaneous measurement of temperature using two-line thermometry
Advisor(s): Rodrigo Sánchez González, Chemistry, St. Olaf College
Co-Author(s):

Abstract: In order to develop safe and reliable high-speed flight, it is important to understand flow behavior under a wide range of conditions. Using Laser Induced Fluorescence (LIF) methods, it is possible to determine velocities and scalar quantities such as flow composition, pressure, and temperature under conditions relevant to high speed wind tunnel testing. Nitric oxide two-line thermometry is a LIF-based technique where two rotational states of NO are sequentially excited by ultraviolet lasers and the resulting fluorescence intensity ratios are used to derive temperature, assuming a Boltzmann distribution. Analysis of images of fluorescence intensity distributions can provide spatially resolved temperature measurements of the flow field under investigation. In order to do so, it is necessary to determine the individual intensities of two LIF images separated in time, which could be problematic in high-speed flow applications. This work proposes the use of Structured Illumination (SI) imaging for the instantaneous measurement of the two fluorescence signals. One of the signals is modulated and then separated from the second signal in the same image using spatial frequency analysis. An image analysis MATLAB code was developed for quantitative instantaneous temperature determination from the simultaneously acquired fluorescence signals.

Presenter(s): Sophie Macfarland, Morgan Reik, University of Chicago
Session: Poster P3.11
Title: The Effects of Thiol Concentration on the Young’s Modulus of Self-Assembled Nanoparticle Films
Advisor(s): Binhua Lin and Stuart Rice, Physics and Chemistry, University of Chicago
Co-Author(s): Morgan Reik

Abstract: Previous experimental studies have shown that dodecanethiol-ligated gold nanoparticles self-assemble into mechanically resilient Langmuir films on an air-water interface. The mechanical properties of these films have been previously reported through experiments involving uniaxial compression of the films. Such experiments demonstrate that the nature of the ligand-ligand and ligand-core interactions of neighboring particles results in increased 2-dimensional compressive and shear moduli of the films with decreased ligand concentrations. However, the nature of systematic variations such as these has not been well-documented for dried films entirely removed from an air-water interface, despite the fact that the optical and electronic properties of these films are relevant for

several categories of electronic devices, for which they would need to be removed from the air-water interface. Therefore, our study strives to examine dried films consisting of dodecanethiol-coated gold nanoparticles, and their mechanical responses to variations in the concentration of dodecanethiol ligands on the surface of the gold spheres. We document variations in the Young's moduli of such films through contact-mode Atomic Force Microscopy (AFM), and demonstrate that lowering the thiol concentration on the surface of the particles increases the Young's moduli of the dried films.

Presenter(s): Nora Madrigal, Grinnell College
Session: Poster P2.10
Title: Detection of triazine herbicides through SPE/LC/MS and ELISA analysis
Advisor(s): Andrew Graham, Elaine Marzluff, Chemistry, Grinnell College
Co-Author(s):

Abstract: Methods of detection for atrazine, a common herbicide and known environmental contaminant, are essential in order to assess the level of concern for ecosystems affected by both atrazine and its degradation products. Solid phase extraction/liquid chromatography/mass spectrometry (SPE/LC/MS) and enzyme-linked immunosorbent assay (ELISA) analysis methods were adapted and optimized to detect atrazine, propazine, simazine, and four degradation products (desethylatrazine, desisopropylatrazine, desetheyl desisopropyl atrazine, and hydroxyatrazine). ELISA detected atrazine concentrations as low as 0.02 ppb, but did not detect degradation products or distinguish among compounds. Compounds were clearly identifiable through LC/MS. The LC/MS detection limit for each of these compounds is about 1.0 ppb; the incorporation of SPE into the LC/MS method resulted in method detection limits as low as 0.005 ppb. Water samples from six locations near the Conard Environmental Research Area in Kellogg, IA were also analyzed with both techniques and found to contain atrazine concentrations from 0.012 ppb to 3.5 ppb and total triazine loads from 0.22 ppb to 5.4 ppb. Good agreement ($R^2 = 0.90609$) was found between the atrazine concentrations determined by ELISA and SPE/LC/MS.

Presenter(s): Gabe McAndrews, Raymond Wieser, St. Olaf College
Session: Poster P3.25
Title: Frictional properties of molybdenum disulfide: a combined indenter probe and quartz crystal microbalance investigation
Advisor(s): Brian Borovsky, Physics, St. Olaf College
Co-Author(s): Brian Borovsky and Raymond Wieser

Abstract: Tribological experiments investigate friction in all size regimes, yet no model links the properties of the atomic and macroscopic length scales. Our experimental technique spans microscopic to macroscopic loads at realistic contact speeds with contact radii from 100 nm to 1 µm. Combining a quartz crystal microbalance with an indenter probe equipped with a 1 mm sapphire tip allowed us to quantify the frictional characteristics by monitoring the crystal's frequency and bandwidth perturbations. We create a procedure to reliably mount substrates, in our case molybdenum disulfide, to the quartz crystal without compromising its quality factor. Using our instrumentation, we can directly measure the static friction and contact area, from which we can calculate the pressure and shear strength. From our analysis, we found a cusp point in the load range of 100 µN to 200 µN. We believe that this corresponds to a shift in the physics of the contact interaction. The data indicates that friction scales with the familiar model $f = \tau A$. Furthermore, we observed that at high loads, shear modulus is independent of pressure. Our experimental setup allows for expansion into other two-dimensional substrates such as graphene, mica, and other transition metal dichalcogenides.

Presenter(s): Matthew Mehrkens, Gustavus Adolphus College
Session: Poster P1.13
Title: Ultrasonic Imaging Using Refracto-Vibrometry
Advisor(s): Thomas M. Huber, Physics, Gustavus Adolphus College
Co-Author(s): Benjamin Rorem, Thomas M. Huber

Abstract: Refracto-Vibrometry was used to make full-field videos of Ultrasound waves and their interactions with different objects in a tank of water. A PSV-400 Laser Doppler Vibrometer superimposed tens of thousands of vibrometric data points which allowed for the visualization of the ultrasonic pressure waves in the tank. A human calcaneus was imaged with the intention of improving osteoporosis diagnosis techniques by measuring bone strength directly with speed of sound measurements. Next, a block of phantom bone material was imaged to test dependencies on an easily controlled and uniform target. Finally, an acrylic block was imaged for the purpose of educational video creation, as well as demonstrating phenomena, such as Snell's law with sound, as opposed to light.

Presenter(s): Leah Mellett, Beloit College
Session: Poster P3.12
Title: Synthesis of AAC(6')-Ib Inhibitors to Combat Bacterial Resistance to Aminoglycosides
Advisor(s): Kristen Jansen Labby, Chemistry, Beloit College
Co-Author(s): Kristen Jansen Labby

Abstract: Antibiotic resistance occurs when bacteria adapt to withstand the effects of antibiotics due to overexposure, and over 2 million individuals are infected with antibiotic resistant bacteria each year. Aminoglycosides (AGs) are a class of antibiotic used to treat infections caused by gram-negative bacteria. AGs fight bacterial infections by binding to the A-site of ribosomes, which disrupts protein synthesis and eventually leads to cell death. Bacteria have adapted to combat AGs by modifying the chemical structure of the antibiotic using aminoglycoside modifying enzymes (AMEs). This modification prevents the antibiotic from binding to bacterial ribosomes, allowing the bacteria to proliferate. AAC(6')-Ib is one of the most clinically relevant type of AME, and it modifies the chemical structure by adding an acetyl group at the 6' position of AGs. Our goal is to synthesize a potential small molecule inhibitor of AAC(6')-Ib, named KJL-5. We have developed and optimized the synthetic route for KJL-5, which involves the synthesis and combination of two small molecule fragments. Developing this synthetic route will lead to synthesis of other analogues. Once tested and found to be successful, and AAC(6')-Ib inhibitor would be taken alongside current AGs, and would modify and prevent AAC(6')-Ib from altering the structure of AGs.

