JMU®

College of Science and Mathematics

2025 REU SUMMER SYMPOSIUM

DEPARTMENT OF BIOLOGY
DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY
DEPARTMENT OF MATHEMATICS & STATISTICS
DEPARTMENT OF PHYSICS & ASTRONOMY

MONDAY JULY 28
&
TUESDAY JULY 29

Keynote Speaker

Taylor Light, Ph.D.
(JMU Class of 2016)
Quality Analytical, Catalent Pharma Solutions
Cell and Gene Therapy
Harmans, MD

Harrisonburg to Baltimore: Breaking Into the World of Clinical Biomarkers

Taylor is a JMU Chemistry alumnus, graduating in 2016 with a degree in Biophysical Chemistry and a minor in mathematics. As an undergraduate student, Taylor researched protein and biomolecule aggregation in response to various solutes and solvents in Gina MacDonald's lab. It was through all the research experiences as an undergraduate at JMU, including a few summers with the REU program, that Taylor gained valuable research skills and informed his decision to pursue a PhD. At Johns Hopkins University, Taylor changed course of study to materials science and engineering with an offer to research in Kalina Hristova's lab studying membrane protein signaling in disease and cancer. After graduate school and with eight years of research experience under his belt, Taylor leapt into a career in industry where he began to develop analytical methods for immunotherapeutic drug testing and biomarker analysis in the pre-clinical and clinical stage. In this seminar, Taylor will share his experiences navigating undergraduate and graduate school, research, the transition to industry, and what he looks forward to in the future.

Monday, July 28th

Multi-Slides Presentations I: King 159		
9:00 AM	Welcome Remarks	*Steven Whitmeyer, Associate Dean for Research & Scholarship, CSM*
9:10 AM	Brian M. Getty, Dr. Maegen A. Borzok, and Dr. Nathan T. Wright	*Characterizing the Desmoplakin-Drug Interaction using NMR Saturation Transfer Difference Experiments*
9:22 AM	Dillon Proxmire and Dr. Thomas DeVore	*Exploration of Acetate Ion Interactions in Solution by FTIR and NMR data*
9:34 AM	Jacob Skinner and Dr. Sachith Dissanayake	*Synthesis and Investigation of Superconducting and Magnetic Properties of Gd and Nd doped Er123 HTSC Cuprate Ceramics*
9:46 AM	Katherine I. Cooper, Ray Enke	*Developmental and Cell-specific Transcriptome Analysis of the Mouse Retina*
9:58 AM	Kaden R. Lopez, Nicholas T. Cheung, I-Cheng Tung, Hua Zhou, Dillon D. Fong, Kendra Letchworth-Weaver	*Energetics of dynamic layer rearrangement and island formation during epitaxial growth on SrTiO3 (001)*
10:10 AM	Tengis Tamir, Emily Nattress, Tristen Bossidy, & Dr. Debra Mohler	*A Novel Synthetic Strategy for Antisense Oligonucleotide Analogs*
10:22-10:37 AM	Break	
10:37 AM	Charles Beattie, Dr. Kristopher Schmidt, Dr. Laura Tiptonr, and Dr. Giovanna Scarel	Random Forest Usage in biostatistics applications
10:49 AM	Peter Henry, Kamrin Shultz, and Dr. Nathan Wright	Characterization of the Obscurin Functional Domain and its Regulatory Pathways
11:01 AM	Elaina X. Manyin and Dr. Isaiah Sumner	Thermodynamics and Kinetics of Boron Esterification
11:13 AM	Davis Stiles, Katherine Cooper, Dr. Marquis Walker, Dr. Ray Enke	Immunohistochemistry Characterization of Phototransduction Proteins in the Mcoln1-/- Mouse Retina
11:25 AM	Owen Phillips, Dr. Barbara Reisner, Dr. Harry Hu, Dr. Thomas DeVore	Hydrated to Anhydrous: Study of the Synthesis and Characterization of $K_2Co_xCu_y(SO_4)_2\cdot 6H_2O$
11:37 AM	Umanga Rupakheti, Rediet G. Abebe, Alyssa A. Afari, Courtney M. Dickens, Eyiakimeh D. Enuameh, Nicholas D. Mayonado, Estefania M. Tapia, Patrick M Lombardi, Christopher E Berndsen	Structural Analysis of the ASCC2 CUE Domain-K63 Diubiquitin Complex Using Small Angle X-ray Scattering
11:49 AM	Break	

Poster Session: King Lobby	
1:00 - 2:00 pm	Group A
2:00 - 3:00 pm	Group B

Poster Session: Group A	
Eva Ackley, Kylie Gill, Cole Kratz, and Dr. Méric Augat	Approaches to the L'vov-Kaplansky Conjecture
Jacob A. Amberg, Alexander Irvine, and Donna S. Amenta	Synthesis of N-Triazolyl and N-Pyrazolyl Derivatives as Chelating ligands for Ruthenium Complexes
Daphne M. Antwi and Gina MacDonald	Amino Acid Influences on Bovine Serum Albumin & Lysozyme Structure and Stability
Jaimin J. Ashra, Kathrine B. Weinstock, Allen C. Shepherd, James T. Whitted, and Dr. Ashleigh E. Baber	Scanning for Order: Can R-2-Butanol Behave on Ni(111)?
Clarissa Azurin, Lois Carpenter, Grace Gorreck, and Dr. Alex Capaldi	Optimizing the Distribution of Fruiting Agave on Bat-Friendly Tequila Plantations
Allen Bao, Jordan Larson, Kelson McBride, and Dr. David Duncan	The Topology of Representation Varieties
Landon Brown, Dr. Masoud Kaveh, Dr. David Lawrence, Dr. Costel Constantin	Refinement of X-Ray Diffraction Data of Gadolinium-doped Indium Tin Oxide Thin Films deposited by DC Magnetron Sputtering in FullProf Suite
Luke Campbell, Emma Foley, Callie Muska, Hui Chen	Aggregation of Short- and Ultrashort-chain Per- and Polyfluoroalkyl Substances (C1-C4 PFAS) by Donnan Dialysis
Erika Cherpes and Dr. Anca Constantin	A WISE Look at Variability of Maser Galaxies
Andrew Christensen, Drew Tobin, Emily Delle, Caleb McCarthy, and Dr. Marquis Walker	Analysis of Mouse Intrinsic Iridial Photoreceptors (IIPs)
Olivia E. Coer and Dr. Brycelyn Boardman	Modulating the Thermal, Mechanical, and Flammable Properties of Chitosan Films with Polyol-Boric Acid Complexes
David W. Compton Jr, James T. Whitted, Katherine B. Weinstock, Jaimin J. Ashra, Emily M. Euler, Allen C. Shepherd, and Dr. Ashleigh Baber	Unraveling the Initial Steps of Water Dissociation on Cu(111)
Drew Cutright and Dr. Costel Constantin	Aerodynamic Efficiency at Variable RPM: Theoretical Comparison Study Between Propellers and Impellers with Computational Fluid
Bethany Droubay and Dr. Alex Capaldi	Modeling Probiotic Bacterial Control of White-Nose Syndrome in Little Brown Bat Colonies
Julia A. Flisiak, Grace M. Hillan, and Oleksandr Kokhan	Optimization of recombinant protein expression with MALDI-MS
Landon Gray, Max Tyree, Elijah Fernands, Dr. Paris Salazar-Hamm, and Dr. Lindsay Caesar	Response of Secondary Metabolism of Bat-Associated Bacteria to Chemical Stimuli
Benjamin D. Grossman, Dr. Ray Enke	Customizable R Shiny Application for Analysis and Visualization of Public Retinal Transcriptome Data
Erin Naman, Juliane A. Calvert, Anna E. Williams, Ethan Dray, Jackson Vickers, Eriberto Osorio, and Dana L. Moseley	Assessing birdsong frequency measurements of sample size, window-sample rate, and timing of frequency shifts in a noise experiment with Gray Catbirds *Dumetella carolinensis*
Anna Williams, Lydia Ritchey, Kylie Bailey, Bernard Lohr, David A. Luther, Brian S. Evans, and Dana L. Moseley	Analyzing the accuracy of AI-powered bird identification systems during the 2021 emergence of 17-year cicada brood

Poster Session: Group B	
Caitlin Gutierrez, Stephanie Schwender and Dr. Brycelyn Boardman	Aggregated induced emission of quinazoline derivatives in the presence of glucosamine and chitosan
Keyvan Harris, Sarah Vollbrecht, Bella Fong, Hui Chen	Development of novel cellulose-based micromotors for maximal nutrient recovery from poultry litter
Courtland Hurley, Sydney Hartman, Katherine Weinstock, James Whitted, Mollie Corbett, Dr. Ashleigh Baber, and Dr. Kendra Letchworth-Weaver	Understanding Oxophilic Pathways of Enhanced Epoxidation Reactions by Optimizing Bimetallic AgCu Catalysts
Carly N. Hemani, Frances E. Homan,& Dr. Lindsay E. Caesar	Mycological Resilience: Evaluation of Heavy Metal Tolerance in Grand Caverns
Elanor K. Kirkland and Dr. Isaiah Sumner	Exploring Interactions between Glucosamine and Differing Plasticizers through Electronic Structure and Molecular Dynamics
Ingrid Larne, Dr. W. Christopher Hollinsed	Synthesizing a Contractile Molecule Using Fluorescein & a Quaternary Ammonium Compound for Atomic Force Microscopy
Alexander F. Lauer, Dr. Jun Yin, and Dr. J. Connor Gilhula	Creating Novel Molecular Plumbates as Potential Catalytic Anions
Lucille McGinnis and Dr. Nathan T. Wright	Characterizing Small Molecule/Desmoplakin Interactions that Prevent Protein Degradation
Nathan E. Morris and Dr. Brycelyn Boardman	Understanding the impact of polyol stereochemistry on plasticized chitosan film morphologies using scanning electron microscopy
Emily Nattress, Tengis Tamir, Tristan Bossidy, William Brown, and Dr. Debra Mohler	Regulating Protein Synthesis: A Novel Synthesis for Antisense Oligonucleotide Analogs
Andrew A. Neumann, Alexander F. Lauer, and Dr. J. Connor Gilhula	Synthesis and Metal Complexation of Regenerative Chelators for Targeted Alpha Therapy
Cameron Page, Gina MacDonald, Yanjie Zhang	Hofmeister Cation and Anion Effects on Caffeine Solvation and Aggregation
Lilija Pflanz, Linette Watkins, and Gina MacDonald	Monitoring The Structure, Stability, and Activity of Horseradish Peroxidase Over Time
Osmond Reindorf-Malm and Dr. Chris Hollinsed	Development and Synthesis of a new class of organic polymeric materials: Synthesizing and purifying a contractile molecule using fluorescein derivatives, transfer hydrogenations techniques, and monomer linkage using a diisocyanate.
Allen C. Shepherd, James T. Whitted, Kate B. Weinstock, Jaimin J. Ashra, David W. Compton, Emily M. Euler, Owen M. Paulson, and Dr Ashleigh E. Baber	Understanding the Reactivity of C2 Molecules on Cu(111) Catalysts
Samuel Stoke, Caleb Fernandes, Audrey Knight, Dr. Behnaz Moradi-Jamei	Deep ReCYCLE: Cycle-Aware Community Detection with RNBRW-Augmented GNNs
Katherine B. Weinstock, James T. Whitted, Allen C. Shepherd, Jaimin J. Ashra, Emily M. Euler, David W. Compton, and Dr. Ashleigh E. Baber	The Selective Catalytic Epoxidation of Ethylene on Ag/Cu(111)
Paige O. Wooten, Elanna F. Smith and Dr. Gina MacDonald	Environmental Influences on α-Chymotrypsin, Myoglobin, & β-Lactoglobulin Structure, Stability, and Aggregation

Monday, July 28th

Multi-Slides Presentations II: King 159		
3:10 PM	Jorge A. Menacho Paz and Dr. Joshua Ducey	Hadamard Matrices: Existence and Equivalence Problems
3:22 PM	Ruhi Rahman, Jonathan Monroe, Christopher Berndsen	Starch Binding Assays and Structure of Carbohydrate-Binding Module of Alpha-Amylase AMY3
3:34 PM	Sara E. Scanlan and Dr. Christopher E. Berndsen	Structural dynamics during the watermelon malate dehydrogenase reaction cycle
3:46 PM	Meriem Dhouibi	Predicting Debris Flow and Landslides in Virginia Using Logistic Regression
3:58 PM	Eva Ackley, Kylie Gill, Cole Kratz, and Dr. Méric Augat	Approaches to the L’vov-Kaplansky Conjecture
4:10-4:25 PM	Break	
4:25 PM	Anna G. Grove, and Dr. Gretchen M. Peters	Targeted cargo loading of supramolecular peptide boronic acid gels
4:37 PM	Sam Robinson and Dr. Chris Hollinsed	Contractile Molecules: Synthesis, Purification, and Analysis
4:49 PM	Alexander J. Hardie, Dr. Despina Louca, Dr. Sachith Dissanayake	$MoTe_2$ Under Uniaxial Pressure
5:01 PM	Emily M. Euler, Haley E. Frankovich, Dr. Kendra Letchworth-Weaver, Dr. Ashleigh E. Baber	Modeling Isomeric Butanol Reaction Pathways on TiO_2/Au(111) Inverse Model Catalysts

Tuesday, July 29th

Keynote Speaker: King 159		
9:00 AM	Taylor Light, Ph.D. (JMU ’16)	*Harrisonburg to Baltimore: Breaking into the World of Clinical Biomarkers*
10:00 -10:15 AM	Break	

Multi-Slides Presentations III: King 159		
10:15 AM	Clarissa Azurin, Lois Carpenter, Grace Gorreck, and Dr. Alex Capaldi	Optimizing the Distribution of Fruiting Agave on Bat-Friendly Tequila Plantations
10:27 AM	Gabriela Niculescu, Sarah Ormond, and Dr. Ioana Niculescu, Dr. Kevin Giovanetti, Dr. Gabriel Niculescu	PbWO4 Crystal Characterization: Data Acquisition and Analysis Workflow
10:39 AM	Brandy L. Davidson and Dr. Gretchen M. Peters	Elucidating the structures of polyol-boric acid complexes in organic solvent using NMR spectroscopy
10:51 AM	Nicholas Luces, Aidan Pisarcik, Dr. Ioana Niculescu, Dr. Kevin Giovanetti, Dr. Gabrial Niculescu	PbWO4 Crystal Characterization: Data Simulation and Analysis
11:03-11:18 AM	Break	

11:18 AM	Hannah Lau, Rhett Sanders, Isaiah Sumner	Molecular Interactions of the plastic PET with a Lysosome Enzyme
11:30 AM	Heather Accorti, Samuel Pearne, and Dr. Ioana Niculescu, Dr. Kevin Giovanetti, Dr. Gabriel Niculescu	PbWO4 Crystal Characterization: Mechanical Design and 3D Modeling
11:42 AM	James T. Whitted, Katherine B. Weinstock, Owen M. Paulson, Emily M. Euler, Jaimin J. Ashra, and Dr. Ashleigh E. Baber	Utilization of Water for Propylene Epoxidation on Ag/Cu(111)
11:54 AM	Allen Bao, Jordan Larson, Kelson McBride, and Dr. David Duncan	The Topology of Representation Varieties
12:06 PM	Samuel Stoke, Caleb Fernandes, Audrey Knight, Dr. Behnaz Moradi-Jamei	Deep ReCYCLE: Cycle-Aware Community Detection with RNBRW-Augmented GNNs
12:18 PM	Announcements	

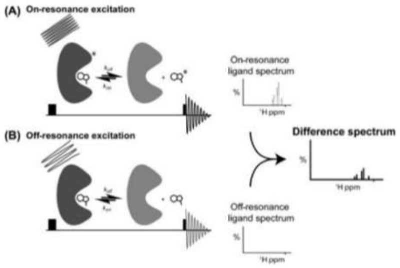
STUDENT ABSTRACTS
Multi-Slide Presentations: Session I

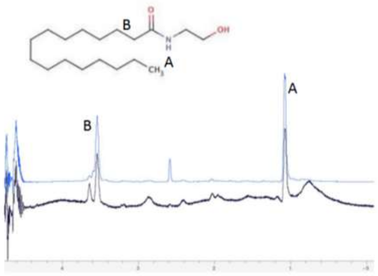
(Student presenters underlined)

Characterizing the Desmoplakin-Drug Interaction using NMR Saturation Transfer Difference Experiments

Brian M. Getty[1], Dr. Maegen A. Borzok[2], and Dr. Nathan T. Wright[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807
[2]Department of Natural Sciences, Mansfield University of Pennsylvania, Mansfield, PA 16933

Desmoplakin (DSP) is a desmosomal protein that plays an integral role in connecting the intermediate filaments from one cardiomyocyte to another. Mutations in DSP underlie about 5% of arrhythmogenic cardiomyopathy (ACM) cases. Recent data from our lab show that some disease-linked DSP mutations result in hypersensitive cleavage in the presence of calpain, an endogenous calcium-dependent protease. The resulting loss of DSP destabilizes the desmosome and leads to weakened cell-cell adhesion, which is correlated with fibrofatty infiltration in ACM. Our lab has shown that DSP mutant hypersensitivity to calpain is dependent upon the exposure of a usually occluded cleavage site on the DSP surface. Previous work found that small molecules stabilize DSP levels in the presence of calpain. Several dozen small molecules specifically inhibit DSP and DSP mutant degradation. However, parameters of how these drugs interact with DSP, including binding affinity, the binding orientation, and bioavailability in our system, are unknown. Here, using NMR saturation transfer difference (STD) experiments, we begin to quantify these characteristics of each DSP degradation-inhibiting small molecule in the presence of wild-type (WT) and mutant DSP strands. Future work will continue identifying these characteristics for each small molecule and calpain-sensitive mutation strain.