Presenter(s): Andrew Molina, University of Chicago
Session: Oral E.2 (2:45)
Title: Molecular mechanism of CNS myelinogenesis: in vitro self-assembly of myelin membrane lipid and protein structures
Advisor(s): Ka Yee C. Lee, Chemistry, Biophysics, University of Chicago
Co-Author(s): Ka Yee C. Lee

Abstract: The long-established theory of central nervous system myelin formation has been put to question by recent in vivo evidence that suggests a new model involving (1) the preformation of myelin membrane tubules that are trafficked to the neuronal axon, where they (2) undergo a transition from tubular to lamellar form and thus form the final compacted myelin sheath. To investigate this mechanism, we designed in vitro experiments to probe the interactions of myelin lipids as they (1) self-assemble into tubules and (2) transition into lamellar form. Using fluid-cell AFM, TEM, and DLS,

we have investigated how self-assembled lipidic tubules can transition into the multilamellar structure characteristic of mature myelin and how this process is modulated by lipid composition and the presence of myelin basic protein. We have found evidence of a galactosylceramide (GalCer) concentration-dependent response in lipid morphology that drives a transition from stable tubules to nonspecific aggregates with decreasing GalCer concentration. Our results at high GalCer concentrations align with in silico results of coarse-grained simulations and the in vivo tubules observed in ovine embryonic oligodendrocytes, suggesting that these structures of major myelin lipids can be stable precursors for myelination.

Presenter(s): Lucas Myers, Lawrence University
Session: Oral F.1 (2:30)
Title: Method for tracking microtubules in gliding assays
Advisor(s): Douglas S. Martin, Physics, Lawrence University
Co-Author(s):

Abstract: Many biological processes which develop over the scale of millimeters can only be understood by resolving details at the nanometer scale. An example of such a process is the transport of proteins through axons via cargo carrying motors. Observing individual steps along the journey of cargo is critical to understanding the details of transport. However, fluorescence microscopy, which can achieve nanometer resolution, is limited to the range of a few micrometers. Here, we present a novel method for extending the range of this technique by tracking fluorescently labeled objects in real time. Currently, the method is being developed specifically for microtubules in gliding assays to achieve a higher precision measurement of bending stiffness. It is expected that this method can be extended to other, similar systems.

Presenter(s): Parveen Narula, Beloit College
Session: Poster P2.11
Title: Clumps in Saturn’s F ring
Advisor(s): Britt Scharringhausen , Physics , Beloit college
Co-Author(s):

Abstract: This summer I did research under my mentor, Britt Scharringhausen, on clumps (dust clouds) in Saturn’s F ring. We used a data set of about 24 hours and 519 images taken by the Cassini spacecraft in 2005, while a ring plane crossing in Cassini’s perspective was occurring (usually can’t see the F ring but during a ring plane crossing it is very visible). My research was mostly statistical using a computer program I made to measure things like vertical width of clumps. I also tracked 5 clumps in about 5 images to see how they moved.

Presenter(s): Lydia Narum, Sydney Grossman, St. Olaf College
Session: Poster P2.12
Title: Stable Maximal Subgroups of Automorphism Groups
Advisor(s): Jill Dietz, Mathematics, St. Olaf College
Co-Author(s): Sydney Grossman, Jill Dietz

Abstract: Factorizations of a group G into a product G=AB, where A and B are subgroups of G, have been greatly studied over the years. An interesting case to study is when A and B are complements of each other, meaning that A intersects B={e} and every element of g in G can be written uniquely as a product g-ab, where a is an element of A and b is an element of B. We focused specifically on factorizations of AutG, the group of automorphisms of G, in terms of certain stable subgroups, and found examples of complements.

If M is the set of all maximal normal subgroups of G, then AutG acts on M in a natural way. Note that the stabilizer of m in M can be denoted as Aut(G;m)={phi in AutG | phi(m)=m}. Using information about group actions, we showed that when G is a p-group for which M has a certain structure, then Aut(G;m) always has a complement in AutG. Moreover, we found specifically that the complement is a cyclic group generated by a p-cycle that transforms one maximal subgroup to another.

Presenter(s): Alec Nelson, Hope College
Session: Poster P3.13
Title: MeV Ion Beam Channeling in Strontium Titanate Crystals by Rutherford Backscattering (RBS)
Advisor(s): S. K. Remillard, Physics, Hope College
Co-Author(s):

Abstract: Rutherford Backscattering Spectrometry (RBS) is an analytical ion beam technique used to characterise materials by backscattered particle energy and counts. In this project, the target is single crystal strontium titanate ($SrTiO_3$), which forms a perovskite crystal structure. By orienting the crystal so that the 2.9 MeV He^+ ion beam at the Hope Ion Beam laboratory (HIBAL) is perpendicular to the crystal plane, the particle backscattering is suppressed by enhanced penetration of the beam into the crystal. Rotational equipment was used to move through a series of tilt and azimuthal angles to create a raster scan of the crystal based on the orientation of the lattice. At the center of the raster scan is the point of maximum suppression, where the beam penetrates the furthest. Around the center of the scan in a grid-like pattern, similar points of suppression are found, likely in accordance with the perovskite structure of $LaAlO_3$, but are not as extreme as the center.

Presenter(s): Kelly Neubauer, Gustavus Adolphus College
Session: Oral A.4 (10:45)
Title: Inverse magneto-caloric effect at the spin reorientation of Fe_2B alloys doped with Co
Advisor(s): Valentin Taufour, Physics, University of California - Davis
Co-Author(s): Peter Klavins, Jackson Badger, and Valentin Taufour

Abstract: The magnetocaloric effect is usually quantified by a negative variation of entropy when applying field at constant temperature. An inverse effect can also be observed near spin reorientations. We describe the solution growth method used for the synthesis of single crystals of Fe_2B alloys with Co substitutions. We can control the spin reorientation temperature using Co doping. The transition occurs in the range 300-0 K for substitutions in the range 11-13%. We report on an inverse magneto-caloric effect at this transition.

Presenter(s): Benjamin November, University of Chicago
Session: Poster P3.14
Title: Effect of co-catalysts and thermal deposition on efficiency of silicon photoelectrodes for water splitting
Advisor(s): Yong Yan, Chemical and Environmental Sciences, New Jersey Institute of Technology
Co-Author(s):

Abstract: Water splitting in photoelectrochemical cells is a commonly researched process for storage of solar energy as H_2, and increasing its efficiency is integral to making solar power a dominant source of clean energy. Co-catalysts are a primary method to improve the efficiency and stability of photoelectrodes via improving charge separation and delivery to the target species. We investigated two co-catalysts, Cobalt imine and Platinum nanoparticle catalyst, on p-doped Si photoanode with varying exposed surface areas. We also investigate the effect of a thermally deposited 50 nm layer of Ag on the back of the Si wafer to improve charge transfer to the counter electrode to complete the redox reaction. Results show the decreased overpotential required to achieve water splitting under dark and light conditions for the molecular Co compared to the Pt nanoparticles. The molecular Co catalyst also exhibited higher turnover number and turnover frequency, making it a stronger catalyst for water oxidation and increasing the efficiency of the overall cell. Photoelectrodes with deposited Ag layer showed higher current density under both light and dark conditions, indicating the stronger ohmic contact between the semiconductor and the copper wire increased conductivity and thus efficiency of the photoelectrode.

Presenter(s): Derrick Obiri-Yeboah, Hope College
Session: Poster P2.13
Title: Synthesis of an EDOT-substituted iron porphyrin for utilization as a redox mediator for glucose sensing
Advisor(s): Elizabeth Sanford, Chemistry, Hope College
Co-Author(s): Elizabeth Sanford, Kenneth Brown, Matthew Ammerman

Abstract: An ethylenedioxythiophene (EDOT)-substituted iron porphyrin was synthesized and electropolymerized to form a redox-active mediation film between glucose oxidase and an electrode for the fabrication of an electrochemical glucose biosensor. The EDOT-substituted iron porphyrin was prepared via a four-step sequence from hydroxymethyl EDOT. The hydroxymethyl EDOT was activated with tosyl chloride and then reacted in a Williamson ether synthesis with 4-hydroxybenzaldehyde. The EDOT-functionalized benzaldehyde was condensed with pyrrole to form the porphyrin. After metallation with iron, the EDOT-substituted iron porphyrin was polymerized electrochemically onto a glassy carbon electrode, functionalized with glucose oxidase, and used for the electrochemical sensing of glucose. The sensor gave a response to glucose at a 0.03 M concentration.

Presenter(s): E. V. Ohstrom, Washington University in St. Louis
Session: Poster P1.15
Title: Nucleosynthesis and Reaction Rates in Core-Collapse Supernovae
Advisor(s): W. Raphael Hix, Department of Physics and Astronomy, University of Tennessee, Knoxville
Co-Author(s): W. Raphael Hix, J. Austin Harris

Abstract: A core-collapse supernova (CCSN) occurs when the pressure of fusion processes within a massive star can no longer withstand gravity, and the star collapses to form a neutron star. In the ensuing blast, layers of nuclear species are emitted, streaming into the surrounding space.

Due to their complexity, the mechanisms of CCSN cannot be replicated in a lab, and so must be simulated. In this project, we used the CHIMERA program, which covers: spectral neutrino transport, to power the explosion (MGFLD-TRANS; Bruenn 1985); shock-capturing hydrodynamics, to follow the supersonic fluid flow (VH-I; Hawley et al 2012); thermonuclear kinetics, to evolve the isotopic concentrations (XNet with 14-species; Hix & Thielemann 1999). CHIMERA also features realistic equations of state, a limited approach to general relativity, and up-to-date neutrino interactions, making it a world class code to study supernova explosions.

Despite the fidelity in CHIMERA, supernova simulations are restricted by their runtime. In this project, we studied the impact of cutoff time on the evolution of a supernova simulation. To accomplish this goal, we compared two simulations with the same initial conditions, but different cutoff times. We developed a set of Python tools to plot and analyze the changing abundances of 150 key species over time. We determined which species were connected by studying which species fluctuated together, sorting them into 11 groups. Analyzing species by group simplifies the process and allows for greater extrapolation later. After grouping, we calculated the species with the largest percentage differences between the two files, and compared that list to the largest species overall. While cutoff time has little impact on abundant species such as helium-4 and nickel-56, an early cutoff forestalls the nucleosynthesis of rarer species that develop unexpectedly in later times and cooler temperatures. Consequently, cutoff times should be extended further than current models permit.

Presenter(s): Emma C. Olson, Grinnell College
Session: Poster P1.14
Title: Synthesis of water soluble rylene derivatives for sensor applications
Advisor(s): Cooper H. Battle, Chemistry, Grinnell College
Co-Author(s): Cooper H. Battle

Abstract: Rylene dyes have been shown to be ideal for fluorescent sensors due to their low native fluorescence and their stability in a variety of environments. However, their insolubility severely limits the scope of their function. In this study, we are synthesizing and characterizing various rylene dye derivatives that incorporate different electronegative atoms in an attempt to improve the solubility of the sensor while maintaining its effectiveness. The synthetic path we've chosen creates three stable products, each of which having unique functional groups for analysis. It begins by the 4-addition of a nitrophenol to naphthalic anhydride, followed by a reduction, and to finish an oxygen heterocycle is formed using a Pschorr reaction.

Presenter(s): Anthony Ortiz, Lawrence University
Session: Poster P1.16
Title: Synthesis and Trapping Studies of Thienonaphthalene Biradicals
Advisor(s): Stefan Debbert, Chemistry, Lawrence University
Co-Author(s):

Abstract: Heterocycles are widely used in medicinal chemistry, and thienonaphthalene biradicals in particular are under-utilized. We propose to form new heterocycles by cyclizing bis-propargyl sulfones to thienonaphthalene biradicals and trapping those biradicals with sulfur dioxide (SO_2). As SO_2 trapping should be reversible, these compounds may be able to deliver SO_2 in vivo. In preparing to synthesize this new compound, three starting materials have been synthesized: phenylpropargyl bromide, bis(3-phenyl-2-propargyl) sulfide, and bis-propargyl sulfoxide. The compounds were characterized via GCMS, IR, and NMR spectroscopy. The synthesis of these heterocycles via a SO_2 donor will open the door to further implementation of SO_2 in medicinal chemistry.

Presenter(s): Dona Pantova, Macalester College
Session: Poster P2.14
Title: UV Photoluminescence Measurements on GaN
Advisor(s): James Heyman, Physics and Astronomy, Macalester College
Co-Author(s): James Heyman

Abstract: We built a UV photoluminescence spectrometer to measure GaN materials produced by our industrial partner Lightwave Photonics. The system uses an inexpensive UV LED as an alternative to a UV laser source. We observe an emission peak at the GaN band edge, as well as defect related luminescence in the yellow.

Presenter(s): John Pavek, Gustavus Adolphus College
Session: Oral C.3 (10:30)
Title: Mercury and Methylmercury Dynamics in the Surface Water of the Saint Louis River Estuary
Advisor(s): Jeff Jeremiason, Chemistry, Gustavus Adolphus College
Co-Author(s):

Abstract: The objective of this project is to develop a clearer understanding of mercury and methylmercury (MeHg) dynamics in the Saint Louis River Estuary (SLRE). Exceedingly high levels of MeHg have been observed in predatory fish residing within the estuary. Fish both in the upper Saint Louis River and in Lake Superior, into which the SLRE flows, have MeHg concentrations much lower than those observed in the estuary. Water, sediment, and biota samples from different habitat zones within the estuary have been, and continue to be, collected, and are analyzed for total mercury (THg), MeHg, and numerous other geochemical parameters. The portion of the overall project that will be discussed is the surface water Hg and MeHg concentrations. The current hypothesis is that sheltered bays are an important source of MeHg to the estuary under low flow conditions, but under high flow conditions the dominant source of MeHg is mobilization from upstream riparian areas. This has been supported by the observation of significantly higher surface water MeHg levels in bays off of the main channel, relative to the main channel itself.

Presenter(s): Benjamin Pederson, Hope College
Session: Poster P2.15
Title: A Model of Reproductive Success for Neotropical Pioneer Plants
Advisor(s): Brian Yurk, H. Greg Murray, Mathematics and Biology (respectively), Hope College
Co-Author(s): Brian Yurk, H. Greg Murray

Abstract: The tropical rainforest is a complex and diverse ecosystem, possessing innumerable species of plants and animals. Treefall and branch breakage open gaps in the dense canopy allowing sunlight to reach the forest floor in places that were previously shaded. In these newly formed gaps, the seeds of pioneer plants that are present in the litter and soil are able to germinate.

For over 30 years, six species of pioneer plants have been studied in the Neotropical Cloud Forest in Monteverde, Costa Rica. These are measured along five 500m transects that are selected such that their topography and climate are representative of the entire forest. Building on an approach taken by Murray (1988), we created a model that estimates the total lifetime reproductive output of a single pioneer plant. To determine an estimate for the potential reproductive success of a single plant, we account for several factors contributing to the germination probability of its seeds and subsequent survival to reproductive size. Germination success is dependent upon gap age, gap size, and distance from the parent plant. Our present work extends the approach of Murray (1988) in several ways, including separately modeling seed populations within the litter layer and the soil, which exhibit different dynamics.

Presenter(s): Jonathan Pekarek, University of Chicago
Session: Oral C.4 (10:45)
Title: Feasibility of wood chip permeable reactive barriers for large scale in-stream denitrification
Advisor(s): Kenneth Foreman, Ecosystems Center, Marine Biological Laboratory
Co-Author(s): Kenneth Foreman

Abstract: Since the Industrial Era, humans have been loading nitrate into streams and groundwater, a practice that leads to problems like eutrophication and toxic algal blooms. Diverting water through wood chip beds that promote growth of denitrifying bacteria has seen increasing use as a way to reduce nitrate in water. These permeable reactive barriers have been used to remove nitrate from groundwater, but have scarcely been used in streams due to larger temperature variations and faster flow rate of stream water. The nitrate removal rate response of these barriers to temperature, residence times of water, and wood chip sizes were tested in microcosms fed with nitrate-spiked stream water. Nitrate removal rate correlated positively with temperature, wood chip size, and residence time, indicating that finding optimal conditions of these variables is important for efficient nitrate removal in these barriers. An equation was created that can predict nitrate removal rates based on these three independent variables. Optima for residence time and wood chip size were found, but modeled nitrate removal rate solely increased with temperature without reaching an optimum. These findings show that these barriers can be effective in summer stream conditions, and display how they can optimally be designed for these conditions.