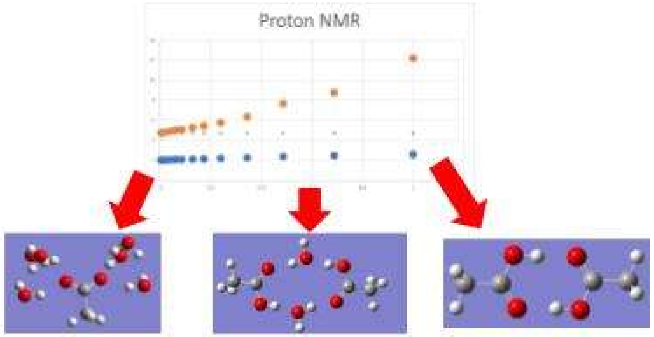




Exploration of Acetate Ion Interactions in Solution by FTIR and NMR data

Dillon Proxmire and Dr. Thomas DeVore
Department of Chemistry and Biochemistry, College of Science and Math, James Madison University, Harrisonburg, VA 22807

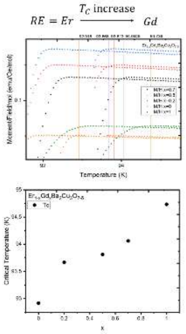
Having a sophisticated understanding for how ions in solution behave has proven, and will continue to be, essential in order to make advancements in many fields of science and medicine. In this study, dilution series of Sodium, Magnesium, and Barium Acetates were analyzed using FTIR, C13, and Proton NMR. Dilution series of acetic acid were also analyzed with the same spectral techniques to offer insights about the acetate ion data. Data trends were identified and compared across all data sets in order to characterize ion-ion interaction and solvation behavior in the solution. Through the experimental lens of spectroscopy and analysis of data trends, 3 different classifications of acetate solvation were identified. At low concentrations, fully-solvated separate ions (FSSI) appear to highly contribute to the solution, with lesser contributions from solvent-separated ion pairs (SSIP). As concentrations increase, the FSSI become less prevalent as ion interactions increase, and eventually contact-ion pairs (CIP) begin to form in solution and increasingly contribute with increasing solute concentration. We identified the FTIR frequency of the fully-solvated, separate acetate ion to be located at 1551 cm-1 and 1415 cm-1. On the C13 NMR, we were also able to identify the location of the carboxylate and methyl peaks of the fully-solvated, separate acetate ion at 181.5 ppm and 23.3 ppm respectively.

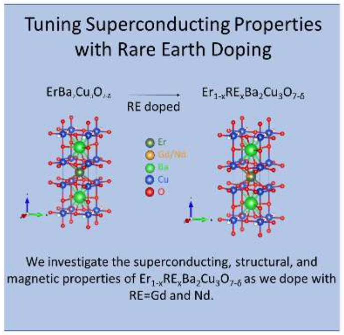


Synthesis and Investigation of Superconducting and Magnetic Properties of Gd and Nd doped Er123 HTSC Cuprate Ceramics

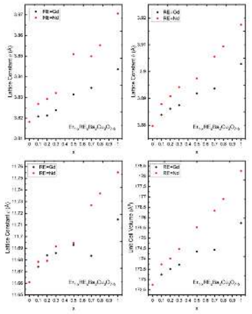
Jacob Skinner and Dr. Sachith Dissanayake
Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

The RE123 (RE=rare earth element) compound is a common form of high-temperature superconducting (HTSC) cuprate ceramic with chemical formula REBa$_2$Cu$_3$O$_{7-\delta}$. This compound makes an excellent superconductor due to its high critical temperature (T_c) in the low 90 Kelvin range, its high critical current density (J_c), stability, non-toxicity, and ease of synthesis, making it viable for use in many industries. In this family, ErBa$_2$Cu$_3$O$_{7-\delta}$ has a critical temperature of 93 K and is known to be one of the best solders for superconducting joint fabrication. In this study, we aimed to investigate the effects of superconducting and magnetic properties of ErBa$_2$Cu$_3$O$_{7-\delta}$ when doped with another RE ion with a different ionic radius. Samples of Gd- and Nd-doped ErBa$_2$Cu$_3$O$_{7-\delta}$ superconductors are prepared systematically using the solid-state reaction (SSR) method, and the sintering parameters for phase formation are determined. The crystal structure of the Gd and Nd doped ErBa$_2$Cu$_3$O$_{7-\delta}$ superconductor is investigated at different doping levels using x-ray diffraction (XRD). Rietveld analysis of XRD data shows that the unit cell volume increases with Gd and Nd doping and orthorhombicity changes. We also measured the superconducting properties of these materials using DC magnetization and compared the critical temperature (T_c), critical field (H_c), and critical current density (J_c) of the material as a function of doping. The relationship between the structure and superconducting properties will be discussed. We also successfully synthesized three RE element RE123 superconductor using Er, Gd, and Nd equal molar ratios as a preliminary effort to synthesize high entropy version of the Er123 superconductor and compare that with our results of Gd- and Nd-doped ErBa$_2$Cu$_3$O$_{7-\delta}$.




Tuning Superconducting Properties with Rare Earth Doping

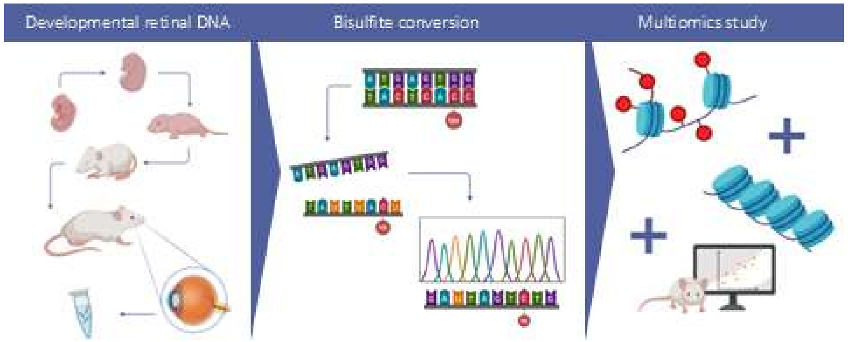
We investigate the superconducting, structural, and magnetic properties of Er$_{1-x}$RE$_x$Ba$_2$Cu$_3$O$_{7-\delta}$ as we dope with RE=Gd and Nd.



Developmental and Cell-specific Transcriptome Analysis of the Mouse Retina

Katherine I. Cooper[1], Ray Enke[1, 2]
[1]Department of Biology, James Madison University, Harrisonburg, VA 22807
[2]Center for Genomics and Metagenomics, James Madison University, Harrisonburg VA 22807

The retina is a neuronal tissue that lines the back of the inner eye. This tissue converts photons of light into electrochemical signals that are sent to the brain resulting in what we perceive as the visual world. This process, called phototransduction, is initiated by highly specialized neurons called photoreceptors (PRs) which can be subclassified as rods and cones. During retinal development, several key transcription factors including Cone-rod homeobox (CRX) and Neural retinal leucine zipper (NRL) are critical for rod and cone differentiation and function. This study analyzes mRNA transcriptome data from the developing mouse retina to better understand how epigenetic regulation impacts PR differentiation and function. Previously published RNA-seq data generated from developing wt, and *Nrl*$^{-/-}$, mouse retinas were obtained from the NCBI SRA database and combined with public ChIP-seq and DNase I hypersensitivity data to visualize areas where epigenetic regulation occur; primarily CRX and NRL binding sites and DNA accessibility. We located nearby regions of interest where DNA methylation may occur as an additional epigenetic regulator. Current experiments focus on mutating DNA samples through bisulfite conversion in preparation for sequencing. Combining DNA methylation assays and the compiled public data will offer a multiomics study of mouse retinal gene regulation.



Energetics of dynamic layer rearrangement and island formation during epitaxial growth on $SrTiO_3$ (001)

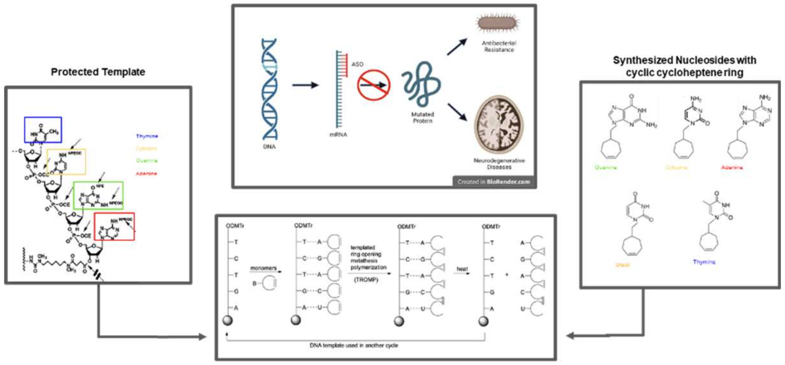
Kaden R. Lopez[1], Nicholas T. Cheung[1], I-Cheng Tung[2,3], Hua Zhou[2], Dillon D. Fong[4], Kendra Letchworth-Weaver[1,5]
[1] Department of Physics and Astronomy, James Madison University
[2] X-ray Science Division, Advanced Photon Source, Argonne National Laboratory
[3] Department of Materials Science and Engineering, Northwestern University
[4] Materials Science Division, Argonne National Laboratory
[5] Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL

Atomic variation in the surface topography of thin films can have significant impact on their electronic structure, macroscopic properties, and potential technological applications. Because strontium titanate ($SrTiO_3$) is a common substrate for growing thin films using Molecular Beam Epitaxy (MBE), we investigate the energetics and kinetics of surface rearrangement during homoepitaxial $SrTiO_3$ growth. We study two different deposition sequences on a bare substrate terminated with double-layer TiO_2. In the sequential deposition sequence a monolayer of SrO is deposited followed by a monolayer of TiO_2 and in the reverse deposition sequence the order is flipped. The structure of the surface is monitored with X-ray Reflectivity (XRR) while models of the surface are energetically minimized with Density Functional Theory (DFT). Using an XRR data inversion procedure constrained to the DFT calculations allows us to determine interfacial structures more accurately than is possible through experiment or theory alone. The observed dynamic rearrangement of the surface, including layer swapping and the formation and subsequent rearrangement of surface islands grants insight into specifics needed to design more effective protocols for MBE growth of novel semiconductors and quantum materials.

A Novel Synthetic Strategy for Antisense Oligonucleotide Analogs

Tengis Tamir, Emily Nattress, Tristen Bossidy, and Dr. Debra Mohler
Department of Chemistry and Biochemistry, College of Science and Math, James Madison University, Harrisonburg, VA 22807

Antisense oligonucleotide analogs (ASOs) are short, modified RNA molecules that have the ability to bind messenger RNA (mRNA) and prevent protein transcription through various mechanisms. ASO technology has been effective at preventing and reducing disease severity for numerous diseases by limiting harmful protein and enhancing helpful protein production. ASOs often face degradation, membrane impermeability, RNase activity, non-specific activities, etc. In an effort to address these challenges, we propose ASO analogs produced via a novel synthetic strategy from nucleoside analogs constructed with a cyclic cycloheptene ring. The synthesis and characterization of the Adenine, Cytosine, Guanine, Thymine, and Uracil derivatives have all been achieved. Currently, the ongoing research involves the synthesis of the solid-state backbone template sequence utilizing protected deoxynucleotides



Random Forest Usage in biostatistics applications.

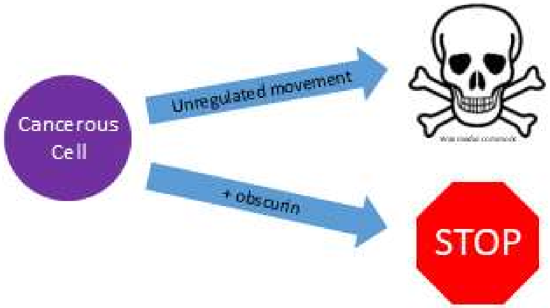
Charles Beattie[1], Dr. Kristopher Schmidt[2], Dr. Laura Tiptonr[3], and Dr. Giovanna Scarel[1]
[1]Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807
[2]Department of Biology, Eastern Mennonite University, Harrisonburg, VA 22802
[3]Department of Biology, James Madison University, Harrisonburg, VA 22807

Random Forest is a machine learning algorithm used in data analysis operations to highlight important variables in datasets with many variables. It is especially useful in datasets with a large amount of unique variables that interact with each other. A good example of application of Random Forest is our research in which this algorithm enabled us to process and reduce a dataset from 4082 variables to 4 variables which characterize the kinematic and postural behavior of C. elegans under red and blue light emitting diodes as well as radio waves. Random Forests algorithm was able to prove that speed differences in C. Elegans under different illumination environments were primarily due to real differences in speed and not an error in the data refinement or recording processes.

Characterization of the Obscurin Functional Domain and its Regulatory Pathways

Peter Henry, Kamrin Shultz, and Dr. Nathan Wright
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

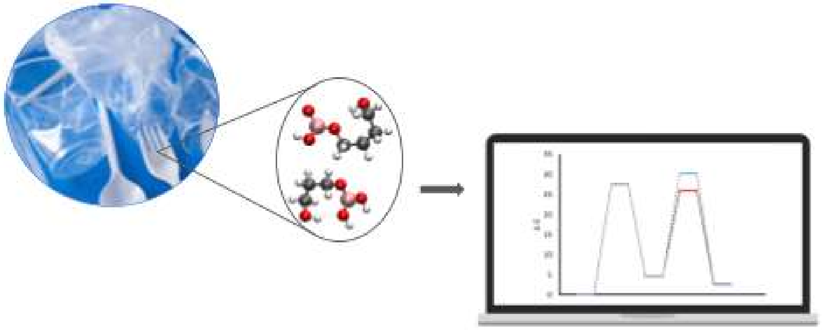
The cytoskeletal protein obscurin has previously been studied only in muscular cells, where it was first characterized. It is known that obscurin plays a role in cell mobility, and if not functioning correctly, can lead to cancer as a result of unregulated movement. Literature has shown that this protein is most often mutated in breast and colorectal cancers. In novel experiments, obscurin is added to cell cultures via adenovirus infection as opposed to previous methods utilizing knockout techniques. The effects of this addition have been measured in colocalization studies, timelapse velocity analysis, and lipid assays. Each of these experiments has shown that there are multiple domains within the obscurin construct that oversee cellular mobility regulation, namely the Rho-GEF and PH domains, as well as certain segments of the unstructured region near the C-terminus of the protein.



Thermodynamics and Kinetics of Boron Esterification

Elaina X. Manyin and Dr. Isaiah Sumner
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

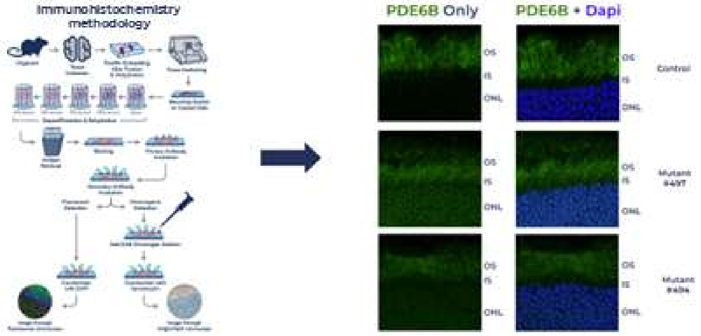
Biodegradable plastic are alternatives to current plastics as they are more environmentally friendly. One such plastic is made from the polymer, chitosan, which comes from crustacean skeletons, and a plasticizer, a small molecule that can tune the properties of chitosan. In a recent set of experiments, borate esters with glycerol were used as plasticizers for the polymer. Although this combination resulted in poor plasticity, borate ester plastics are stiff and thermally stable. These are desirable properties that warrant more investigation. However, the molecular-level understanding of borate ester synthesis is unexplored. For instance, borate esters synthesized from boric acid and diols can form open-chain molecules or cyclic compounds. Experimental data showed reactions with ethane glycol and 1,3-propanediol seemed to form only closed complexes, whereas reactions with 1,4-butanediol seemed to form only open-chain complexes. To explain this experimental data, Gibb's free energies were calculated using density functional theory (DFT) at the M06-2x/6-311+G(2d,p) level-of-theory. The difference in Gibb's free energy between open and closed complexes was calculated by subtracting the closed structure plus a free water molecule needed to balance the reaction by the open structure ($\Delta G= (G_{closed}+G_{H2O}) - G_{open}$). The ΔG values for Ethane Glycol Boric Acid, 1,3-Propanediol Boric Acid, and 1,4-Butanediol Boric Acid were -1.45 kcal/mol, -6.86 kcal/mol,and -0.69 kcal/mol, respectively. These computational findings did not match experimental data, however the trend of how favored the closed complex was did. Based on these results, the reaction barrier heights were explored to understand the kinetics of the formation of these reactions. In all reaction schemes the calculations indicated two transition states and two different intermediates to form the product for each reaction. However, the barrier heights were very high in energy which may indicate a more complicated reaction mechanism forms these complexes.