Presenter(s): Hoang Anh Phan, Macalester College
Session: Poster P2.16
Title: Interactions of Copper (I) with Zinc-finger Domains of Transcription Factor Sp1
Advisor(s): Kathryn E. Splan, Chemistry, Macalester College
Co-Author(s):

Abstract: Copper is an essential trace element in the functioning of many metalloproteins and biological processes. Deficient or excess copper levels can lead to copper stress and disrupt copper homeostasis, which has been strongly associated with many diseases. Nevertheless, limited research has been done to fully decipher all possible copper toxicity pathways. A possible mechanism for copper toxicity, which has been investigated in the Splan lab, entails the displacement of Zn(II) in zinc fingers (ZF) by Cu(I). We focus on Specificity Protein 1 – Sp1, which is constituted of three different ZF domains: Sp1-f1, Sp1-f2, and Sp1-f3. We hope to characterize the metal-binding ability and protein-DNA interaction of Sp1 with all three ZF domains as well as of the individual ZF domains Sp1f1-f3. Techniques such as protein induction and purification (cation-exchange column & HPLC), UV-Vis spectroscopy, and electrophoretic mobility shift assay, have been utilized. We have successfully expressed in E.coli and purified protein Sp1 (619-712) via both strategies: one with the Glutathione-S-Transferase (GST) tag to Sp1 and the other with the non-tagged codon-optimized Sp1. Preliminary results indicate that Sp1 binds Zn(II) in a tetrahedral geometry, interacts with the promoter region of the hCtr1 gene, and that Sp1's individual ZF domains bind Cu(I).

Presenter(s): Mark Powers, Hope College
Session: Poster P1.17
Title: Graph pebbling algorithms and Lemke graph construction
Advisor(s): Charles Cusack, Computer Science, Hope College
Co-Author(s): Charles Cusack, Airat Bekmetjev, Aaron Green

Abstract: On a connected graph, a configuration places a nonnegative number of pebbles on each vertex. A move between adjacent vertices removes two pebbles from one and places one pebble on the other. A configuration is solvable if a sequence of pebbling moves can be made to place a pebble on any given vertex. The pebbling number of a graph is the minimum number of pebbles so that any configuration is solvable. A graph satisfies the two-pebbling property if any configuration of twice the pebbling number minus the number of vertices with pebbles allows for placing two pebbles on any vertex after applying pebbling moves. If a graph does not have the two-pebbling property, it is a Lemke graph. We present a new algorithm for determining if a configuration is solvable, as well algorithms to determine pebbling number and whether or not a graph has the two-pebbling property. Using these algorithms on all connected graphs through 9 vertices, we find many previously unknown Lemke graphs. Additionally, we have developed a new way to construct Lemke graphs that differs from previous known infinite families of Lemke graphs.

Presenter(s): Tatiana Proksch, Zachary Martin, Joshua Jackson, Luther College
Session: Oral F.3 (3:06)
Title: Charm meson production from bottomonium decays
Advisor(s): Todd Pedlar, Physics, Luther college
Co-Author(s):

Abstract: Centered in Tsukuba, Japan, the Belle experiment collected a great deal of data using the KEKB particle accelerator. With access to this data, a great many interesting studies of bottomonium, wherein a bottom quark is bound by the strong force to an anti-bottom quark, may be conducted. We have examined official continuum Monte Carlo samples at the Y(2S) energy level to characterize the production of various charm mesons, or D mesons, as a function of the particle's reduced momentum. Through additional analysis of Monte Carlo associated with the decay chain Y(2S)→γχbj(1P)→D+X, with X as any other particle, we have characterized the yield of these D mesons from the various decays of the χbj(1P) states as a function of the energy of the photon emitted by the Y(2S). These results will be used in future analyses as we carry out an identical analysis on the true data collected by the Belle detector in an effort to better understand the strong force.

Presenter(s): Nicolette Puskar, Lawrence University
Session: Oral C.5 (11:00)
Title: Tropospheric Ozone Production in Rural Wisconsin: An Air Quality Study on Adams Farm
Advisor(s): Deanna Donohoue, Chemistry, Augustana College - BA Chemistry, Rosenstiel School of Marine and Atmospheric Science - PhD Marine and Atmospheric Chemistry
Co-Author(s): Fry Intia, Deanna Donohoue

Abstract: Tropospheric ozone is an air pollutant that damages human health, vegetation, and is a core ingredient in photochemical smog. It is formed near industrial hubs in a chemical reaction cycle involving sunlight, nitrogen oxides (NOx), and volatile organic compounds (VOCs). Adams Farm, located in rural Wisconsin, has recently seen an increase in industrial activity due to the opening of a hydraulic fracture sand mining site and a granary construction site near the property. We deployed our mobile lab, ARTEMIS (Atmospheric Research Trailer for Environmental Monitoring and Interactive Science), for two months to collect data on the local air quality to see if we could detect a rise in tropospheric ozone concentrations on the farm. The instrumentation included a gas monitors for ozone and nitrogen oxides, an optical particle sizer, and a mobile weather station. Our data indicated no rise in both tropospheric ozone concentrations and NOx concentrations over the two-month period. We believe these results were likely due to the large amount of rainy weather, effectively washing NOx out of the atmosphere and eliminating a primary ingredient needed for the catalytic cycle. We concluded that the air quality on Adams Farm is currently not compromised by the nearby industrial activity.

Presenter(s): Emily Reasoner, Nathan Campbell, Luther College
Session: Poster P3.15
Title: Effects of ligand substitution on CdSe nanocrystal optical properties
Advisor(s): Molly Wilker, Chemistry, Luther College
Co-Author(s): Nathan Campbell

Abstract: The unique optical properties of semiconductor nanocrystals have prompted their use in a wide range of technological devices. With their growing popularity, it has become increasingly important to understand how the surface chemistry of nanocrystals can be altered to control the ways in which nanocrystals interact with their environment. In this study, the native ligands from as-synthesized CdSe nanocrystals were substituted for a series of shorter, thiol-based ligands with

different functional groups. We measured the optical properties of the nanocrystals as new ligands were introduced onto the nanocrystal surfaces. The extent of ligand exchange was monitored by time-resolved and steady-state photoluminescence spectroscopy and the stability of the nanocrystals was assessed using absorption spectroscopy. These data were used to gain insight into the ligand binding mechanisms and to understand how the nature of the binding mechanism is influenced by ligand functionality.

Presenter(s): Alexander Reiter, Jack Haggett, Carthage College
Session: Poster P1.18
Title: Synthesis of an Alkene-Terminating Steroidal Surfactant Designed for Micelle-Catalyzed Organic Synthesis
Advisor(s): David Brownholland, Chemistry, Carthage College
Co-Author(s): Jack Haggett

Abstract: Organic solvent accounts for approximately 80% of hazardous waste generated in the pharmaceutical industry. This reality underscores the necessity of finding alternatives to organic solvent as reaction media. Water is an excellent alternative, as it is abundant, non-toxic, and non-hazardous. Unfortunately, water is often unsuitable because many organic reactants and reagents are water-insoluble. Aqueous micellar solutions can help mitigate the insolubility challenges, as water-insoluble starting materials and reagents are entropically driven into the hydrophobic micelle interior, which can facilitate organic reactions. Micelles have not only been shown to catalyze organic reactions, but often do so more efficiently, with fewer side-products, and at ambient temperatures. We are designing and synthesizing novel surfactants that self-aggregate into micelles capable of reversibly immobilizing starting materials or catalysts within the micelle. We report success on the synthesis of an alkene-terminating steroidal-PEG surfactant synthesized from lithocholic acid with a 50% yield in 5 steps. This synthesis was accomplished through an oxidation-decarboxylation pathway followed by PEG headgroup installation through the Fischer esterification pathway. We also report the progress of a more efficient and green synthetic route from lithocholic acid in only 3 steps involving the addition of allyl alcohol to the carboxylic acid of lithocholic acid to introduce the alkene. This approach removes the need for the protecting group strategy and use of lead (IV) tetraacetate used in our original synthesis.

Presenter(s): Megan Roozeboom, Emily Fuller, Luther College
Session: Poster P2.17
Title: Using UV-vis spectrophotometry and fluorescence spectroscopy to analyze the binding relationship of Curcuminoids and HSA.
Advisor(s): Olga Michels, Chemistry, Luther College
Co-Author(s): Emily Starman

Abstract: Curcuminoids are a family of photosensitive organic molecules that have potential application in Photodynamic Drug Therapy (PDT). To determine each curcuminoid derivative’s efficacy as a drug in PDT, binding affinity for the carrier protein Human Serum Albumin (HSA) was explored through UV-vis spectrophotometry and steady-state fluorescence spectroscopy. This study suggests that there is an inverse relationship between the presence of hydroxyl groups in the curcuminoid derivative and binding affinity for HSA.