Immunohistochemistry Characterization of Phototransduction Proteins in the Mcoln1$^{-/-}$ Mouse Retina

Davis Stiles, Katherine Cooper, Dr. Marquis Walker, Dr. Ray Enke
Department of Biology, James Madison University, Harrisonburg, VA 22807

Age-related macular degeneration (AMD) is a disease that leads to loss of retinal neurons and is the most prominent cause of irreversible blindness among elderly in the western world. There is currently no cure and limited treatment options for AMD. One of the barriers to studying AMD is the lack of an established animal model system to study disease onset and progression. The *Mcoln1-* mutant mouse does not produce the TRPML1 membrane protein and exhibits defects in intracellular autophagy in all cells, including retinal neurons. Preliminary studies in our lab have demonstrated that the*Mcoln1-* mouse retina displays cellular, molecular and physiological phenotypes similar to the human AMD retina. This project is focused on further characterizing the *Mcoln1-* mouse as a potential animal model to study AMD. Here we have conducted immunohistochemistry (IHC) characterizing localization and expression of four critical proteins in photoreceptor retinal neurons. The RHO, GUCA1B, RCVRN, and PDE6B proteins were determined to have dysregulated expression and localization in mutant mice compared to controls. Current and future work will focus on conducting western blot experiments on these phototransduction proteins to confirm if there is a decrease in protein expression, along with exploring the expression and localization of complement pathway of proteins by both IHC and western blot assays.



Hydrated to Anhydrous: Study of the Synthesis and Characterization of $K_2Co_xCu_y(SO_4)_2·6H_2O$

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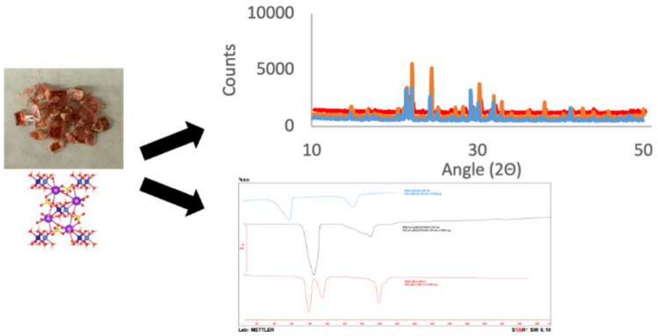
Tutton salts are a family of double salts with applications in waste heat recovery and solar energy storage. In this study, mixed-metal Tutton salts with the formula $K_2Co_xCu_y(SO_4)_2·6H_2O$ were synthesized in various ratios of Co/Cu by slow evaporation. The synthesized salts were then analyzed and characterized using as Powder X-ray Diffraction (PXRD), Infrared Spectroscopy (IR), Scanning Electron Microscopy/Energy Dispersive X-ray Spectroscopy (SEM/EDS), and Differential Scanning Calorimetry (DSC). DSC analysis gave a range for dehydration enthalpies from 341-348 kJ/mol for the 50:50 ratio of metals, and a range of 320-323 kJ/mol for the 75:25 and 25:75 ratios. Aside from initial characterization of the salt, PXRD and IR were used to determine the change in the structure of the salt as it was heated to different temperatures. It was found that when heating the salt becomes amorphous to x-rays before becoming crystalline again at higher temperatures. Additionally, the dehydrated salts were able to be rehydrated indicating that the salts could be used in thermal storage situations.



Structural Analysis of the ASCC2 CUE Domain-K63 Diubiquitin Complex Using Small Angle X-ray Scattering

Umanga Rupakheti[1], Rediet G. Abebe[2], Alyssa A. Afari[2], Courtney M. Dickens[2], Eyiakimeh D. Enuameh[2], Nicholas D. Mayonado[2], Estefania M. Tapia[2], Patrick M Lombardi[2], Christopher E Berndsen[1]
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DNA damage is one of the precursors to cancer and other diseases. Alkylation of nucleotides where a methyl group is added to the base group of the nucleotide is one form of damage which can cause mutations in DNA and RNA. Activating Signal Cointegrator 1 Complex Subunit 2 (ASCC2) complex can repair alkylation damage but the structure of this complex and the mechanism of action is not clear. During the repair process, ASCC2 interacts with Lysine63 (K63) linked ubiquitin chains through the CUE domain of ASCC2 however the specific interaction site and mode is not known. Our goal is to describe the structure of the complex of K63-linked ubiquitin and ASCC2 CUE domain complex using small angle X-ray scattering. We want to propose a model to provide more information about how the complex forms and functions. We collected SAXS data on K63 diubiquitin and the ASCC2 CUE domain expressed in E.coli along with a mixture of the proteins with the aim of characterizing the complex. We used normal mode analysis to adjust the conformation of the existing NMR model of ASCC2 to better fit to the SAXS data. This adjusted conformation of ASCC2 better matches the structure of known CUE domains. Preliminary analysis of the data on the complex suggests a 1:1 Ub2:ASCC2 stoichiometry and we are currently developing models to fit to the data in order to propose an interaction site. These structures will be useful in describing how DNA damage is repaired in humans and potentially provide information for the development of anticancer agents.

STUDENT ABSTRACTS
Poster Session: Group A

Listed in alphabetical order by presenter's last name
(Student presenters underlined)

Approaches to the L'vov-Kaplansky Conjecture

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The L'vov-Kaplansky Conjecture is a longstanding open question in the field of Algebra, which asks if the image of a multilinear polynomial acting on the space of $n \times n$ matrices is a subspace. We consider a weakening of the conjecture using an analytic lens: the Density Dimension-Free L'vov-Kaplansky Conjecture. This asks whether any multilinear polynomial eventually attains density in a subspace for large enough matrices with complex entries. Using an auxiliary map, we prove that density of the image on 2 × 2 matrices is guaranteed by a linear independence condition. Moreover, we give conditions on factorizations of multilinear polynomials that, if satisfied, guarantee density of the image within the traceless matrices or full matrix algebra. We provide concrete open problems that would shed further insight into the conjecture.

Synthesis of N-Triazolyl and N-Pyrazolyl Derivatives as Chelating ligands for Ruthenium Complexes

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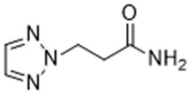
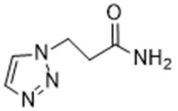
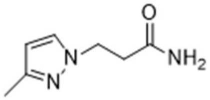
Chelating hemilabile ligands are of interest for applications in organometallic catalysis. N-pyrazolyl and N-triazolyl derivatives have been studied as potential metal chelates particularly for platinum and palladium. In this study, the reaction of 1,2,3-triazole with acrylamide produced isomeric N-triazolylpropanamides L1 and L2. The synthesis of the L1/L2 mixture in dioxane was accomplished by a Michael addition in six minutes using a microwave reactor and Cs_2CO_3 as a catalyst. In a similar microwave reaction, the synthesis of the isomers 3-(3-methylpyrazolyl)propanamide (L3) and 3-(5-methylpyrazolyl)propanamide (L4) was accomplished in sixteen minutes. Both reactions gave good yields. When a mixture of L1 and L2 was allowed to react with n-butyllithium followed by dichlorotris(triphenylphosphine) ruthenium (II), a new phosphorus compound was obtained. The identity of the new compound is presently under investigation as is the reaction of L3 and L4 with n-butyllithium and dichlorotris(triphenylphosphine)ruthenium (II).



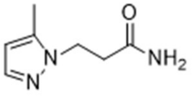
L1



L2



L3

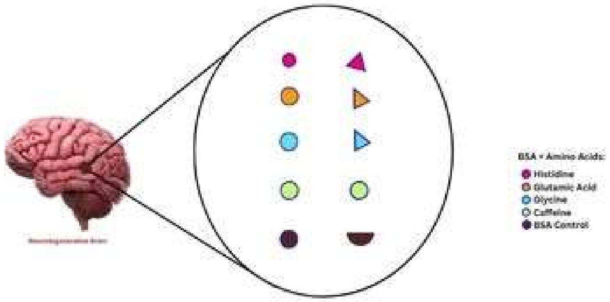


L4

Amino Acid Influences on Bovine Serum Albumin & Lysozyme Structure and Stability

Daphne M. Antwi and Gina MacDonald
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Neurological diseases have continued to be a critical issue for many Americans. Unfolded, aggregated proteins are characteristics of many neurological diseases. Previous research has demonstrated that changing the solution conditions of different proteins affects their structure, stability, and aggregation. Additional investigations have shown that different amino acids alter protein stability and aggregation. Previous studies in our lab have focused on how salts and metals specifically influence protein stability and aggregation. Most previous studies have used heat to denature proteins and observe how their structure changes with increasing temperature. This research investigated whether the incubation of the model protein Bovine Serum Albumin (BSA) with the addition of amino acids altered the structure and stability of the protein. Additionally, current research used model proteins BSA and Lysozyme to compare thermal induced unfolding changes to changes associated with prolonged incubation at 37° C. These studies used Circular Dichroism (CD) to monitor protein structural transitions. The CD results show that the presence of amino acids slightly alters protein structure and stability after incubation over time.



Scanning for Order: Can R-2-Butanol Behave on Ni(111)?

Jaimin J. Ashra, Kathrine B. Weinstock, Allen C. Shepherd, James T. Whitted, and Dr. Ashleigh E. Baber
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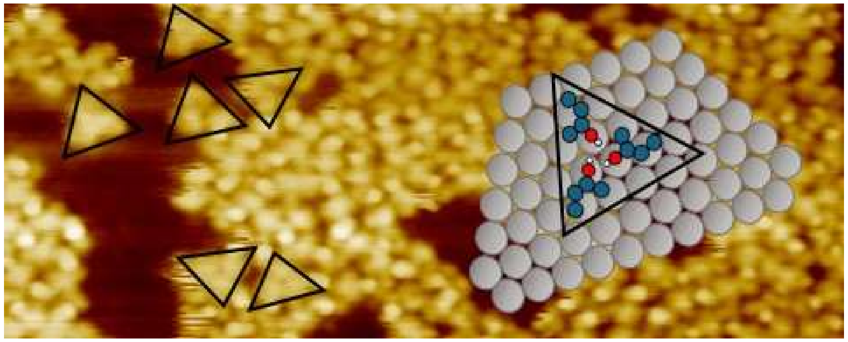
Self-assembly interactions play a vital role in natural processes such as the protein folding and micelle formation. To better understand the complexity of self-assembly, simpler model systems, such as small alcohols are often used. Previous studies have examined the self-assembly of alcohols such as R-2-butanol (R-2-BuOH) on Au(111), which forms long range, hydrogen-bonded tetramer networks. Au(111) is an inert surface with an oxophilicity of 0.0 that does not disrupt intermolecular hydrogen-bonding, allowing self-assembly interactions to dominate. To explore how surface reactivity affects self-assembly, scanning tunneling microscopy (STM) was employed to study R-2-BuOH on the more reactive Ni(111) surface. In addition to being more reactive, Ni(111) is also more oxophilic, with an oxophilicity value of 0.2. These properties result in stronger interactions between the surface and the hydroxyl group of the alcohol, which compete with intermolecular hydrogen-bonding among R-2-BuOH molecules. This competition between molecule-surface and molecule-molecule interactions interrupts long range order and inhibits self-assembly. STM imaging reveals these differences in adsorption and organization, highlighting how surface reactivity influences molecular self-assembly. Due to its higher reactivity, Ni(111) prevents extended ordering, allowing only short-range pockets of organized structures to form.



Optimizing the Distribution of Fruiting Agave on Bat-Friendly Tequila Plantations

Clarissa Azurin[1], Lois Carpenter[2], Grace Gorreck[3], and Dr. Alex Capaldi[4]
[1]Department of Mathematics & Computer Science, College of the Holy Cross
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Bat-friendly tequila plantations aim to feed pollinating bats like the Mexican Long-nosed Bat (*Leptonycteris nivalis*) by allowing a portion of their crop to flower at the expense of the final harvest size. We seek to determine if the spatial distribution of flowering agave has any impact on the number of bats a plantation could support, so that farmers interested in preserving nectarivorous bats could do so more efficiently. We created an agent-based model, a type of computer simulation, to study the interaction of *L. nivalis* bats and *Agave tequilana*. The model is informed by phenology and empirical parameters from the literature such as energetics. We compared four different spatial arrangements of flowering agave and determined spatial distribution does impact bat populations, with the most efficient arrangements yielding population estimates consistent with conservationist predictions, validating our model. Finally, the emergent bat carrying capacity of a plantation is directly proportional to the amount of flowering agave meaning that farmers need not worry about diminishing returns from their conservation efforts.

The Topology of Representation Varieties

Allen Bao, Jordan Larson, Kelson McBride, and Dr. David Duncan
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Representation varieties are geometric objects used to study symmetries. Our projects analyze various topological properties (e.g., the number of connected components) of several representation varieties. This talk will report on some of our results.

Refinement of X-Ray Diffraction Data of Gadolinium-doped Indium Tin Oxide Thin Films deposited by DC Magnetron Sputtering in FullProf Suite

Landon Brown[1], Dr. Masoud Kaveh[1], Dr. David Lawrence[2], Dr. Costel Constantin[1]
[1]Dept. of Physics and Astronomy, James Madison University
[2]Dept. of Integrated Science and Technology, James Madison University

In this study, we refined X-Ray Diffraction (XRD) data of Gadolinium-doped Indium Tin Oxide (ITO) thin films to observe any structural changes in the ITO due to varying concentrations of Gd-doping. The software used for the refinement of our data was FullProf suite, in which we used the LeBail method to extract and select peak intensities that are suitable to determine the atomic structure and refine the intensities of our films without considering structural parameters. Our analysis reveals a general increase in lattice constants as dopant concentration is increased due to Gd substituting in place of either Sn or In atoms, which is consistent with results from other studies we have reviewed. This insight gives more context to the role that Gd-doping concentration plays in ITO systems and shows the effectiveness of refinement techniques such as the one used in this study.

Aggregation of Short- and Ultrashort-chain Per- and Polyfluoroalkyl Substances (C1-C4 PFAS) by Donnan Dialysis

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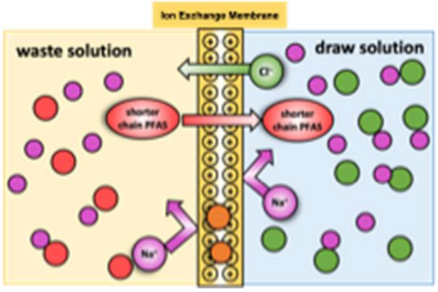
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Removal of ultrashort-chain Per- and polyfluoroalkyl substances (PFAS) has shown low efficiency with emerging adsorbents and ion exchange resins since they are highly mobile and less hydrophobic. Generally, with the existence of longer chain PFAS, the adsorption of ultrashort-chain PFAS is always inhibited due to competing effect. In this work, we employed Donnan dialysis, an ion exchange membrane process based on electrochemical potential gradient, to aggregate ultrashort-chain PFAS from waste solution to a cleaner draw solution for further target removal. A mixture of C1-C4 PFAS solution containing 500 ug/L of TFA, TFMS, PFPrA, PFEtS, PFPrS, PFBA and PFBS were prepared as waste solution, and 1 M NaCl solution was put in the draw chamber. Anion exchange membranes FAA-3-PK-130 (IEC = 1.30 ± 0.15 meq/g) and FAD-PET-75 (IEC = 1.40 ± 0.10 meq/g) were investigated in this process. It is observed that the kinetics of all PFAS removal from waste solution is rapid, confirmed by pseudo first order mechanism. In the draw side, interestingly, the aggregation rate of PFAS decreases when chain length increases, which can be attributed to the increasing hydrophobicity and higher selectivity of the longer chain PFAS. Therefore, ultrashort-chain PFAS diffuses quickly through the membrane while longer chain PFAS was stuck in the membrane, allowing ultrashort-chain PFAS to be target treated with selective adsorbents in our future work. Overall, this work highlighted, for the first time, selective aggregation of ultrashort-chain PFAS via ion exchange membranes for target treatment.



A WISE Look at Variability of Maser Galaxies

Erika Cherpes and Dr. Anca Constantin
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Current cosmological models for the fate of the universe and its geometry lack constraints that can be found with observations of powerful laser-like microwave emission (maser) from galaxy centers. These so called megamasers are however very rare, with detections in only about 3% of all surveyed galaxies. We explore here ways of efficiently detecting megamasers via a possible connection between this type of emission and accreting matter on supermassive black holes at galaxy centers, known as Active Galactic Nuclei (AGN). An important feature of AGNs is light variability, which can now be exploited with multi-epoch observations in mid-infrared from the Wide-field Infrared Survey Explorer (WISE). We present here results from our calculations and parameterization of the Structure Function for galaxies with and without maser emission, as a tool to identify and compare the most prominent variability features, and therefore AGN emission, associated with maser activity.

Analysis of Mouse Intrinsic Iridial Photoreceptors (IIPs)

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The eye is the sensory organ that initiates visual function in all vertebrate animals. Within the eye, the iris is a thin pigmented smooth muscule tissue layer that controls the amount of light entering the eye and protecting it from light-dependent photoreceptor degeneration. The actions of the iris are mediated through two light-dependent signaling pathways. The most characterized pathway involves photoreceptors in the retina sending light signals to the brain to drive iridial constriction. This neurological pathway controls a behaviour known as the pupillary light reflex (PLR). A lesser-known pathway found in sub-primate vertebrates is an intrinsic pathway, where photoreceptors within the iris tissue drive pupil constriction without input from the brain. Intrinsic iridial photoreceptors (IIPs) are the cells that initiate the light signaling to drive constriction activity. We hypothesize that this IIP driven pathway is a light signaling mechanism in the vertebrate iris that preexisted the neurological input that drives the PLR behavior. We have designed experiments to label the IIP cells in the mouse iris to measure their abundance and morphological dimensions. We have also begun to characterize structural overlap between the neurological and intrinsic pathways that drive pupil constriction. Our results show that a small subset of photoreceptive iris sphincter cells are sufficient to drive pupil constriction and suggest that there is structural convergence between the neurological and intrinsic signaling pathways in vertebrate iris.

Modulating the Thermal, Mechanical, and Flammable Properties of Chitosan Films with Polyol-Boric Acid Complexes

Olivia E. Coer and Dr. Brycelyn Boardman
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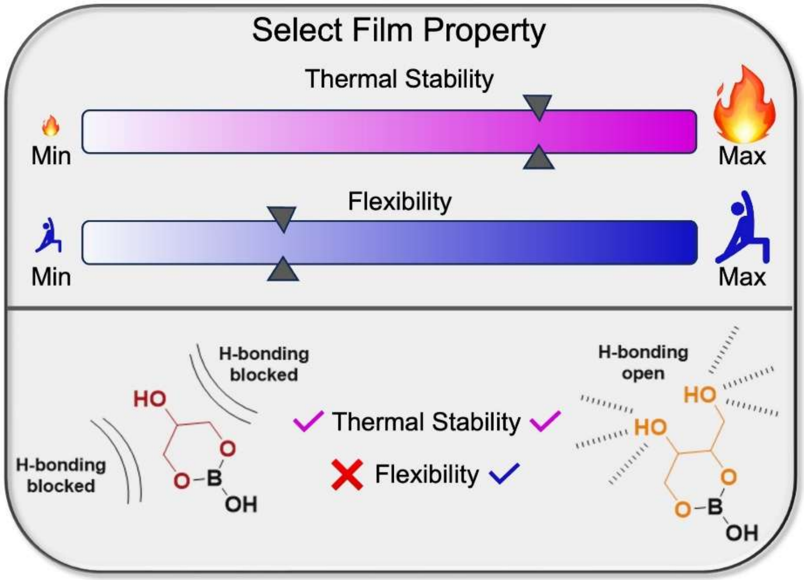
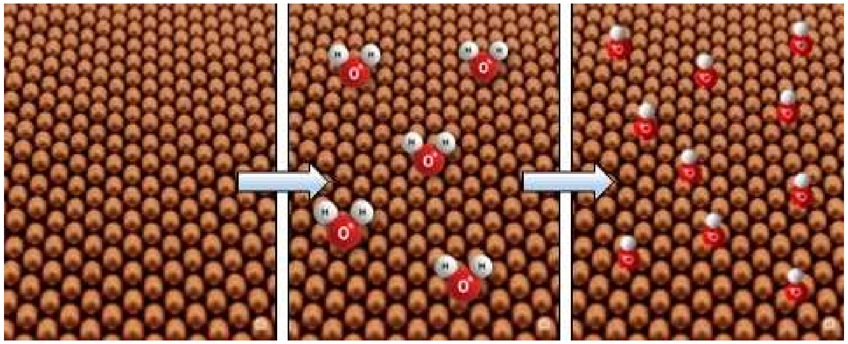
Chitosan, a natural biopolymer derived from the exoskeletons of crustaceans, is an eco-friendly alternative to petroleum-based plastics that are widely used today. However, optimizing the properties of chitosan materials with plasticizers to fit particular applications remains a significant challenge. Here, we report the ability to control the binding potential of alcohol-rich plasticizers with boric acid. Polyols can form neutral complexes with boric acid (BA) that alter the hydrogen-bonding face of the plasticizer, resulting in changes to the effectiveness of the plasticizer. Glycerol-BA and erythritol-BA systems were previously studied to investigate the impact of increasing the polyol chain from 3 OH to 4 OH units. In chitosan, films with glycerol-BA complexes displayed a decrease in flexibility and an increase in thermal stability, whereas films containing erythritol-BA complexes showed an increase in both thermal stability and flexibility comparatively. Linear polyols xylitol, sorbitol, and mannitol contain 5 and 6 OHs, respectively. Films containing each polyol were prepared with increasing concentrations of BA (0.5 eq - 2 eq). Structural, thermal, and mechanical characterization of the films were performed using ATR-FTIR, TGA, DSC, and DMA. Xylitol-BA-containing films exhibited increased flexibility when compared to erythritol-BA with a decrease in Young's moduli at all concentrations, while the thermal stability was maintained. However, the stereoisomers mannitol and sorbitol do not show the same trends, exhibiting inconsistent behavior with an increase in BA concentration. This may be due to the complex mixture of neutral boron complexes as a result of the increase in polyol length. Additionally, all films were tested for flame retardancy by exposing them to an open flame and establishing whether they were capable of self-extinguishing. In the absence of BA, all films at various polyol concentrations (25 mM - 100 mM) ignited and burned completely indicating no correlation between polyol length and flammability. Similar tests were performed with all polyols at increasing concentrations of BA, results showed that most films containing 0.5 and 1 eq of BA self-extinguished, while films containing 2 eq of BA did not ignite. The combined results demonstrate the ability of BA to modulate the specific hydrogen-bonding interactions between the plasticizer and the polymer resulting in tunable, thermal, mechanical, and flammable properties of chitosan materials.



Unraveling the Initial Steps of Water Dissociation on Cu(111)

David W. Compton Jr, James T. Whitted, Katherine B. Weinstock, Jaimin J. Ashra, Emily M. Euler, Allen C. Shepherd, and Dr. Ashleigh Baber
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Copper is used in a wide range of catalytic applications, such as selective epoxidation, but results in overoxidation of reactants to combustion. Cu catalysts often depend on promoters, including Cl, Na, and Cs to reduce CO_2 emissions and enhance selectivity. However, these promoters pose environmental risks. Alternative materials have been explored to improve catalytic performance without relying on environmentally harmful promoters. The addition of Ag to Cu catalysts boosts epoxidation without the use of promoters. While Ag(111) is highly selective for epoxidation, it has a high barrier for O_2 dissociation. Cu, on the other hand, easily oxidizes. The reactive oxygen species for epoxidation are not well understood on AgCu catalysts. Exploring atomic oxygen and hydroxyl species for epoxidation will uncover the reactive oxygen necessary for selective reactions on AgCu. To systematically investigate the adsorbed atomic oxygen and hydroxyl species on model catalysts, experiments were conducted first on a Cu(111) surface. Cu(111) readily dissociates O_2, forming atomic O on the surface, yet due to a high energy barrier, Cu(111) cannot easily dissociate H_2O. Water desorbs molecularly from Cu(111) with zero-order kinetics and a T_{des} = 145-157 K. Molecular oxygen can be dosed at room temperature to promote H_2O dissociation on O/Cu(111), forming a hydroxylated surface. Temperature-programmed desorption (TPD) experiments under ultra-high vacuum (UHV) conditions show that atomic oxygen increases the desorption temperature of water by 12-15 K, stabilizing OH on the surface. The higher desorption temperature results from hydroxyl groups on the surface undergoing disproportionation. These results suggest that the stabilization of hydroxyl on the O/Cu(111) surface makes it a viable reactive oxygen species for the study of epoxidation on model catalysts. [Graphical abstract generated by Gemini AI and then modified.]



Aerodynamic Efficiency at Variable RPM: Theoretical Comparison Study Between Propellers and Impellers with Computational Fluid Dynamics

Drew Cutright[1] and Dr. Costel Constantin[2]
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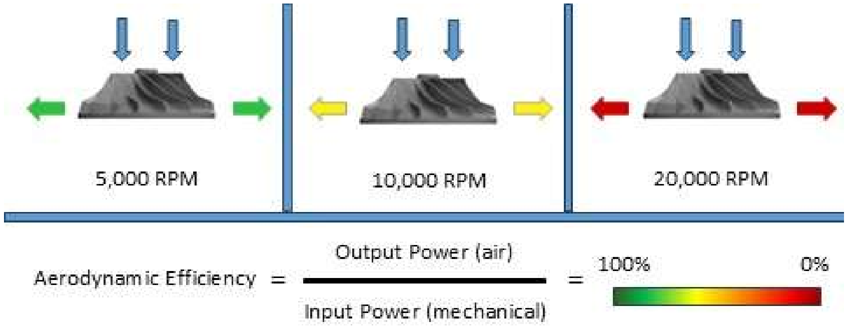
Propellers and impellers generally have applications in moving volumes of liquid or gas, such as in aerospace, compression systems, and cooling systems. Propellers push the air along one axis. Impellers take in air axially and, by enacting centrifugal forces, emit the air radially. Propellers are used in applications requiring thrust, while impellers are used in centrifugal compression systems such as automotive turbochargers and air compressors. Although there are differences in applications, this study aims to investigate the trends in aerodynamic efficiencies over eight design points involving a set of rotation per minute (RPM) values and draw conclusions on their trends. Aerodynamic efficiency is a means of calculating the ratio of the effective output power by the input power of the system and, therefore, determining how effective the system is at transferring rotational kinetic energy to the pressure, density, and velocity of the air. Energy can be lost through heat, turbulence, and phenomena like surge, which is a violent reciprocation of airflow reversing directions due to downstream and upstream pressure differences.



Modeling Probiotic Bacterial Control of White-Nose Syndrome in Little Brown Bat Colonies

Bethany Droubay and Dr. Alex Capaldi
Department of Mathematics & Statistics, James Madison University, Harrisonburg, VA 22807

Since 2006, white-nose syndrome (WNS) has been spreading across North America, devastating many bat species and killing millions of individual bats. WNS is caused by the invasive psychrophilic fungus *Pseudogymnoascus destructans* (*Pd*), which grows well in caves and on bat skin during cold seasons. The little brown bat, *Myotis lucifigus*, is a species severely harmed by the disease, experiencing 90-100% mortality in many colonies. In 2019, a bacterial probiotic using *Psuedomonas fluorescens*, an antifungal bacterium naturally present in the bat skin microbiome and cave environments, was field-tested as a control method against WNS, and shown to be effective in enabling survival among treated bats. We analyze the effects of implementing this probiotic as a long-term control for WNS by adapting a mathematical model based on the phenology of little brown bats to include a class of bats treated with the probiotic alongside a class of untreated bats. We also compare the effectiveness of application magnitude and perform a sensitivity analysis to support our results. We find that a probiotic control using *P. fluorescens* is theoretically effective in mitigating the severity of the outbreak of WNS and has the potential to restore populations of little brown bats.

Optimization of recombinant protein expression with MALDI-MS

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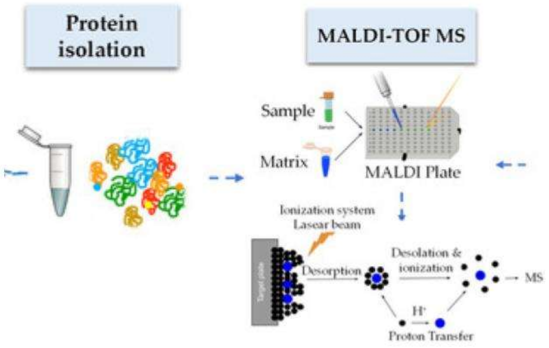
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

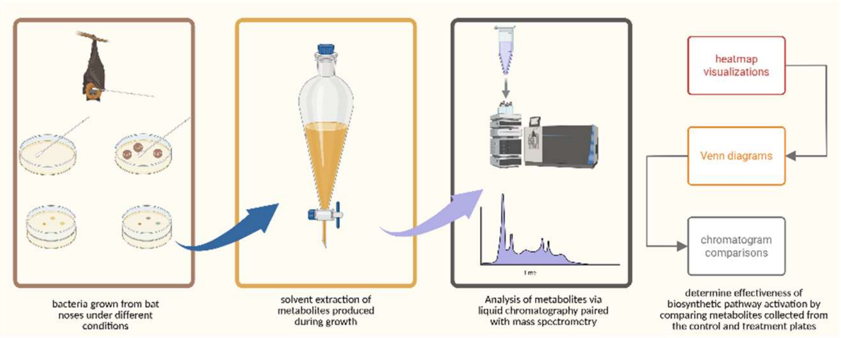
Recombinant protein expression enables the production of specific proteins by introducing target genes into non-native host organisms, a process with broad applications in research, medicine, and biotechnology. Optimization of protein expression is essential for reproducible and cost-effective large-scale protein production. This study aimed to optimize conditions for the expression of PpcA, a 3-heme cytochrome native to *Geobacter sulfurreducens,* using *Escherichia coli* as the host system and matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) for protein detection. Variables including growth duration, IPTG concentration and induction time, buffer composition, and sample loading volume were evaluated. Based on our MALDI-MS analysis, the optimal PpcA expression was achieved with 22–23 hours of cell growth at 30°C, 6–8 hours of induction with 20-100 μM IPTG, 1:2 (v/v) ratio of salt-containing lysis buffer to bacterial culture volume, and 1.5 μL of protein solution per MALDI-MS sample spot. These results provided not only the most reproducible MALDI-MS data, but also demonstrated the highest PpcA expression yield.



Response of Secondary Metabolism of Bat-Associated Bacteria to Chemical Stimuli

[1]Landon Gray, [2]Max Tyree, [3]Elijah Fernands, [4]Dr. Paris Salazar-Hamm, and [2]Dr. Lindsay Caesar
[1]Dept. of Biology, James Madison University
[2]Dept. of Chemistry and Biochemistry, James Madison University
[3]Dept. of Health Sciences, James Madison University
[4]Dept. of Biology, New Mexico Tech

Microbial natural products, small molecules that are not essential to survival but rather provide a competitive advantage, are a pivotal source of medicinal lead compounds with diverse biological activities including antifungal, antibacterial, and anti-cancer activities. Genomic studies have revealed the vast biosynthetic potential of microorganisms, but most biosynthetic pathways responsible for producing natural products are turned off under laboratory conditions. To overcome the limitations of traditional culturing methods, we took advantage of the “One Strain Many Compounds” (OSMAC) approach, in which culture conditions are altered to activate previously silent biosynthetic pathways. To maximally express natural products in twelve strains of bat-associated bacteria, we grew bacteria under standard conditions, with the histone deacetylase inhibitor suberoylanilide hydroxamic acid (SAHA), or with lanthanum (III) chloride. Chemical changes were evaluated using mass spectrometry-based metabolomics. In the twelve strains under study, 3 strains were significantly impacted by treatment with SAHA. Treatment with lanthanum led to less notable impacts, though 12 metabolites were identified as potentially upregulated with this treatment. Using publicly available natural products databases, we have putatively identified 21 molecules that are reproducibly upregulated or completely unique to SAHA- or lanthanum-treated cultures. Future studies evaluating the impact of scandium (III) chloride and N-acetylglucosamine will be to reveal stimulus-induced production of natural products from bat-associated bacteria.



Customizable R Shiny Application for Analysis and Visualization of Public Retinal Transcriptome Data

Benjamin D Grossman[1] and Dr. Ray Enke[1,2]
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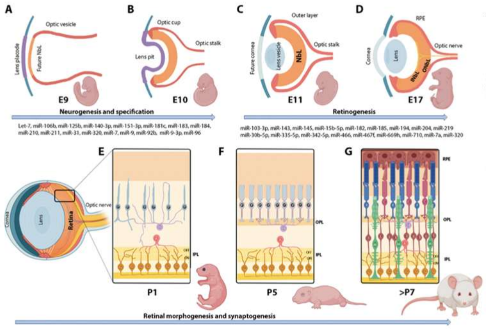
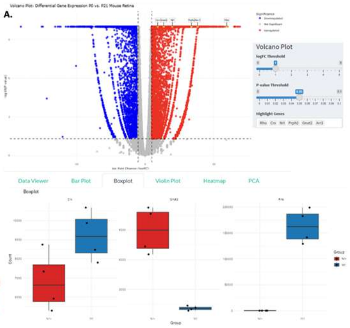
The mouse retina undergoes complex developmental changes marked by dynamic shifts in gene expression, particularly during photoreceptor (PR) neuronal development. Although large-scale retinal transcriptome data are publicly available, the tools needed for effective analysis and visualization often pose a barrier to many researchers. To address this, we developed a customizable, user-friendly R Shiny application that enables exploration of bulk RNA-seq datasets through interactive dashboards where no coding experience is required. Utilizing open-access mouse retina transcriptome datasets spanning embryonic to postnatal stages, our app integrates differential gene expression (DGE), gene ontology (GO), KEGG pathway enrichment, principal component analysis (PCA), and K-nearest neighbor (KNN) clustering. The application reveals key developmental patterns, such as the postnatal upregulation of general PR, cone-specific, and rod-specific genes (e.g., *Rho*, *Gnat2*, *Crx*), as well as the cone-dominant phenotype of *Nrl*-knockout retinas. This platform supports reproducible, intuitive analysis of bulk RNA-seq data and is especially well-suited for educational settings and early-stage researchers seeking to expand their skills in bioinformatics.