Presenter(s): Leah Sanford, Carthage College
Session: Poster P3.16
Title: Size-matched nanoparticles for the detection of small organic compounds
Advisor(s): John S. Kirk, Chemistry, Carthage College
Co-Author(s):

Abstract: The field of nanoscience is applicable to many different technologies. These include electronics, drug delivery, structural materials, and sensors. The research presented here is the development of a sensor based on nanoparticles that will detect small organic compounds such as pesticides, herbicides, and fungicides. Silica nanoparticles will be used as the main component of these sensors due to their ability to self-assemble into nanoporous crystals, thus effectively creating a filtration system. The sensing surface of the device consists of gold nanoparticles, which were chosen due to their optical properties and ease of surface modification. In order to create a uniform colloidal crystal with consistent pores, the nanoparticles must be similar in size. Nanoparticle syntheses, however, are very sensitive to reaction conditions, making it difficult to accurately size-match particles. The work presented here explores the different variables to control and achieve size matching between silicon dioxide and gold nanoparticles.

Presenter(s): Nivedina Sarma, University of Chicago
Session: Poster P1.19
Title: Silicon Nanowire Scaffold for Active Support of Cardiac Muscle
Advisor(s): Bozhi Tian, Chemistry, The University of Chicago
Co-Author(s): Kelliann Koehler, Tom Hayes, Ramya Parameswaran, Bozhi Tian

Abstract: The Center for Disease Control reports heart disease as the leading cause of death, with myocardial infarction being the most prominent form of coronary failure. Cardiac muscle cannot divide to replace injured cells, so current treatments cause scar tissue to develop over heart muscle. Scar tissue hinders contractile activity, and therefore impedes functioning. Advances in cardiac tissue engineering promise materials that support hearts' contractile activity, and scaffold materials prove to be more supportive than cardiac grafts However, many scaffolds are limited by insulating materials and passive materials, therefore failing to provide cohesive beating between cell patches. We introduce a silicon nanowire scaffold that can be photothermally or photoelectrically stimulated, and these semiconductor properties allow us to stimulate synchronized beating among heart cells. Our lab has tested the nanowires' ability to pace neonatal rat heart cells by placing the cardiomyocytes on silicon nanowires that have been coated with fibronectin. We show the cells are aligned on the scaffold by staining them with troponin, and we stain with connexin to confirm they are connected to each other through gap junctions. Our silicon nanowire scaffold provides new insight for treating effects of heart tissue damage, such as myocardial scarring and arrhythmia.

Presenter(s): Erik Schoonover, Rebecca Johnson, Hope College
Session: Poster P2.18
Title: Development of rhodium-catalyzed carbon-carbon single bond activation via in situ generated imine directing groups.
Advisor(s): Jeffrey B. Johnson, Chemistry, Hope College
Co-Author(s): Kimberly DeGlopper

Abstract: Carbon-carbon bonds are ubiquitous in nature, but few methods for functionalizing these bonds exist. Previous work in the Johnson lab has demonstrated that aryl ketone carbon-carbon bonds can be activated using rhodium catalysis. However, this method of activation requires quinolone directing groups which restricts the scope of accessible ketones. To expand the utility of this methodology, the use of removable imine directing groups was explored. Initial results indicate that an alkene can undergo addition across the carbon-carbon bond of an aryl ketone. Ketone functionality can then be restored upon hydrolysis of the imine product. The scope of ketone, amine, and alkene substrates is currently being explored.

Presenter(s): Jacob Schulz, Luther College
Session: Poster P2.19
Title: Non-invasive Characterization of Mixed Renal Kidney Stones using Dual Energy CT and Photon Counting CT
Advisor(s): Cynthia McCollough , CT Clinical Innovation Center, Mayo Clinic, University of Wisconsin, Madison
Co-Author(s): Andrea Ferrero, Cynthia McCollough

Abstract: Dual-energy (DE) CT uses the CT number ratios (CTR) of the CT numbers at high and low energies to identify in vivo the mineral composition of renal stones. This analysis provides almost 100% accuracy in discriminating uric acid (UA) from non-uric acid (non-UA) stones, but is limited for stones with mixed mineral composition. In this study, we investigated whether the CTR distribution and the ultra-high-resolution (UHR) mode of a photon-counting-detector (PCD) CT would improve the classification of small mixed stones.

Fourteen small renal stones of variable composition were scanned using DECT and UHR-PCD-CT. Each scan was performed at clinical dose levels. Image noise and sharpness were varied to identify the most accurate approach to classifying mixed stones using the CTR distribution. Mixed stones were identified by fitting double Gaussian curves to the CTR distribution. Previously reported CTR thresholds were applied to the DECT data to compare the performance of the proposed UHR-PCD-CT approach with the clinically-accepted DECT method.

Preliminary data showed that the proposed UHR-PCD-CT approach could correctly identify mixed UA and non-UA stones, provided that at least 25% of the stone consisted of the least prevalent component. Unlike the clinical DECT approach, all three pure stones were properly classified with the proposed method as not having a second component.

Presenter(s): Shuruthi Senthil, Macalester College
Session: Poster P3.17
Title: An Investigation of Distant Inductive Effects on Donation into Group VI Metals in Tris(diphenylphosphinomethyl)phenylborate Complexes
Advisor(s): Paul J. Fischer, Chemistry, Macalester College
Co-Author(s): Jeremy T. Stephan, McKinley L. Swift, Emily T. Chan, Matthew V. Vollmer, Victor G. Young, Jr. and Paul J. Fischer

Abstract: Tris(diphenylphosphinomethyl)phenylborate ligands have been dubbed as strongly donating scorpionates towards cationic metal fragments. To assess this donor capability towards lower valent metals, our research group synthesized and characterized salts of zerovalent group VI metal complexes of tris(diphenylphosphinomethyl)phenylborate ligands. IR spectroscopy and the oxidation potentials of the metal complexes suggest that tris(diphenylphosphinomethyl)phenylborate is significantly less donating than scorpionates towards zerovalent metals. However, the boron negative charge, via a through-space inductive effect, apparently plays a role in altering the donation capability of this ligand at phosphine-bound metal centers. The introduction of substituents on the bridgehead phenyl substituent offers a way of changing the electron density at the negatively charged boron. To this end, two new ligands with methyl and trifluoromethyl substituents on this phenyl group have been synthesized, fully characterized and coordinated to group VI metals. The IR spectral data and oxidation potentials that probe metal electronics seems to indicate that replacement of a trifluoromethyl substituent by a methyl substituent has a tangible impact at the phosphine-bound metal fragment, suggesting a new inductive strategy for tuning tris(diphenylphosphinomethyl)phenylborate donation.

Presenter(s): Kaung Shein, Beloit College
Session: Poster P1.20
Title: Simple superhydrophobic coating process on copper
Advisor(s): George Lisensky, Chemistry, Beloit College
Co-Author(s): Alexander Knapp

Abstract: Hydrophobic materials can be found in nature for its self-cleaning and drag-reducing abilities. Leaves self-clean by having water roll-off the surface, dragging dirt and other particles with it. Lotus leaves and rose petals, in particular, are well-known for its hydrophobicity. Inspired by this, the water-repelling feature can be applied to man-made materials. In this experiment, we coated Cu(OH)2 and CuO on a copper plate for an environmentally-friendly process of obtaining a superhydrophobic surface. Coated copper surfaces were examined using Scanning Electron Microscope and X-ray Powder Diffraction. The water contact angles were captured with a microscope, and analyzed using Low-bond Axisymmetric Drop Shape Analysis. The copper surfaces had contact angles up to 168 degrees under 5 minutes of lab procedure.