Assessing birdsong frequency measurements of sample size, window-sample rate, and timing of frequency shifts in a noise experiment with Gray Catbirds *Dumetella carolinensis*

Erin Naman, Juliane A. Calvert, Anna E. Williams, Ethan Dray, Jackson Vickers, Eriberto Osorio, and Dana L. Moseley
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Measuring song in the context of anthropogenic noise can be difficult to do accurately and precisely especially when the focal species is a complex, continuous singer and vocal mimic. Gray catbirds imitate, improvise, and invent sounds within their song bouts which can last from three syllables to three minutes without a 1-second break. In the context of an immediate flexibility experiment in which we recorded freely singing catbirds for 1-3 minutes (pre-noise) and then played back low-frequency “urban” noise, we investigated three questions: 1) How many song elements are necessary to obtain an accurate and precise measure of song minimum frequency? We used a bootstrapping method in R and found that 100 song elements yields a frequency similar to a large sample. 2) Is there a significant difference between processing with a window-sample size of 512 or 1024 when measuring minimum frequency? While there are slight differences, minimum frequency did not differ significantly between windows of 512 vs 1024. 3) How long does it take catbirds to adjust their minimum frequency in response to low-frequency noise playback compared to pre-noise? Catbirds adjusted their frequencies nearly immediately and within the first 1-min of playback. These methodical explorations confirm that we are adequately sampling a sufficient amount of catbird song, using the correct sampling parameters within spectrographic analysis, and show the immediacy with which catbirds adjust their songs in response to urban noise.

Analyzing the accuracy of AI-powered bird identification systems during the 2021 emergence of 17-year cicada brood

Anna Williams[1], Lydia Ritchey[1], Kylie Bailey[1], Bernard Lohr[2], David A. Luther[3], Brian S. Evans[4], and Dana L. Moseley[1,4]
JMU[1], UMBC[2], GMU[3], Smithsonian Migratory Bird Center[4]

Acoustic communication is vital for mediating territory defense, mate attraction, and predator avoidance. However, communication can be disrupted by acoustic interference from natural and anthropogenic sources. Mass emergences of periodical cicadas, such as 2021 Brood X, create significant interference with their loud choruses overlapping avian vocal frequencies. This study investigates how bird communities adjust vocal strategies in response to cicada-generated acoustic disturbances using Automated Recording Units across cicada-active and inactive years in the Mid-Atlantic. Initial analyses reveal variability in species detection accuracy by automated software (BirdNET, Merlin) during cicada emergence. Preliminary results suggest training BirdNET for target species significantly enhances detection accuracy. Recordings are quantitatively assessed to determine if birds alter song frequencies or reduce singing duration during cicada activity. Confirming these behavioral changes would demonstrate short-term adaptive plasticity and avian resilience to intense natural acoustic interference, informing conservation efforts amid increasingly noisy ecosystems.

STUDENT ABSTRACTS
Poster Session: Group B

Listed in alphabetical order by presenter's last name
(Student presenters underlined)

Aggregated induced emission of quinazoline derivatives in the presence of glucosamine and chitosan

Caitlin Gutierrez, Stephanie Schwender and Dr. Brycelyn Boardman
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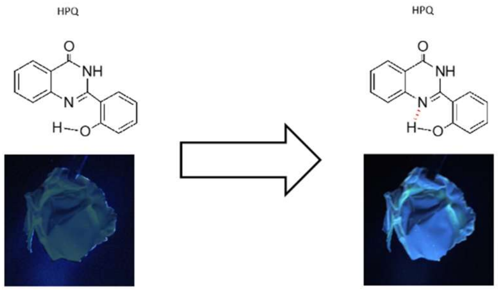
Antisense Amine sensing bio-plastics are potentially powerful materials that can help solve the food and plastic waste crises simultaneously. Quinazoline derivatives, acetylated 2-(2-hydroxyphenyl)quinazolin-4(3H)-one (HPQ-Ac) and 2-(2-hydroxyphenyl)quinazolin-4(3H)-one (HPQ) have previously been studied as amine sensors. In the presence of amine vapor, HPQ-Ac is converted to HPQ, which promote aggregation-induced emission (AIE) in HPQ turning the sensor to the "on" state. HPQ-Ac was incorporated into chitosan films, however these films fluoresced in the absence of amine. To further investigate the lack of an "off" state of the sensor in these materials, glucosamine (GlcN), the repeat unit of chitosan, was used as a model system. Fluorescence and nuclear magnetic resonance (NMR) spectroscopy were used to investigate these interactions. The model system has elucidated that there are strong interactions between HPQ-Ac and GlcN which are likely the cause of the observed AIE in the chitosan films. Additional quinazoline derivatives were prepared to investigate the impact of hydrogen bonding capability and steric bulk on the interaction of these sensor molecules with GlcN and chitosan. 2-(Phenyl)quinazolin-4(3H)-one (PQ), acetylated 2-(2-hydroxy-3,5dit-butylphenyl)quinazolin-4(3H)-one (BPQ-Ac) and 2-(2-hydroxy-3,5dit-butylphenyl)quinazolin-4(3H)-one (BPQ) were prepare under similar reaction conditions to HPQ and HPQ-Ac. Even in the absence of hydrogen bonding capabilities, PQ still displays fluorescence intensity in solution, in the presence of GlcN, in chitosan solution and films. This result suggests that hydrogen bonding interactions with the chitosan chains are not responsible for the "on" state of the fluorophore, but that the molecule is capable of pi-pi stacking that initiates the AIE. Both BPQ and BPQ-Ac have reduced fluorescence intensity in solution when compared to HPQ and PQ. Interestingly, BPQ shows an increase in fluorescence intensity in the presence of GlcN while BPQ-Ac does not. Additionally, chitosan films containing BPQ-Ac have a significantly reduced emission intensity compared to other derivatives. These films were then exposed to amine vapor and fluorescence was turned "on" These combined results indicate, that steric bulk is the most promising structural modification for use of quinazoline derivatives as sensors in chitosan films.



Development of novel cellulose-based micromotors for maximal nutrient recovery from poultry litter

Keyvan Harris, Sarah Vollbrecht, Bella Fong, Hui Chen
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Nutrient pollution from animal manure significantly contributed to eutrophication and aquatic dead zones due to excessive nitrogen and phosphorus. Simultaneously, global phosphorus reserves are rapidly consuming, and the Harbor-botch processes for ammonia production is energy intensive. Hence, there is the critical need for sustainable nutrient management strategies. In this work, we targeted poultry litter as the manure sample, in which NH4+, H2PO4- and urea are main source of nutrient. Novel cellulose-based micromotors with urease modification were developed to enhance nutrient recovery from poultry litter. First, cellulose was oxidized to 2,3-dialdehyde cellulose (DAC), subsequently, urease was grafted onto the DAC based on Schiff base reaction. The DAC-urease composite was well characterized with FTIR, powder XRD and SEM. The content of aldehyde groups and modified urease were determined by titration and urease assay, respectively. The resulting composite with 75% aldehyde contents and 50% urease modified rapidly reacted with urea in the poultry litter slurries to produce NH_3 and CO_2 gas, which is the driving force of the micromotors. NH3 gas dissolved to form NH_4^+, the total NH_4^+ ions (monitored by ion chromatography) throughout the experiment were increasing until the micromotors were not moving, indicating constant nitrogen release from poultry litter to aqueous phase. Additionally, these micromotors are effective to reduce the presence of solids and organic matter, thereby minimizing membrane fouling issue when further implemented to membrane techniques. This work highlighted, for the first time, the efficacy of employing urease-modified cellulose-based micromotors for advancing sustainable nutrient recovery from animal manure waste.

Understanding Oxophilic Pathways of Enhanced Epoxidation Reactions by Optimizing Bimetallic AgCu Catalysts

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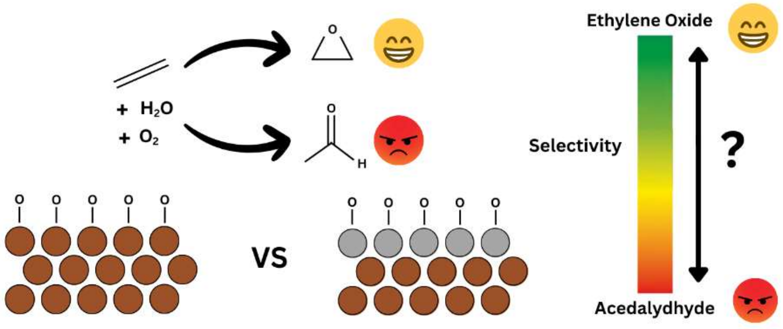
Ethylene epoxidation is a major industrial process that traditionally utilizes Ag or Cu catalysts; however, this reaction requires promoters that are often expensive and toxic (Cl, Na, Cs) to increase selectivity and reduce greenhouse gas emissions. Recently, AgCu bimetallic catalysts have gained attention as a potential solution due to copper's oxygen dissociation properties and silver's favorable selectivity, but many questions regarding their mechanics and functionality remain. DFT (Density Functional Theory) is a quantum mechanical approach to determining the ground state and relative energy of a given system by calculating the electron density distribution. Previous DFT studies have shown that the easily oxidizing nature of Cu (111) can help promote epoxidation since Ag does not easily oxidize; however, too much O coverage increases combustion (producing CO_2). Our goal is to determine whether a heterogenous AgCu catalyst could provide an optimal amount of O coverage and lower activation energies to allow more selective epoxidation. Preliminary results from TPD (temperature-programmed desorption) experiments indicate that the addition of water plays a role in the oxidation of Cu (111), and DFT can provide an atomic-scale model for this process. This project's joint theoretical and experimental approach offers insights into commercial-scale application of bimetallic catalysts for epoxidation, ultimately increasing industrial efficiency and reducing environmental impact.



Mycological Resilience: Evaluation of Heavy Metal Tolerance in Grand Caverns

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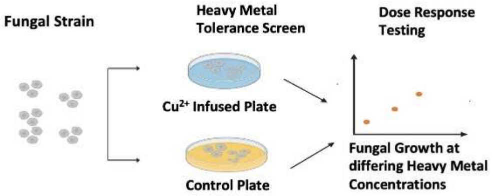
Over the last 40 years, there has been a shift from the theory that subterranean environments are lifeless and unchanging with the discovery of diverse microbial communities that have adapted to survive and thrive in these extreme environments over millions of years. Caves and karst systems contain heavy metals due to both natural and anthropogenic reasons, and fungi tolerant of heavy metals and metalloid compounds may have the potential for bioremediation use once they are isolated from subterranean ecosystems. The Shenandoah Valley has a history of improper disposal of heavy metal waste by commercial businesses, which has led to the Shenandoah River being designated as a Superfund site by the Environmental Protection Agency. Heavy metals pose a significant risk to public safety for all humans, animals, and living organisms in the environment. The effective detoxification and removal of metal contaminants from polluted environments has increasingly moved towards bioremediation by specialized microorganisms as a sustainable solution to mitigate the negative environmental impacts of mining. In an effort to identify subterranean fungi with unique bioremediative potential, we isolated and screened 17 fungal strains from Grand Caverns for heavy metal tolerance using chloride salts of copper, nickel, cadmium, and manganese. After three heavy metal tolerance screens with increasing concentrations of heavy metal salts, three strains were selected for dose-response testing to establish the maximum concentration of heavy metals the organisms can withstand. Following dose-response testing, heavy metal bioaccumulation will be quantified using ICP-OES to evaluate the bioremediative potential of fungi from Grand Caverns.



Exploring Interactions between Glucosamine and Differing Plasticizers through Electronic Structure and Molecular Dynamics

Elanor K. Kirkland and Dr. Isaiah Sumner
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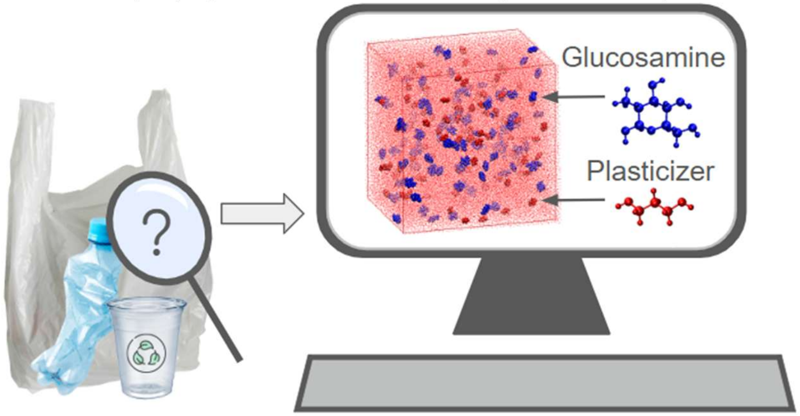
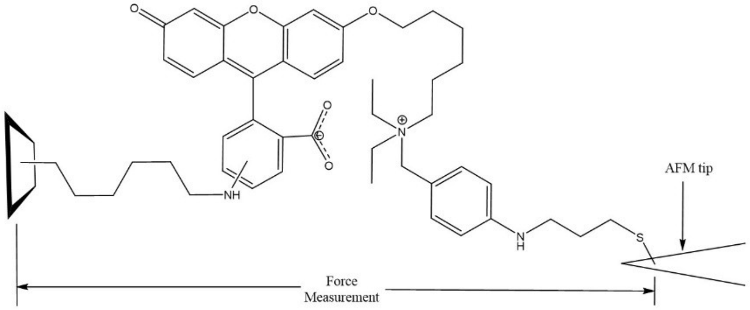
Chitosan based bioplastics have emerged as an alternative to traditional petroleum based synthetic polymers due to their biodegradability and renewable sources. One promising bioplastic is made from two main parts, chitosan – an abundant biopolymer derived from chitin found in the exoskeleton of arthropods – and a plasticizer – an additive that can change the physical properties of chitosan. However, the molecular interactions between the chitosan and the plasticizer, as well as how they affect the bioplastic's properties, remain poorly understood. To address this, we previously performed computational experiments to quantify the interactions between β-D-glucosamine (the base unit of chitosan) and several polyol plasticizers (glycerol, 1,2-propanediol, 1,3-propanediol, and ethylene glycol). To understand the molecular-level interactions between these diols and glucosamine, and to find the most stable structures, optimization and frequency calculations were run using the M06-2X density functional combined with two basis sets: 6-31+G(d) and 6-311+G(2d,p). Results indicated that the diols seem to drive glucosamine aggregation. To further advance this research, molecular dynamics simulations are being used to investigate the dynamic behavior of the interactions between chitosan and glycerol. Several different concentrations ranging from 50mM to 200mM glucosamine and glycerol in water provide deeper insight into how these components interact in a larger, more complex system. However, due to limited intermolecular interactions, the results of these simulations were inconclusive, prompting future research conducted with higher concentrated systems.



Synthesizing a Contractile Molecule Using Fluorescein & a Quaternary Ammonium Compound for Atomic Force Microscopy

Ingrid Larne, Dr. W. Christopher Hollinsed
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

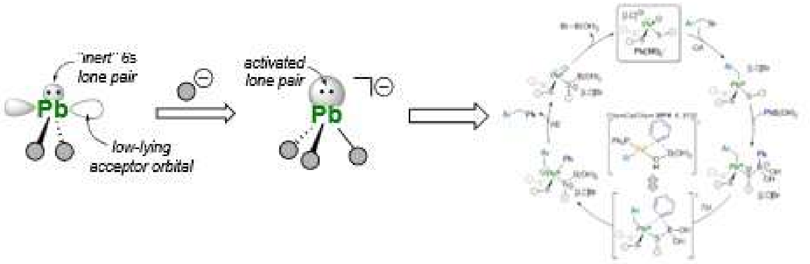
The Hollinsed lab is working closely with fluorescein and an original quaternary ammonium compound, 6-bromohexyldiethyl-(4-nitrobenzyl)ammoniumbromide, in order to synthesize a contractile molecule known as Fluorescein-O-hexyl-6-diethylnitrobenzylammoniumbromide. The 3-step synthesis consists of: (1) electrophilic aromatic substitution using 3-substituted phthalic anhydride with resorcinol to give the substituted fluorescein, (2) alkylation of a dialkyl amine to provide a tertiary amine, and (3) Menshutkin reaction to make the quaternary ammonium salt. When the molecule is completed, the strength of the attractive force will be measured using Atomic Force Microscopy (AFM). The intention is to polymerize this monomer unit and create a chain that can attract and repel / contract and relax from end to end on command, not unlike an artificial muscle. Next steps include attaching a sulfur group and an amino group to prepare the molecule for AFM. The sulfur group will be used to attach the molecule to the gold AFM tip. The amino group will mount the molecule to the gold AFM plate. To confirm the structure and purity of the molecules, ^{1}H NMR and ^{13}C NMR spectroscopy are utilized.