Presenter(s): Andrew Smith, University of Chicago
Session: Poster P2.20
Title: Grain Growth in Sintered Uranium Dioxide for Fuel Performance Code Validation
Advisor(s): Kun Mo, Nuclear Engineering Division, Argonne National Lab,
Co-Author(s): Kun Mo, Linyun Liang

Abstract: New and well-controlled grain growth data for Uranium Dioxide was collected for validation of the MARMOT mesoscale fuel performance code for in-reactor grain growth, developed at Idaho National Lab. Uranium Dioxide is typically used as a nuclear fuel in Light Water Reactors. The grain growth behavior of the material as a function of time of is an important parameter for code validation purpose. Depleted UO_2 fuel pellets, fabricated according to standard Light Water Reactor UO_2 fuel pellets processes, were used. The samples were sintered in a furnace at a pressure of approximately $5*10^{-6}$ Torr, and a temperature of 1900˚C. The average grain diameter was measured for each of these samples using a linear intercept method, and compared to an as-recieved (unsintered) sample. All grain size measurements were performed based on ASTM standard (E-112-13). Significant grain growth was observed, and the trends observed showed good qualitative agreement with data collected at the same temperature reported in the literature.

Presenter(s): Madison Stamos, University of Chicago
Session: Poster P3.18
Title: HCV Screening and Linkage-to-Care Best Practices
Advisor(s): Ellen Almirol, Department of Medicine, Section of Infectious Diseases, University of Chicago
Co-Author(s): Mai T. Pho, Ellen Almirol, David Pitrak

Abstract: Background: The prevalence of Hepatitis C (HCV) has increased in the US, however linkage to care (LTC) of infected patients remains challenging.

Methods: In January 2017, the University of Chicago medicine (UCM) adopted an intensive case management (ICM) model involving near real-time chart reviews of patients with positive HCV antibody and/or RNA tests and referral to HCV providers. Out-of-network ICM patients were referred to the Hepatitis C Community Alliance to Test and Treat (HepCCATT). We compared percent linkage of in- and out-of-network patients undergoing ICM to patients linked prior to the ICM model (non-ICM). Linkage was defined as attending an outpatient visit with an HCV provider. Chi-square tests were used to compare differences between groups.

Results: Between 2014-8/2017, 24,571 patients were screened for HCV. 1272 (5.2%) were antibody positive, and 739 (3.0%) had a confirmed infection. 248 (55.6%) of eligible patients were linked. The mean number of days between HCV test and LTC was 86.5±135.1 for in-network ICM, 172.5±217.8 for out-of-network ICM (HepCCATT), and 128.4±163.4 for non-ICM ($p<0.01$).

Conclusion: In-network ICM shortened the time between HCV test and LTC versus non-ICM patients. Identification and management of barriers faced by out-of-network patients must be addressed to improve linkage in this population.

Presenter(s): Lauren Stierman, Colorado College
Session: Oral D.5 (11:00)
Title: Harmonic mappings from generalizations of hypocycloids
Advisor(s): Jane McDougall, Mathematics, Northwestern University
Co-Author(s):

Abstract: A family of generalized hypocycloids called rosettes display unique mathematical properties. The rosette is a harmonic mapping with canonical decomposition identical to the simple polynomials that generate the harmonic hypocycloid, but with additional factors that are hypergeometric 2F1 series. While the hypocycloid is well-known in the mathematical realm, the rosette was only discovered in 2016. This project explores the intricacies of rosettes and their relationship with hypocycloids, through an analysis of the relationships between relevant formulae and the use of the computer algebra system Mathematica. The graphics of hypocycloids and rosettes that this system generates are of particular significance to this research endeavor. Important findings include the following properties of the rosette: its nested behavior, the mirror image property on the boundary of its mappings, the equal and opposite tangent vectors that produce this property, and the distinct shapes that are generated based on the relative angle rotation of the functions of the canonical decomposition.

Presenter(s): Shining Sun, University of Chicago
Session: Poster P2.21
Title: Hierarchical Equations of Motion Approach to the Mechanism of Tyrosine Oxidation in Photosynthesis
Advisor(s): Yoshitaka Tanimura, Chemistry, Kyoto University
Co-Author(s):

Abstract: Proton-Coupled Electron Transfer (PCET) is a common process that appears in many natural and artificial systems. Due to the strong influence of quantum coherence and system-bath interaction, it is hard to treat PCET processes using conventional Markovian and perturbative methods. Therefore, the Hierarchical Equations of Motions (HEOM) approach, which does not make Markovian or perturbative assumptions, will be used to solve for the time evolution of the PCET system. This project focuses on the PCET process of tyrosine-Z in photosynthesis. We model the PCET process as a four-level system coupled to a harmonic oscillator bath, which imitates the protein environment. The time evolution of the density matrix is then solved to understand the mechanism of the PCET process.

Presenter(s): Ian Sutherland, St. Olaf College
Session: Poster P3.19
Title: Boltzmann Analysis of Gadolinium II Spectra
Advisor(s): David Nitz, Physics, St. Olaf College
Co-Author(s):

Abstract: New atomic data, particularly transition probabilities, are needed for Rare-Earth elements to increase reliability of spectral modeling used for analysis of stars as well as advances in industrial lighting. In this project, four Gadolinium spectra from the digital archives of the National Solar Observatory in Kitt Peak, Arizona were analyzed to determine the excited state population distributions of the emission sources. The intensities of approximately 400 emission lines were determined by numerical integration using custom software and, in combination with published atomic transition probability data, fitted to a Boltzmann distribution. Of the four spectra, two show acceptable Boltzmann fits, another does not, and the fourth lacks adequate data points for a statistically meaningful answer. The fact that the population levels in the first two spectra were found to follow a Boltzmann distribution implies that these spectra can be used to measure new transition probabilities in a continuation of this project.

Presenter(s): Aileen Szczepanski, Carthage College
Session: Poster P3.20
Title: Organic Synthesis of O-acylated Amino Acid Surfactants to Examine Antibacterial Properties
Advisor(s): David Brownholland, Chemistry, Carthage College
Co-Author(s):

Abstract: Surfactants are surface-active materials with numerous applications, including: detergents and soaps, cosmetics, fabric softeners, pharmaceutical creams and ointments, and plasticizers. Amino acid-surfactants have generated interest as antibacterial agents, chiral resolution, chelating agents, and as switchable surfactants. These surfactants are of particular interest because they are largely biodegradable, due to a relatively labile ester or amide bond. We describe the synthesis of O-acylated amino acid surfactants with hydrophobic ω-alkenyl chains. Amino acids were acylated with ω-undecylenyl alcohol using a Fischer esterification reaction and purified using silica-gel chromatography as well as an amine-selective resin. Future work will include the evaluation of their antimicrobial activity by doing an agar disc diffusion assay using the Kirby-Bauer method, and a broth micro dilution susceptibility assay.

Presenter(s): Austin Szczodrowski, Carthage College
Session: Poster P1.21
Title: Synthesizing PSLA-mPEG-550 a designer surfactant for optimizing micellar catalysis through an immobilized Proline-derivative catalyst
Advisor(s): David Brownholland, Chemistry, Carthage College
Co-Author(s):

Abstract: In many ways, water is an ideal solvent: it is cheap, abundant, renewable, non-toxic, and non-flammable, making it an excellent alternative to the organic solvents used in organic synthesis. Unfortunately, the insolubility of most organic compounds in water limits its use as a solvent. Significant progress has been made in micellar catalysis, in which organic reactions take place in the hydrophobic medium in the interior of the micelle. We are designing a surfactant that will generate micelles containing immobilized catalysts capable of catalyzing stereoselective reactions within the interior of the micelle and are able to be immediately recycled without any purification of isolation.

Specifically, we report our progress on the six-step synthesis of PSLA-mPEG-550, a surfactant synthesized from Lithocholic acid with a proline-derivative linked to the A-ring of the steroid. We hypothesize that this new surfactant can be introduced into a solution of commercially available surfactants in a small mole percent to minimize waste and maximize efficiency. Future work will focus on the catalytic ability and recyclability of these micelles. The physical properties of the micelles will be characterized by dynamic light scattering (DLS), cryo-TEM, and pulse-field gradient (PFG) NMR.

Presenter(s): Peter Timperman, Hope College
Session: Poster P2.22
Title: PyScan: Interfacing Laboratory Instruments using Python
Advisor(s): William F. Polik, Chemistry, Hope College
Co-Author(s): William F. Polik

Abstract: Modern laboratory instruments can be interfaced with and controlled from a personal computer. Several programs to scan spectroscopic instruments and acquire data have been written by students in the Polik Lab. However, the existing software can only be run on Windows 98 and uses older ISA hardware. These programs must be replaced to run on modern operating systems and computers.

PyScan is a laser instrument interface program intended to replace the Polik Lab's current software. It allows the user to control the laser, setup a scan, acquire data, and store the data for subsequent analysis. PyScan is written purely in Python 2.7 and is designed with strict adherence to the Model-Controller-View pattern. The user interface is built using Tkinter, Python's default graphic user interface library. Pyscan also makes extensive use of PySerial and Measurement Computing data acquisition libraries.

Presenter(s): Judith Tong, Grinnell College
Session: Poster P3.21
Title: Analysis of organic pigments within art works using surface enhanced Raman spectroscopy
Advisor(s): Corasi Ortiz, Chemistry, Grinnell College
Co-Author(s):

Abstract: Surface Enhanced Raman Spectroscopy (SERS) is a scattering spectroscopy technique that is used to obtain Raman spectra of organic colorants that were commonly used historically. These organic colorants were some of the first to be discovered and used as art materials and dyes for textiles and cultural artifacts. Analyzing the use and the properties of these organic colorants provides art historians and curators with vital historical and conservational information about ancient art works and artifacts. The Raman spectra obtained from SERS can be used to identify unknown natural dye materials as well as give vibrational and structural information about the molecules. A library of SERS spectra of organic dyes is created as a potential resource in identifying unknown materials. Silver colloids are synthesized using the Lee-Meisel procedure as the metal substrate. The dye is analyzed in a solution of Silver colloids, Magnesium Nitrate or Potassium Sulfate as an activation agent, and the dye solution itself. The dyes are also tested on a Silver surface that is roughened with sandpaper, and another roughened electrochemically using the Weaver method. Using a rough silver surface eliminates the need for silver colloids, eliminating interfering signals from sodium citrate. Methods in extracting dyes from textiles are also developed, allowing the comparison between the spectra of the dyes on their own and spectra taken from dyes extracted from textiles.

Presenter(s): Victoria Vivtcharenko, Luther College
Session: Poster P1.22
Title: Dopamine Quantification in Caenorhabditis elegans with High-Performance Liquid Chromatography
Advisor(s): Molly Wilker, Chemistry, Luther College
Co-Author(s): Molly Wilker, Stephanie Fretham

Abstract: The loss of dopamine, a significant neurotransmitter, is a hallmark of neurodegenerative diseases such as Parkinson's disease, however the etiology is unclear. Evidence has shown that the insulin signaling pathway, a central regulator of metabolism and oxidative stress response, may be dysregulated in the disease state. In order to determine the influence of this pathway on dopamine, we quantified dopamine in wild type and insulin signaling mutant strains of the nematode model system Caenorhabditis elegans (C. elegans). Due to the molecular complexity of the cellular mixture, it is difficult to quantify dopamine in multicellular organisms. Standard absorption spectroscopy is not effective because many compounds in the cellular mixture absorb in the same wavelength range as dopamine. We have developed a protocol to quantify dopamine in C. elegans worms using High-Performance Liquid Chromatography (HPLC) with UV-vis detection. HPLC is an effective method because of its high sensitivity and selectivity, as well the possibility to detect several analytes at once. In this study, we correlated dopamine levels in C. elegans with activity of the insulin signaling pathway. Both the development of our HPLC protocol for dopamine detection and our results from analysis of C. elegans mutant strains will be presented.

Presenter(s): Anne Wampler, Washington University in St. Louis
Session: Poster P2.23
Title: Exploring the antimicrobial activity of beta-lactones to combat antibiotic resistance
Advisor(s): Timothy Wencewicz, Department of Chemistry, Washington University in St. Louis
Co-Author(s): Erin Gemmell

Abstract: Antibiotic resistance is one of the world's most urgent health crises. By their very nature, antibiotics tend to select for resistance in bacteria, killing off non-resistant strains in the process of fighting infection and leaving only resistant strains to reproduce, making each successive generation harder to treat. In the past, antibiotic drug development has focused on a few classes of antibiotics, directly combating bacterial resistance mechanisms by modifying the functional groups surrounding the drug's active core. However, diminishing returns in these alterations' efficacy have driven development to branch out into new classes of antibiotics that hit different targets within the bacteria, circumventing evolved resistance mechanisms. I am studying one such under-explored class: beta-lactones. Although a few beta-lactone lipase inhibitors have been approved for clinical use as anti-obesity drugs, the antibiotic activity of beta-lactones is not well characterized. In order to explore this property, we synthesized a library of simple beta-lactones to test their antimicrobial activity. I used the Mitsunobu cyclization on L-serine followed by an acylation to synthesize simple substituted beta-lactones. These compounds were assayed with E. coli and showed dose dependent activity. This suggests that beta-lactones, even in their simplest form, possess bacteriostatic antimicrobial activity.

Presenter(s): Jue Wang, Grinnell College
Session: Oral E.3 (3:00)
Title: Conformational analysis of MTHFR mutants with substrate binding utilizing hydrogen-deuterium exchange and mass spectrometry
Advisor(s): Elaine Marzluff, Chemistry, Grinnell College
Co-Author(s): Elizabeth Trimmer, Chemistry, Grinnell College

Abstract: MTHFR is a homotetramer, which is the only known enzyme to catalyze the folate reduction reaction in human bodies using FAD as a cofactor. This study uses Hydrogen-Deuterium Exchange and mass spectrometry (HDX-MS) to study if mutations along the MTHFR catalytic triad near the folate binding site cause conformational changes. We are specifically interested in two mutations at the 28th position: E28Q and E28D, when the glutamate (E) is replaced by similar amino acids glutamine (Q) or aspartate (D). Prior kinetic studies have shown both E28Q and E28D bind to the folate but do not carry out the reduction reaction. HDX-MS was used to determine the conformational changes upon folate binding to the free enzyme. The rate of HDX depends on the solvent accessibility where peptides embedded in the core or hydrogen bonded tightly gets less deuterium labels added. Differences in HDX between free and folate bound enzyme allow us to determine where the folate binding affects the local conformation. Among the 15 reference peptides identified in this project, residues near the MTHFR protein-protein binding surface, the FAD and folate binding site show the most changes HDX extent, which indicates the folate binding has an extensive effect on MTHFR conformation.

Presenter(s): Yuan Wang, Grinnell College
Session: Poster P1.23
Title: New ASTRAL-III: scalable distance-based species tree estimation method
Advisor(s): Siavash Mirarab, Electrical and Computer Engineering, University of California - San Diego
Co-Author(s): Siavash Mirarab

Abstract: Phylogenetic trees show how species have emerged from common ancestors through evolution. The reconstruction of phylogenetic trees is a computational task with complications, a common one of which is the gene tree and species tree incongruence caused by incomplete lineage sorting (ILS). We have improved a widely accepted software, ASTRAL-III, which is statistically consistent under multi-species coalescent (MSC), a model for ILS. While the core algorithm is dynamic programming that performs an optimization task, ASTRAL-III has a distance-based preprocessing step. We improved the preprocessing step of ASTRAL-III by incorporating the advanced distance techniques from USTAR and PhyD*/BIONJ*, and designed new algorithms that run on polytomies and missing data in gene trees. The improved software is the New ASTRAL-III. New ASTRAL-III first computes a distance matrix based on the topological distances between all pairs of vertices. It then uses that matrix to infer a tree. Comparing to the original ASTRAL-III, the New ASTRAL-III increases scalability and reduces runtime, while maintaining the original accuracy. Moreover, it implements a better normalization method. These advantages enable New ASTRAL-III to be a useful computational tool for a variety of phylogenetic studies in analyses of real biological datasets.

Presenter(s): Collin Wassilak, Hope College
Session: Poster P3.22
Title: Functionalization of electrode surfaces using iron-based redox mediating films for glucose detection
Advisor(s): Elizabeth M. Sanford, Chemistry, Hope College
Co-Author(s): Kenneth L. Brown, Elizabeth M. Sanford

Abstract: Organometallic redox mediators are integral to the construction and efficacy of biosensors because they facilitate electron movement between the biological and electrochemical transducers of the sensor leading to improved signal. Electropolymerization of a redox-active monomer can be used to form a polymer film to mediate charge transfer between glucose oxidase and an electrode. Two monomers were prepared to form redox mediation films; tris(5-amino-1,10-phenanthroline)iron(II) and a 3,4-ethylenedioxythiophene (EDOT)-substituted ferrocene. Preparation and characterization of these monomers were completed. The monomers were then electropolymerized to form films on electrodes and the electrochemical properties were characterized. After further functionalization with glucose oxidase, biosensors for glucose were prepared. Glucose sensitivity tests were carried out using cyclic voltammetry down to 1.0 mM glucose solutions. Both mediation layers successfully mediated charge transfer down to 1.0 mM glucose solutions, a concentration suitable for detecting glucose in blood.