Creating Novel Molecular Plumbates as Potential Catalytic Anions

Alexander F. Lauer, Dr. Jun Yin, and Dr. J. Connor Gilhula
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Lead (Pb), is one of the most abundant elements in the Earth's crust, is well poised to overcome the challenges presented by precious metal shortages caused by current geopolitical tensions if compounds that exhibit Pb^{II}/Pb^{IV} redox cycling can be established. Molecular plumbates are tricoordinate, anionic organolead species that are known to react as Pb nucleophiles that have potential to induce a catalytic cycle similar to platinum and palladium. These lead plumbates would present a more cost-effective and sustainable catalyst for the formation of carbon-carbon bonds than the current precious metal alternatives. We have taken on the challenge of "resurrecting" these under-investigated compounds by expanding the scope of known plumbates in a synthetic chemistry campaign. We found that homoleptic trithiolatoplumbates are formed by treating polymeric, insoluble $Pb(SR)_2$ with a suitable thiolate salt in methanol. So far, three molecular plumbate anions have been successfully created with this procedure. We have identified these compounds unambiguously by ^{207}Pb NMR spectroscopy, which is a new analytical capability that we have established for JMU. Future work will investigate the synthesis, characterization, and reactivity of tricoordinate lead organochalcogenides. We envision that these preliminary studies will represent a first step towards establishing a catalytic cycle that is hypothesized to be similar to a Sizuki-Miyaura palladium catalyzed cross coupling at a mononuclear Pb center.



Characterizing Small Molecule/Desmoplakin Interactions that Prevent Protein Degradation

Lucille McGinnis and Dr. Nathan T. Wright
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Desmoplakin is a protein in the desmosome that plays an integral role in connecting the intermediate filaments from one cardiomyocyte to another. Some desmoplakin mutations have been linked to arrhythmogenic cardiomyopathy and fragile skin disease. Specific mutations in DSP (R451G, S507F, S442F, and S299R) result in hypersensitive cleavage in the presence of the protease calpain. To block this cleavage event, we have screened drugs for their ability to specifically inhibit calpain-dependent DSP degradation. STD-NMR experiments further confirm that 12 of the drugs bind to DSP in the µM range. Here we begin studies designed to interrogate where the most promising drugs bind to desmoplakin, using biomolecular crystallography experiments.

Understanding the impact of polyol stereochemistry on plasticized chitosan film morphologies using scanning electron microscopy

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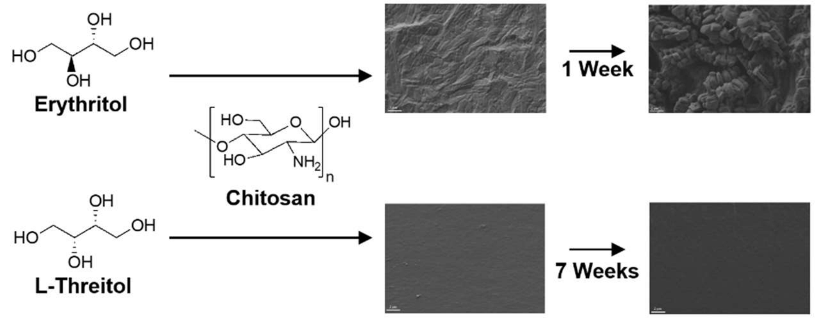
Correlating physical and mechanical properties to surface morphologies can be very challenging in complex polymer systems whereas cross-sectional images are much more valuable. Herein we describe the investigation of both surface and cross-sectional morphologies of chitosan films plasticized with the stereoisomers L-threitol (L-Thr), and erythritol (Ery) in the presence and absence of boric acid (BA). Our previous results have shown that the addition of glycerol reduces the pore-like structures observed in pure chitosan films, while the addition of BA to the system yields a more uniform morphology and reduction of pore size. SEM images were collected overtime on the same chitosan film samples which contained increasing amounts of the polyols (25 mM-100mM). Visible aging of the films from transparent to opaque was correlated to the increasing presence of microstructures on the surface and cross-section of the films in the SEM images. L-Thr films displayed significantly different rates of microstructure formation compared to Ery, indicating that stereochemistry does play a role in the interaction of the polyol with the chitosan chains and the migration of the polyol through the polymeric network. Similar experiments were performed with films containing chitosan, polyols (25 mM-100mM) and the addition of BA (0.5 eq-2.0 eq). SEM images indicate that as BA equivalents are increased, the aging process is inhibited, with little to no microstructure formation observed, even at extended time points. Differences in the pore-sizes were also observed when compared to previously studied Glycerol-BA films. Both L-Thr-BA and Ery-BA containing films showed a significant reduction in pore-size and an increase in the smoothness of the cross-sections. Additional films containing stereoisomers sorbitol and mannitol also revealed significantly different cross-sectional morphologies, further supporting that the stereochemistry of the polyol does impact the interactions between the plasticizer and the chitosan chains even in extended polyol systems. This study continues to aid in our development of a methodology for tuning and optimizing chitosan materials.



Regulating Protein Synthesis: A Novel Synthesis for Antisense Oligonucleotide Analogs

Emily Nattress, Tengis Tamir, Tristan Bossidy, William Brown, and Dr. Debra Mohler
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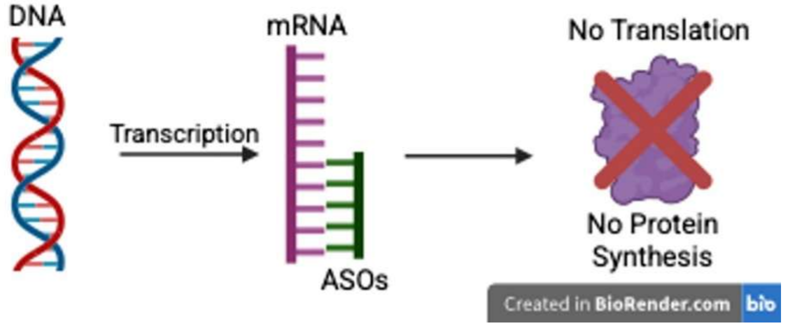
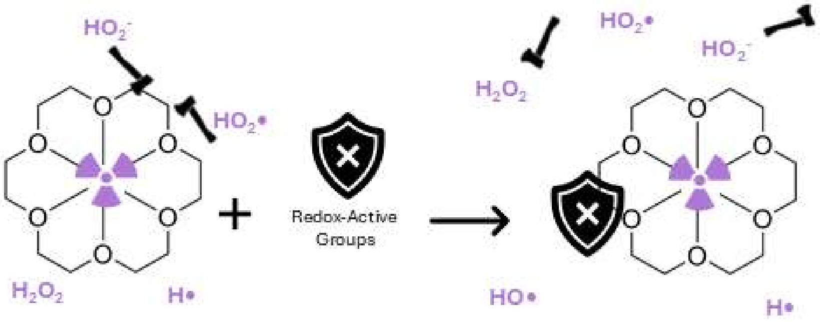
Antisense oligonucleotide analogs (ASOs) are synthetic modified DNA or RNA molecules with the ability to modulate gene expression by binding to messenger RNA (mRNA) to inhibit protein synthesis. ASOs are emerging as a promising strategy for eliminating genetic diseases and genetic mutations by regulating gene expression. ASOs come with challenges like degradation and membrane permeability, to aid these challenges a novel synthetic strategy to attach a seven membered carbon ring to the nucleoside analogs were performed and characterized Adenine, Cytosine, Guanine, and Uracil. To form the ASOs, a DNA template will also be synthesized utilizing protecting group chemistry. Currently protected deoxyadenosine and deoxyuridine have been successfully synthesized.



Synthesis and Metal Complexation of Regenerative Chelators for Targeted Alpha Therapy

Andrew A. Neumann, Alexander F. Lauer, and Dr. J. Connor Gilhula
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

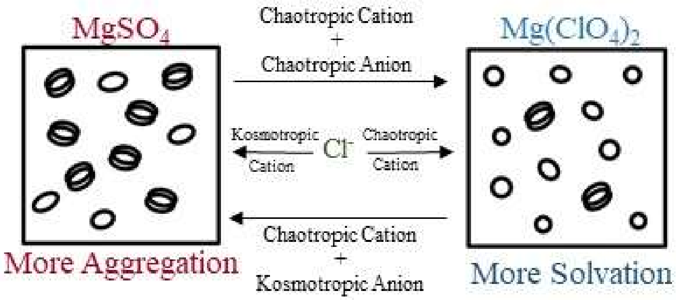
New advances in radiotherapy are moving further down the periodic table in search of innovative approaches to cancer treatments. Targeted alpha therapy is one such method that uses high energy alpha particles from the radioactive decay of chelated (i.e., complexed) atoms to attack cancerous tissue, leaving neighboring cells largely unharmed. However, few chelators in aqueous environments can withstand the effects of ionizing radiation without breaking apart and releasing their radioactive isotope due to the creation of reactive oxygen species (ROS). To address this problem, we have made progress toward novel dibenzo-18-crown-6 derivatives that utilize redox-cyclable anthraquinone and metalloporphyrin groups to catalytically neutralize ROS. Initial experiments were successful in rapidly binding non-radioactive surrogates La^{3+}, Ba^{2+}, and Sr^{2+} to a simplified phosphonate-substituted macrocycle. We established a new radioanalytical capability (radio-TLC) at JMU to demonstrate that ions of uranium-238 are also bound by this crown ether derivative. Future work in the project will consist of completing our proposed synthesis of redox-active complexing agents, evaluating their stability under radiolytic conditions at Madison Accelerator Laboratory, and binding clinically suitable isotopes like radium-223 and actinium-225 to these self-regenerative chelators.



Hofmeister Cation and Anion Effects on Caffeine Solvation and Aggregation

Cameron Page, Gina MacDonald, Yanjie Zhang
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

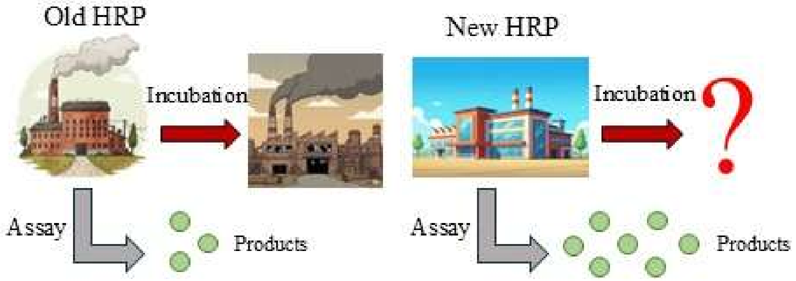
The Hofmeister Series is a list of ions ranked based on their ability to salt in or salt out proteins. Caffeine was used as a model compound to investigate how different combinations of various kosmotropic and chaotropic ions influence caffeine solvation and aggregation. Anionic effects on caffeine have been previously studied in depth, however fewer studies have been performed using cations. Attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) was utilized to study the relative solvation or aggregation of the caffeine molecules in solution with various salts. Our results demonstrate that a chaotropic cation with a chaotropic anion ($Mg(ClO_4)_2$), leads to a decrease of the two carbonyl stretching peaks at ~1698 cm^{-1} and ~1638 cm^{-1}, indicating increased caffeine solvation. On the other hand, a chaotropic cation with a kosmotropic anion ($MgSO_4$), leads to an increase of the two peaks, indicating increased caffeine aggregation. Our results suggest for most combinations that the anionic effects dominated the cationic effects, with the exception of the chloride anion. As expected from previous studies, kosmotropic anions (SO_4^{2-}) lead to the most caffeine aggregation, and chaotropic anions (ClO_4^-) lead to more caffeine solvation. Interestingly for the chloride anion, our results showed that the cationic effects dominated the anionic effects, with kosmotropic cations (NH_4^+, Na^+) increasing caffeine aggregation and chaotropic cations (K^+, Mg^{2+}) increasing caffeine solvation.



Monitoring The Structure, Stability, and Activity of Horseradish Peroxidase Over Time

Lilija Pflanz, Linette Watkins, and Gina MacDonald
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg VA 22807

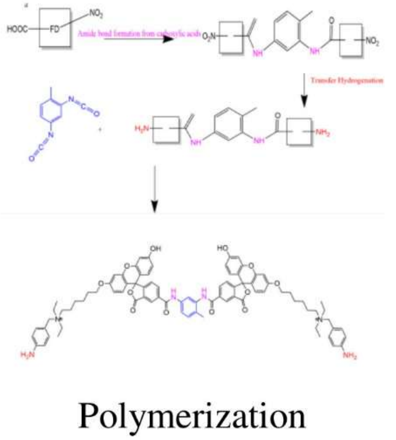
Proteins and enzymes are vital for brain and bodily function. Protein misfolding and aggregation can alter the progression of neurodegenerative diseases. Many studies have used Circular Dichroism (CD) and Infrared Spectroscopy (IR) in combination with increasing temperature to monitor protein unfolding and stability. However, fewer studies have monitored protein structure after incubation at 37° C. The model protein Horseradish Peroxidase (HRP) was used to study how incubation over time altered protein structure and activity. CD was used to study structural changes over time and correlated with activity assays. Two different HRP samples were studied and it was found that HRP stored long term had significant decreases in structure and activity as compared to recently acquired HRP samples. The differences in structure in the HRP samples directly correlated with changes in enzyme activity.



Development and Synthesis of a new class of organic polymeric materials: Synthesizing and purifying a contractile molecule using fluorescein derivatives, transfer hydrogenations techniques, and monomer linkage using a diisocyanate.

Osmond Reindorf-Malm and Dr. Chris Hollinsed
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

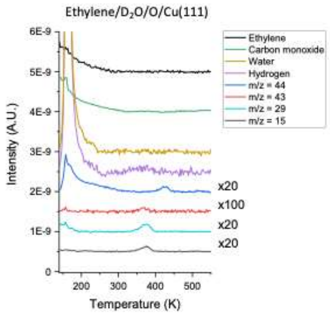
The Hollinsed Group is engaged in the design, development, and synthesis of a unique class of organic polymeric materials with the capability to operate under electrical stimuli in a manner comparable to, and in certain respects exceeding, the capabilities of natural physiological muscle. Central to our effort is the creation of a functional monomer, which has been successfully designed, synthesized, and replicated in the laboratory. Our monomer exhibits several key structural features critical to its performance: a molecular hinge for conformational flexibility, an anionic quinone-carboxylate group, a complementary cationic ammonium side chain for electrostatic attraction between the two ion charges, and the addition of structural fluorescein derivatives. To enable the polymerization of our monomer into a responsive polymeric material, several modifications and synthetic strategies are required. Strategic projects this term include purification of the crude monomer product, reduction of aromatic nitro groups to amines, conversion of carboxylic acid functionalities into amide bonds, and the incorporation of bifunctional structural linkers. Significant progress has been made in these areas: a high-purity purification method was developed, although current yield remains low; a preliminary yet promising pathway for nitro group reduction was identified and experimentally validated in initial trials; and a diisocyanate linker was selected for its bifunctional isocyanate groups, which are ideally suited for connecting monomer units through amide bond formation. Additionally, techniques for amide bond formation from carboxylic acids were studied and tested over the course of this term's work. These advances lay essential groundwork for the future assembly of polymeric systems with biomimetic actuation potential, contributing to the broader goal of developing synthetic materials capable of dynamic, electrically-driven mechanical response.

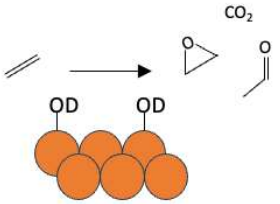


Understanding the Reactivity of C_2 Molecules on Cu(111) Catalysts

Allen C. Shepherd, James T. Whitted, Kate B. Weinstock, Jaimin J. Ashra, David W. Compton, Emily M. Euler, Owen M. Paulson, and Dr Ashleigh E. Baber
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Epoxidation is a commercially critical reaction in the chemical industry, with widespread applications such as chemical synthesis, pharmaceuticals, and polymers. Copper-based catalysts oxidize easily leading to prevalence of surface-bound reaction oxygen species for epoxidation reactions. In this study, Cu model catalysts were investigated for C_2 oxidation, aiming to reduce carbon emissions via overoxidation and enhance product selectivity. Clean Cu(111) leads to the complete combustion of ethylene, while partial oxidation or epoxidation is desired. Different surface oxygen species were explored to achieve selective epoxidation, including atomic oxygen and hydroxyl groups. Using temperature programmed desorption in an ultra-high vacuum system, reactions were examined on Cu(111) surfaces under various surface treatments: oxidized, hydroxylated, and hydrated. Our results show that hydroxylation enhances both reactivity and oxygen incorporation into C_2 reactants. Moreover, surface conditions strongly influence selectivity. Notably, the copper surface with oxygen, hydroxyls, and molecular water shows potential to selectively oxidize ethylene.





Deep ReCYCLE: Cycle-Aware Community Detection with RNBRW-Augmented GNNs

Samuel Stoke[1], Caleb Fernandes[2], Audrey Knight[3], Dr. Behnaz Moradi-Jamei[4]
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In the interconnected world around us, from social media networks to biological systems, communities naturally form through complex patterns of relationships. However, one hammer doesn't fit all in community detection**.** Different domains exhibit structurally distinct mechanisms for community formation that require domain-specific approaches. In meaningful cycle-rich domains, such as social networks, biological systems, and knowledge graphs, cycles carry semantic meaning: friendship triangles indicate trust, feedback loops represent functional pathways, and citation circles reveal research communities. These graphical topologies are essential in community formation. Traditional methods apply universal algorithms that ignore domain-specific structural patterns. More critically, in meaningful cycle-rich graphs, **l**earning and reasoning with cycles is essential for understanding network organization. While classical algorithms like Louvain are fast but domain-agnostic, modern Graph Neural Networks typically use generic message-passing that washes out the very cycle patterns that encode meaningful community signals.

Our **Deep ReCYCLE** framework bridges this gap by integrating meaningful cycle reasoning into learnable deep-learning architectures. We adapt RNBRW to efficiently quantify connection participation in meaningful cycles and integrate this cycle-awareness into neural networks through: (1) attention to cycle-rich connections during information aggregation, and (2) training objectives that reward cycle-based community structure, both tailored for domains where cycles encode semantically meaningful signals.

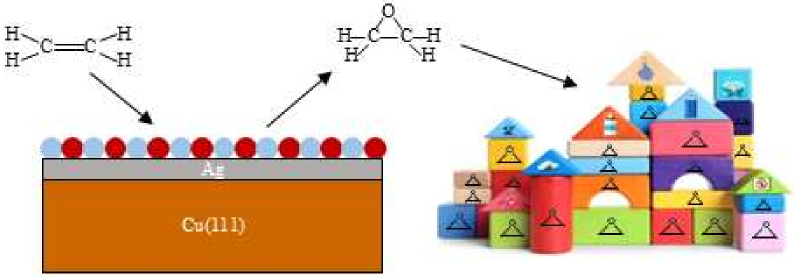
Current evaluation on benchmark datasets demonstrates that domain-tailored, meaningful cycle-aware learning consistently outperforms generic methods, achieving ARI scores of 0.8823 on Karate Club and 0.7565 on Political Books. Ablation studies confirm both cycle reasoning components are essential. We are extending experiments to larger-scale networks to demonstrate scalability.

This work recognizes that effective community detection requires domain-specific reasoning, and in meaningful cycle-rich domains, the cycles we overlook may be the very patterns that matter most for revealing hidden community structures.

The Selective Catalytic Epoxidation of Ethylene on Ag/Cu(111)

Katherine B. Weinstock, James T. Whitted, Allen C. Shepherd, Jaimin J. Ashra, Emily M. Euler, David W. Compton, and Dr. Ashleigh E. Baber
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

The production of ethylene oxide is a major industrial process that plays an integral role in the formation of insecticides, detergents, adhesives, and other products. Although it is vital, the mass production of ethylene oxide is the fifth largest producer of CO_2, and its synthesis requires dangerous and expensive promoters. Due to this controversial environmental impact, alternative approaches to promoters are being investigated. The use of AgCu catalysts is promising for ethylene epoxidation without promoters. Although the AgCu materials are active for epoxidation, the oxygen species responsible for the reaction remains elusive. To uncover the nature of the oxygen that leads to epoxidation rather than combustion, model Cu(111) catalysts were modified with Ag prior to oxidizing the surface with atomic O and hydroxyl groups. The products of the reaction of ethylene over hydroxylated and oxidized Ag/Cu(111) were monitored using temperature programmed desorption (TPD) under ultrahigh vacuum conditions. TPD revealed that hydroxylated Ag successfully suppressed CO_2 while simultaneously enhancing the selectivity of ethylene epoxidation.

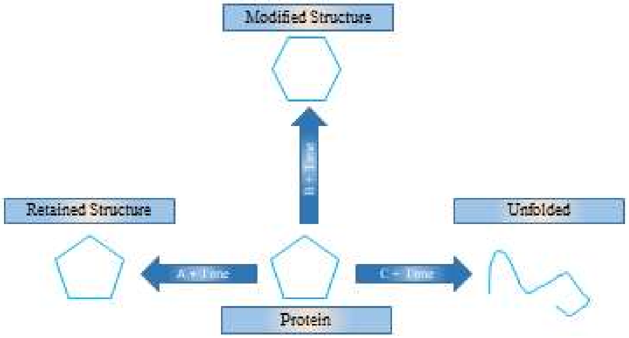


Environmental Influences on α-Chymotrypsin, Myoglobin, & β-Lactoglobulin Structure, Stability, and Aggregation

Paige O. Wooten, Elanna F. Smith and Dr. Gina MacDonald

Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Unfolded and aggregated proteins are associated with numerous neurological diseases. Understanding environmental factors that influence protein stability is crucial for understanding how the environment is related to disease progression. This study investigates how different molecules affect protein structure. Model proteins used for this study were α-Chymotrypsin (ACT), Myoglobin (Mb), and β-Lactoglobulin (BLG). Infrared (IR) and Circular Dichroism (CD) spectroscopies were used to monitor changes in protein stability and structure. Proteins were incubated at 37°C with various molecules including brilliant blue (Acid Blue 9), glycine, histidine, sunset yellow FCF (FD & C Yellow 6), and caffeine. CD and IR were used to determine if the different incubation conditions altered the structures and stabilities of the proteins as compared to proteins incubated in the absence of molecules. Brilliant blue decreased overall secondary structure of α-Chymotrypsin and Myoglobin, while histidine increased structure, and glycine, caffeine, and sunset yellow retained structure similar to the control. Sunset yellow and brilliant blue decreased BLG structure, while caffeine retained structure similar as compared to the control BLG. Interestingly, BLG incubated in the presence of glycine and histidine resulted in increased beta sheet as compared to the control BLG.



STUDENT ABSTRACTS
Multi-Slide Presentations: Session II

(Student presenters underlined)

Hadamard Matrices: Existence and Equivalence Problems

Jorge A. Menacho Paz and Dr. Joshua Ducey
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Hadamard matrices are interesting objects with many relations to other parts of mathematics such as designs, graphs, and groups. In this talk we will define Hadamard matrices, explore its connections to other math objects, present some open questions related to the existence and equivalence of Hadamard matrices, show some recent progress, and describe our approach to these problems.

Starch Binding Assays and Structure of Carbohydrate-Binding Module of Alpha-Amylase AMY3

Ruhi Rahman, Jonathan Monroe, Christopher Berndsen
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Starch is a crucial plant carbohydrate that serves as an energy reserve, supporting growth and development. Plants have enzymes that perform both starch synthesis and breakdown, with α-amylase3 (AMY3) being a plastidic amylase that contains an N-terminal tandem carbohydrate-binding module (CBM) from the CBM45 family. This domain is conserved in AMY3 homologs in most land plants but the structure and function of the CBM are unknown. Some enzymes involved in starch remodeling may be targeted to specific sites within the starch by the CBMs to control and coordinate starch synthesis and degradation precisely. We expressed and purified the N-terminal region of Arabidopsis AMY3, which contains the CBM, to investigate the structure of this domain and its role in AMY3 function. After purification, glutaraldehyde crosslinking and size exclusion chromatography indicated that the protein was dimeric, a unique property among CBMs. We further characterized the structure and size of the AMY3 CBM using small-angle X-ray scattering and developed a dimeric model of the CBM to fit these data. To identify potential functions, we performed a carbohydrate binding assay, finding that the CBM could bind a variety of glucose polymers but preferred to bind amylose, another unique property. Understanding how CBMs function could enhance our understanding of starch remodeling and aid in the development of more effective tools for work at the molecular level, such as carbohydrate sensors.

Structural dynamics during the watermelon malate dehydrogenase reaction cycle

Sara E. Scanlan and Dr. Christopher E. Berndsen
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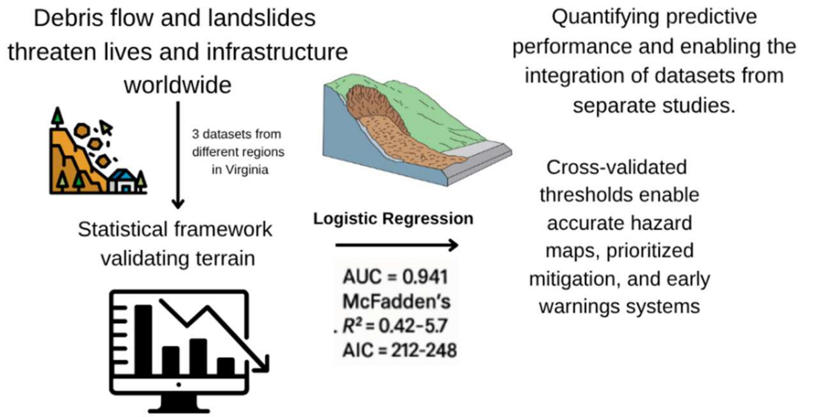
Malate dehydrogenase is an enzyme responsible for the interconversion of malate and oxaloacetate, coupled to redox chemistry involving NAD(H) or NADP(H). This enzyme is conserved across all domains of life, as it plays a crucial role in the citric acid cycle and other metabolic pathways involving malate and oxaloacetate. In eukaryotes, these enzymes are homodimeric and isoforms exist in the mitochondria and the cytosol. Plants have additional isoforms localized to the chloroplasts or peroxosomes (also known as glyoxysomes). Although little is known about the structural mechanism of catalysis, it has been suggested that the active site contains two highly dynamic regions, commonly referred to as the "active site loop" and the "thumb loop". Some of the crystal structures of MDH enzymes are missing the electron density for loop residues, suggesting this region is dynamic. In addition, it has been proposed that catalysis occurs via a reciprocating or half-of-sites mechanism, where the active sites of each subunit in MDH are in different yet coordinated stages of the reaction. This mechanism has yet to be described in detail. To investigate the structural basis for MDH catalysis and explore the reciprocating mechanism, we ran molecular dynamics simulations of MDH in the presence and absence of MDH substrates. We utilized Python and R packages to calculate the distance between residues on the loop and thumb, as well as the active site, during the reaction cycle, and performed principal component analysis to compare the structural ensembles that occurred during the simulations. Analysis of the simulations reveals substrate binding to the active site promotes changes in conformation to the loop and thumb. Furthermore, we found that there is structural coupling between the two active sites of the MDH dimer, whereby the completion of the reaction in one active site appears to prime the other to initiate the reaction. Interestingly, this effect was dependent on the loop not being in the open position. These studies will influence future work aimed at targeting MDH with therapeutics and provide a foundation for comparison to MDH enzymes found in other compartments, which have distinct loop sequences.

Predicting Debris Flow and Landslides in Virginia Using Logistic Regression

Meriem Dhouibi

Landslides and debris flows cause billions in damage annually, yet most prediction models rely on single regional datasets, limiting their reliability. This research develops a statistical framework validating terrain metrics across three independent Virginia datasets, comparing equivalent variables measured through different methods to identify universal predictors that transcend geographic limitations.

Results demonstrate remarkable consistency, with Elevation Variability and Slope Variability showing the lowest AIC values (ranging from 212-248) and the highest pseudo R-squared values (McFadden's R^2 = 0.42-0.57) across all datasets.
These cross-validated metrics derived from this approach support managers in creating more precise hazard maps, prioritizing interventions in high-risk zones, and utilizing early warning systems with quantified uncertainty. By leveraging logistic regression models, my framework not only quantifies predictive performance but also enables the integration of datasets from separate studies, thereby enhancing the reliability of debris flow and landslide predictions.



Approaches to the L'vov-Kaplansky Conjecture

Eva Ackley[1], Kylie Gill[2], Cole Kratz[3], and Dr. Méric Augat[4]
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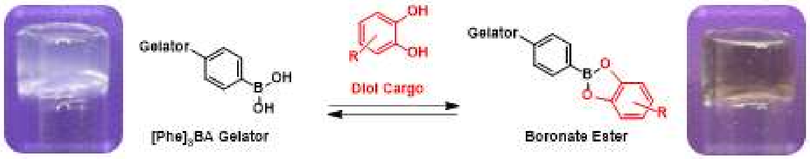
[4]Department of Mathematics and Statistics, James Madison University

The L'vov-Kaplansky Conjecture is a longstanding open question in the field of Algebra, which asks if the image of a multilinear polynomial acting on the space of $n \times n$ matrices is a subspace. We consider a weakening of the conjecture using an analytic lens: the Density Dimension-Free L'vov-Kaplansky Conjecture. This asks whether any multilinear polynomial eventually attains density in a subspace for large enough matrices with complex entries. Using an auxiliary map, we prove that density of the image on 2×2 matrices is guaranteed by a linear independence condition. Moreover, we give conditions on factorizations of multilinear polynomials that, if satisfied, guarantee density of the image within the traceless matrices or full matrix algebra. We provide concrete open problems that would shed further insight into the conjecture.

Targeted cargo loading of supramolecular peptide boronic acid gels

Anna G. Grove, and Dr. Gretchen M. Peters
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

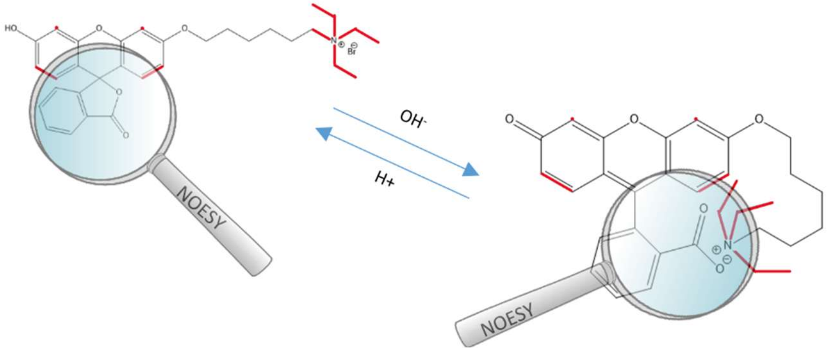
Supramolecular gels have been widely used for cargo-loading applications, including drug delivery and environmental clean-up. Peptide gelators are particularly attractive for this function, as they generally have high biocompatibility, low critical gelation concentrations (CGC), and are stimuli-responsive. Generally, incorporation of target molecules into peptide gels has utilized diffusion mechanisms and hydrophobic forces, which lack specificity and are difficult to control. Here we report a supramolecular peptide hydrogel capable of selectively binding to diol-rich cargo via reversible boronate ester bonds. Triphenylalanine boronic acid ($[Phe]_3BA$) was found to form stiff, stable hydrogels at concentrations greater than 2 mM at neutral pH. Spectroscopic studies indicate that $[Phe]_3BA$ forms β-sheets and that the $B(OH)_2$ group is free and accessible for binding. A variety of catechol derivatives, an important class of compounds commonly used as pharmaceuticals, pesticides, and dyes, were incorporated into the $[Phe]_3BA$ gel via covalent B-O bond formation. We found that in all cases, self-supporting hydrogels were formed with up to 1 equivalent of a catechol derivative, and in several systems, greater than 20 equivalents were successfully incorporated into the $[Phe]_3BA$ gel. However, in materials with greater than 1 equivalent of diol, the gelation time increased and gel stiffness varied. Structurally, we observed that catechol derivatives with alkyl, amine, or aldehyde substituents were well-tolerated in the gel, having little to no impact on the rheological properties. In contrast, carboxylic acid-containing catechol derivatives notably decreased the material stiffness. We theorize that these functional groups disrupt the noncovalent interactions between the peptide units and thus destabilize the gel network. These results provide important insights into using boronic acid units in peptide gels for targeted cargo loading. Additionally, we have demonstrated that $[Phe]_3BA$ gels have outstanding potential as materials for cargo-based applications. Currently, we are evaluating mechanisms for triggered release of these compounds for targeted drug therapies and environmental remediation applications.



Contractile Molecules: Synthesis, Purification, and Analysis

Sam Robinson and Dr. Chris Hollinsed
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

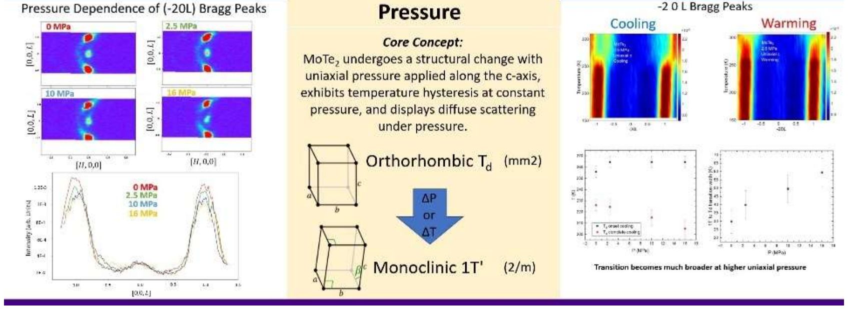
Having achieved the larger molecule of a resorcinol phthalein and a quaternary ammonium last summer, this summer the Hollinsed lab attempts two goals. One is attaching hooks to our molecule from last summer in the form of reducing a nitro group to an amine on the quaternary ammonium side, and reacting a carboxylic acid with a bisisocyanate group on the resorcinol phthalein ring side. We are also attempting to create a smaller scale version of our molecule this summer without the functional groups to turn into hooks in order to publish a paper on the contraction of said molecule.



$MoTe_2$ Under Uniaxial Pressure

Alexander J. Hardie[1], Dr. Despina Louca[2], Dr. Sachith Dissanayake[1]
[1]Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807
[2]Department of Physics, University of Virginia

$MoTe_2$ is shown to have extreme magnetoresistance because of a phase change from the monoclinic 1T'-$MoTe_2$ phase to the orthorhombic T_d-$MoTe_2$ phase upon cooling. This magnetoresistance has been demonstrated to be tunable through the application of mechanical hydrostatic pressure as well as chemical pressure through doping Mo sites with W; however, the effects of uniaxial pressure along the c-axis have yet to be extensively documented through diffraction techniques. Uniaxial pressure on $MoTe_2$ may prove to be more relevant to understanding the phase transitions between 1T' and T_d as tensile strain along the a- or b- axes has been reported to decrease and increase the transition temperature respectively. It is unclear how the application of uniaxial pressure along the c-axis would affect its structural properties. In this talk, we will explore the analysis of our data collected from Oak Ridge National Lab's Wide Angle Neutron Diffractometer (WAND) and what it says about $MoTe_2$'s structural properties and phase stability.