Presenter(s): Benjamin Wollant, St. Olaf College
Session: Poster P2.24
Title: Characterization of SU-8 Spin Coating over High Aspect Ratio Substrate Topography
Advisor(s): David L. Dickensheets, Electrical and Computer Engineering, Montana State University
Co-Author(s): Tianbo Liu

Abstract: A parametric study of spin coating SU-8 over high aspect ratio trenches and vias is presented. The coating of trench and via features is investigated based on the experimental parameters of feature width, depth, radial location on the wafer, angular orientation, resist viscosity, and spin velocity. An optical microscope, profilometer, and scanning electron microscope are used to measure and examine coated features. The effects of parameters on feature bridging and non-planarity are investigated.

Presenter(s): Qifan Xiao, Macalester College
Session: Poster P1.24
Title: Toward Carboxylic Acid-Functionalized Naphthalene Diimides
Advisor(s): Dennis D.Cao, Chemistry, Macalester College
Co-Author(s):

Abstract: Core-functionalized naphthalene diimides (cNDIs) are promising candidates as organic redox materials that could be used in applications including OLEDs, photovoltaics, and other organic electronic devices.

A diverse variety of cNDIs exhibiting varying degrees of electron deficiency and intramolecular charge transfer features have been reported in the literature. However, functionalization of the NDI core with imide groups has not been explored to date. We hypothesize that the crowding of imide groups on the naphthalene core to form naphthalene tetraimides may lead to new chemical and physical properties. To synthesize the naphthalene tetraimide, we first targeted the synthesis of NDI tetracarboxylic acids using three strategies.

Presenter(s): Haoru Yang, Washington University in St. Louis
Session: Poster P2.25
Title: Synthetic Scheme of Graphite Oxide Using Hummers' Method
Advisor(s): Julio D'Arcy, chemistry, Washington University in St. Louis
Co-Author(s):

Abstract: Graphite oxide (GO) is an allotrope of carbon comprised of oxygen and hydrogen and it is produced by exposing graphite to strong oxidizing conditions resulting in the attachment of functional groups to the graphitic surface. This process expands the interlayer distance of graphite and makes GO easy to exfoliate into single layers, i.e., graphene oxide sheets. Although the exact structure of GO and the mechanism of its formation are still unclear, various approaches to oxidation have been reported. We chose the Hummers' synthetic method due to its safety and efficiency at oxidizing carbon; this protocol was modified to increase product yield. To determine the best path for synthesis, the product GO was characterized using atomic force microscopy (AFM) and Raman spectroscopy. Through optimization, we managed to exfoliate the product GO without reducing it due to prolonged exposure in heat. Finally, we generated a synthetic protocol to be referenced for future synthesis.

Presenter(s): Junze Yao, Grinnell College
Session: Poster P3.23
Title: Growth and analysis of single crystal TbCuAl alloy
Advisor(s): Charles E. Cunningham, Physics, Grinnell College
Co-Author(s):

Abstract: A series of Tb:Cu:Al ternary alloys were flux-grown as single crystals from a range of melt compositions. These materials were subjected to structural and magnetic analyses. Lower Tb:Cu ratios yielded orthorhombic $Tb_3CuxAl_{(11-x)}$ with $0.9 < x < 1.2$, while higher Tb:Cu ratios yielded tetragonal $TbCu_{(4+x)}Al_{(8-x)}$, with $0.5 < x < 0.9$. The antiferromagnetic ordering temperature is depressed with increasing x in the alloy with nominal 1:4:8 stoichiometry, but it appears independent of x in the alloy with nominal 1:11 stoichiometry.

Presenter(s): Lyujiangnan Ye, Hanbo Shao, Colorado College
Session: Poster P1.25
Title: On Computing Slice Genus of Non-alternating Prime Knots
Advisor(s): Kathryn Bryant, Department of Mathematics and Computer Science, Colorado College
Co-Author(s): Hanbo Shao

Abstract: Knot genus, in both the 3- and 4-dimensional settings, is a well-studied knot invariant. In this project, we calculate the smooth slice genus of the last remaining non-alternating prime knots of twelve or fewer crossings for which this invariant is previously unknown - 11 in all. We do this by performing band moves - additions and deletions - on a knot K to produce a torus cobordism in 4-ball with another knot J, and the slice genera of two knots are merely differed by one. Regarding different types of knots, we applied various methods to deduce the slice genus of K via analysis of J.

Presenter(s): Xiaoqi Yu, Gustavus Adolphus College
Session: Oral C.2 (10:18)
Title: Decomposed Velocity Field in $f(R)$ Cosmology
Advisor(s): Jie Wang, National Astronomical Observatories of China; Baojiu Li, Institute for Computational Cosmology, Durham University
Co-Author(s):

Abstract: Inspired by Zhang et al (*PhRvD* 87, 3526,2013), we tried to distinguish the modified gravity $f(R)$ cosmology from Λ CDM cosmology using decomposed components of peculiar velocity field. We used N-body simulations run by Dr. BaoJiu Li at Durham University to predict the density and velocity field of both cosmologies. By decomposing peculiar velocity in the simulations into three eigen-components, an irrotational component completely correlated with the density field V_{δ}, an irrotational component completely uncorrelated with density field V_{S}, and a rotational component V_{B}, the velocity power spectra of these components are compared and contrasted for different cosmological models. A close investigation of the contrast among cosmological models for three components at shows that the V_{S} component is the most powerful one to indicate $f(R)$ cosmology. We find that, even for an $f(R)$ model with $|f_{R0}|= 10^{-6}$, the power spectrum of V_{S} component can reach 13% higher than General Relativity at k=0.2h/Mpc. The difference between $f(R)$ and GR in the V_{S} get larger as the scales gets smaller. This signal is significant and could be checked in forthcoming observational data, which promises a new way to constrain the gravity models.

Presenter(s): Kaiyuan Zhang, Beloit College
Session: Poster P3.24
Title: Characterization of ω-3 Fatty Acids in Fish Oil Dietary Supplements with FTIR Spectroscopy and 2D Correlation Analysis
Advisor(s): Rongping Deng, Chemistry, Beloit College
Co-Author(s): Andrew Collins

Abstract: This study experiment provided the evidence to identify the Omega-3 fatty acids from other forms of unsaturated fatty acids in fish oil dietary supplements by using Fourier Transform Infrared Spectroscopy and 2 Dimensional Correlation Analysis. The experimental method in this study shows the advantage of the minimum instrument requirement, less chemical waste, low cost, non-destructive, fast and direct measurement to identify the contents of Fatty Acids. It could have the applications in the analyses of other chemicals.

Presenter(s): Junmian Zhu, Grinnell College
Session: Poster P1.26
Title: NMR Measurements of Ion Transport for Organosilicon Nitrile Electrolytes
Advisor(s): Leslie J. Lyons, Chemistry, Grinnell College
Co-Author(s): Leslie J. Lyons

Abstract: Organosilicon (OS) nitrile solvents have low flammability, broad electrochemical windows and excellent thermal stability, which make them promising materials for lithium ion battery (LIB) electrolytes. However, little is known about ion transport and salt dissociation of the lithium salts in organosilicon nitrile electrolytes. In this presentation, we report on the temperature dependence of the self-diffusion coefficients of lithium and fluorine for 6 pure OS nitrile solvent/$LiPF_6$ salt electrolytes from 295.0 K to 330.0 K measured by Pulsed Field Gradient Stimulated Echo (PFG-STE) NMR experiments. Electrolytes were prepared from 3 OS nitrile solvents with varying levels of fluorination and having a concentration of $LiPF_6$ salt at Li-solvent molar ratios of 1:5 or 1:20. We found that mono-fluorinated solvent electrolytes have the highest Li and F diffusion coefficients. In addition, all dilute samples have higher salt dissociation and Li and F diffusion coefficients than their concentrated counterparts. Our studies on the Li cation and PF_6^- anion diffusion help to illustrate the ion transport processes of lithium salts in the organosilicon nitrile solvent-based electrolytes.

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