Pressure Dependent Change

Pressure Dependence of (-20L) Bragg Peaks

$MoTe_2$ Under Uniaxial Pressure

Core Concept:
$MoTe_2$ undergoes a structural change with uniaxial pressure applied along the c-axis, exhibits temperature hysteresis at constant pressure, and displays diffuse scattering under pressure.

Temp. Dependent Change

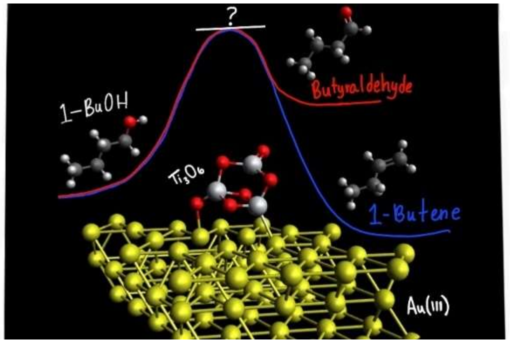
-2 0 L Bragg Peaks

Transition becomes much broader at higher uniaxial pressure

Modeling Isomeric Butanol Reaction Pathways on TiO_2/Au(111) Inverse Model Catalysts

Emily M. Euler[1], Haley E. Frankovich[1], Dr. Kendra Letchworth-Weaver,[2] Dr. Ashleigh E. Baber[1]
[1]Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807
[2]Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

Biobutanol, or butanol sourced from biomass, can produce butene which serves as a viable chemical precursor for a fossil-fuel free route to plastic production. Developing a deeper understanding of the fundamental thermal catalytic processes of butanol over heterogeneous model catalysts aids in the design of more efficient catalysts. Temperature-programmed desorption (TPD) experiments demonstrate differences in both reactivity and selectivity for butanol isomers. 1-BuOH reveals little reactivity and high selectivity for butene (reduced) products, whereas 2-BuOH displays high reactivity and low selectivity, producing both 2-butanone (oxidized) and butene (reduced) products. To gain an atomically-detailed perspective on these processes, density functional theory (DFT) was used to investigate energetic trends and identify comparisons between 1- and 2-BuOH as they adsorb on Ti_3O_x nanoparticles supported on a Au(111) surface. Findings suggest Ti-O_{BuOH} bonding, van der Waals interactions between the alkane chain and the Au surface, and electrostatic interactions between H and the nanoparticle all impact butanol's interactions on the catalyst material. Adsorption energies of both BuOH isomers place greater significance on Au surface interactions over Ti coordination number in determining favorability. The configuration of 2-BuOH enables it to interact more favorably with both the nanoparticle and Au surface compared to 1-BuOH, influencing reactivity and selectivity. Transition state energetics support experimentally observed trends for the thermodynamic favorability of 2-BuOH forming oxidized products compared to 1-BuOH.



STUDENT ABSTRACTS
Multi-Slide Presentations: Session III
(Student presenters underlined)

Optimizing the Distribution of Fruiting Agave on Bat-Friendly Tequila Plantations

Clarissa Azurin[1], Lois Carpenter[2], Grace Gorreck[3], and Dr. Alex Capaldi[4]
[1]Department of Mathematics & Computer Science, College of the Holy Cross
[2]Department of Mathematics, Statistics & Computer Science, Hollins University
[3]Department of Mathematics, Marist University
[4]Department of Mathematics & Statistics, James Madison University, Harrisonburg, VA 22807

Bat-friendly tequila plantations aim to feed pollinating bats like the Mexican Long-nosed Bat (*Leptonycteris nivalis*) by allowing a portion of their crop to flower at the expense of the final harvest size. We seek to determine if the spatial distribution of flowering agave has any impact on the number of bats a plantation could support, so that farmers interested in preserving nectarivorous bats could do so more efficiently. We created an agent-based model, a type of computer simulation, to study the interaction of *L. nivalis* bats and *Agave tequilana*. The model is informed by phenology and empirical parameters from the literature such as energetics. We compared four different spatial arrangements of flowering agave and determined spatial distribution does impact bat populations, with the most efficient arrangements yielding population estimates consistent with conservationist predictions, validating our model. Finally, the emergent bat carrying capacity of a plantation is directly proportional to the amount of flowering agave meaning that farmers need not worry about diminishing returns from their conservation efforts.

PbWO4 Crystal Characterization: Data Acquisition and Analysis Workflow

Gabriela Niculescu, Sarah Ormond, and Dr. Ioana Niculescu, Dr. Kevin Giovanetti, Dr. Gabriel Niculescu
Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

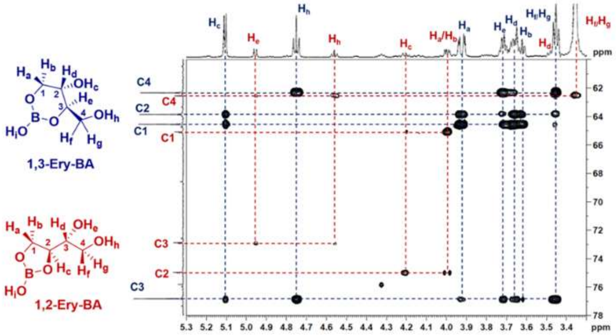
For the summer of 2025, the main thrust of the experimental work in the JMU Particle and Nuclear Physics Group (Drs IN, KG, and GN) was designing and building a test stand for characterizing the properties of Lead Tungstate (PbWO4) crystals. These modern, high-resolution, and radiation hard detectors will form the backbone of high-performance electromagnetic calorimeters to be used in current and planned nuclear and particle experiments. We designed and built a testing process to evaluate the uniformity of the crystal's response along its longest axis. This is accomplished using a Na-22 source and comparing the PbWO4's signal to a known (witness) NaI detector, as the two detectors move with respect to one another.

This project can be divided into three intertwined subsections: computer modelling of the testing stand, building the test stand itself, and providing a robust data acquisition and analysis workflow. Our work focused on the latter task. To this end, the data acquisition (DAQ) system was completely rewired, the coincidence signals were timed in, and the DAQ software was updated. Furthermore, we wrote Python code to integrate the DAQ with the linear actuator movement. We made substantial strides in writing the analysis code, which ultimately will provide the characterization of these PbWO4 crystals.

Elucidating the structures of polyol-boric acid complexes in organic solvent using NMR spectroscopy

Brandy L. Davidson and Dr. Gretchen M. Peters
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA 22807

Boric acid (BA) readily forms reversible, covalent B-O bonds with polyols, yielding complexes with broad implications for drug delivery, materials science, and polymer chemistry. While this chemistry is well-established in aqueous environments, less is known about the formation of neutral boron complexes with BA in organic solvents. Our previous work has shown that the diol binding face impacts both the product distribution and rate of this reaction, with 1,2-diols forming fastest and 1,3-diols being thermodynamically preferred. Here, we describe an NMR spectroscopic study into the complexation of polyols combined with BA. We have employed 2D NMR techniques (i.e., COSY, HSQC, and HSQC-TOCSY) to identify and fully characterize the B-O complexes formed with BA and glycerol (Glyc), erythritol (Ery), D-threitol (D-Thr), L-threitol (L-Thr), xylitol (Xyl), and mannitol (Man). Notably, the major complexes formed with these polyols are not always consistent with the trends established with diols. For example, though we would anticipate that the 1,3-isomer would predominate, Glyc forms a ~50:50 of the 1,2-Glyc-BA and 1,3-Glyc-BA complex when BA is added. We theorize that this is the result of stabilizing interactions between the free OH of the polyol and the B-O ring. Support for this hypothesis has been seen computationally and via spectroscopic methods with triols of longer tail length, such as 1,2,4-butanetriol (1,2,4-BT). With 1,2,4-BT, the expected ratio of 1,3- to 1,2-complex was observed (~90% and 10%, respectively). Stereochemistry was also found to impact the isomeric ratio of B-O complexes. While Ery forms ~85% of the 1,3-Ery-BA complex as its major product, D- and L-Thr form predominately the 2,3-Thr-BA complex (~50%). We speculate that the 2,3-Thr-BA complex is highly stabilized by the aforementioned secondary interactions, having two free OH's on both sides of the B-O ring. Control experiments with the isomers of 2,3-butanetriol showed the *meso* compound formed significantly less complex relative to the D- and L-isomers. This suggests that steric interactions are inhibiting the formation of the 2,3-complex with Ery. In combination, these findings highlight the impact of structural features within the polyol on the formation of B-O complexes. In the future, we will use these results as a scaffold for solving more complex structures and will evaluate the thermodynamics and kinetics of polyol-BA complexation.



PbWO4 Crystal Characterization: Data Simulation and Analysis

Nicholas Luces, Aidan Pisarcik, Dr. Ioana Niculescu, Dr. Kevin Giovanetti, Dr. Gabrial Niculescu
Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

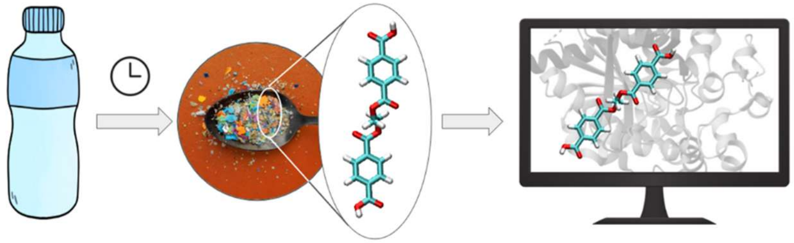
For the summer of 2025, the main thrust of the experimental work in the JMU Particle and Nuclear Physics Group (Drs IN, KG, and GN) was designing and building a test stand for characterizing the properties of Lead Tungstate (PbWO4) crystals. These modern, high-resolution, and radiation hard detectors will form the backbone of high-performance electromagnetic calorimeters to be used in current and planned nuclear and particle experiments. We designed and built a testing process to evaluate the uniformity of the crystal's response along its longest axis. This is accomplished using a Na-22 source and comparing the PbWO4's signal to a known (witness) NaI detector, as the two detectors move with respect to one another.

This project can be divided into three intertwined subsections: computer modelling of the testing stand, building the test stand itself, and providing a robust data acquisition and analysis workflow. The aspect in this project that we were tasked with working with was on simulating , the first being able to simulate radiation from a point source through a medium onto a "receiver" to observe differing attributes of radiation. Second, being able to simulate a peak of good data over a background and using python to fit the peak and observe the characteristics of the fit. Lastly, using that code used for the fits to be applied to actual data obtained from Jefferson Lab to find similar characteristics.

Molecular Interactions of the plastic PET with a Lysosome Enzyme

Hannah Lau, Rhett Sanders, Isaiah Sumner
Department of Chemistry and Biochemistry, James Madison University, Harrisonburg, VA

Plastics continuously decompose into tiny, tiny pieces called microplastics which are absorbed into our bodies by oral intake, inhalation, and skin contact. They then travel into our bloodstream and interact with organelles and proteins in our cells, which may cause damage and lead to disease. Unfortunately, we currently do not have a detailed understanding of how microplastics interfere with our biochemistry, although some details are emerging. For example, there is evidence that polyethylene terephthalate (PET), a common plastic which makes up much of the food and beverage packaging, slows down the lysosome, an organelle that disposes of cellular waste, but there is currently no molecular-level understanding of this process. We hypothesize that PET may inhibit the normal function of lysosomal enzymes that digest molecules with structures similar to PET. To test this hypothesis, we focused our efforts on interactions between PET and Lysosomal Acid Lipase (LAL), an enzyme that cleaves large fatty substrates into small nutrients. We are investigating this interaction through docking software (AutoDock Vina and Diffdock), molecular dynamics simulations (AMBER), and binding energy calculations. First, the PET was placed into LAL's binding pocket with docking software. Second, molecular dynamics simulations were used to see if the PET would remain bound to the active site and to quantify active-site interactions. Finally, binding energy calculations were initiated. Our simulations show that it is likely that PET does bind to LAL's active site.



PbWO4 Crystal Characterization: Mechanical Design and 3D Modeling

Heather Accorti, Samuel Pearne, and Dr. Ioana Niculescu, Dr. Kevin Giovanetti, Dr. Gabriel Niculescu
Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807

For the summer of 2025, the main thrust of the experimental work in the JMU Particle and Nuclear Physics Group (Drs IN, KG, and GN) was designing and building a test stand for characterizing the properties of Lead Tungstate (PbWO4) crystals. These modern, high-resolution, and radiation hard detectors will form the backbone of high-performance electromagnetic calorimeters to be used in current and planned nuclear and particle experiments. We designed and built a testing process to evaluate the uniformity of the crystal's response along its longest axis. This is accomplished using a Na-22 source and comparing the PbWO4's signal to a known (witness) NaI detector, as the two detectors move with respect to one another.

This project can be divided into three intertwined subsections: computer modelling of the testing stand, building the test stand itself, and providing a robust data acquisition and analysis workflow. Our part in this project was to design and assemble experimentation hardware to fit the project's goals. We received hardware from the JMU Physics Department's workshop and adapted it to our needs. Furthermore, we analyzed the Na-22 source constraints related to the PbWO4 crystal and created unique 3D printed parts using Solidworks computer aided design (CAD). Our final product went through multiple iterations to ensure that the project had reliable mechanics and consistent data readings.

Utilization of Water for Propylene Epoxidation on Ag/Cu(111)

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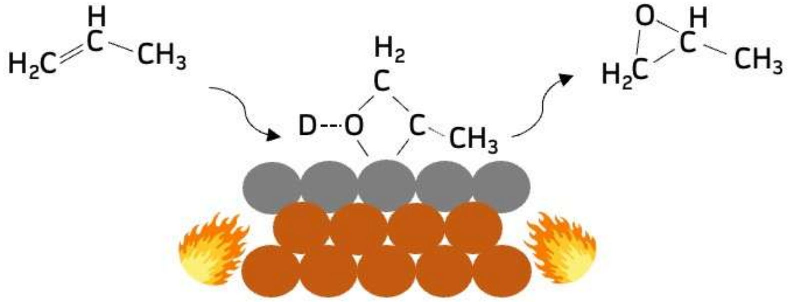
The selective catalytic epoxidation of alkenes using Ag and Cu catalysts are major industrial processes, with value-added products worth a combined $77 billion global market value. Cu-based heterogeneous catalysts are known to enhance propylene (C_3H_6) epoxidation, but struggle to simultaneously suppress the combustion pathway without the presence of toxic promoters (Cl, Na, Cs). The highly selective epoxidation of various olefins occurs on oxidized Ag(110) and Ag(111), while sequentially limiting the combustion pathway. Ag(111) is not easily oxidized, yet is selective for epoxidation, while Cu(111) readily oxidizes but leads to combustion. By combining these two materials, oxophilic Cu with the epoxide-selective Ag, into a bifunctional AgCu near surface alloy, inadvertent CO_2 production could be limited while sustaining propylene oxide formation. Ultra-high vacuum temperature programmed desorption (UHV-TPD) spectra were gathered on partially oxidized Cu(111) and Ag/Cu(111) after dosing propylene. These results showed that atomic O does not lead to selective epoxidation and therefore is not likely the reactive oxygen species of interest. The role of surface-formed hydroxyls for propylene reactivity was explored by conducting TPDs on a D_2O/O/Ag/Cu(111) surface. Without the presence of Ag, the combustion and epoxidation pathways were present at high temperatures (~360 K). By depositing 1 ML of Ag on Cu(111) via physical vapor deposition, the combustion pathway was fully minimized while retaining the epoxidation pathway. Future work will focus on utilizing scanning tunneling microscopy to image the complex surface and elusive intermediates. Our collaborators will conduct reactor studies to explore scaling the reaction to industrially relevant conditions and computational modeling to create a better understanding of reaction pathways.



The Topology of Representation Varieties

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Representation varieties are geometric objects used to study symmetries. Our projects analyze various topological properties (e.g., the number of connected components) of several representation varieties. This talk will report on some of our results.

Deep ReCYCLE: Cycle-Aware Community Detection with RNBRW-Augmented GNNs

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In the interconnected world around us, from social media networks to biological systems, communities naturally form through complex patterns of relationships. However, one hammer doesn't fit all in community detection. Different domains exhibit structurally distinct mechanisms for community formation that require domain-specific approaches. In meaningful cycle-rich domains, such as social networks, biological systems, and knowledge graphs, cycles carry semantic meaning: friendship triangles indicate trust, feedback loops represent functional pathways, and citation circles reveal research communities. These graphical topologies are essential in community formation. Traditional methods apply universal algorithms that ignore domain-specific structural patterns. More critically, in meaningful cycle-rich graphs, learning and reasoning with cycles is essential for understanding network organization. While classical algorithms like Louvain are fast but domain-agnostic, modern Graph Neural Networks typically use generic message-passing that washes out the very cycle patterns that encode meaningful community signals.
Our **Deep ReCYCLE** framework bridges this gap by integrating meaningful cycle reasoning into learnable deep-learning architectures. We adapt RNBRW to efficiently quantify connection participation in meaningful cycles and integrate this cycle-awareness into neural networks through: (1) attention to cycle-rich connections during information aggregation, and (2) training objectives that reward cycle-based community structure, both tailored for domains where cycles encode semantically meaningful signals.
Current evaluation on benchmark datasets demonstrates that domain-tailored, meaningful cycle-aware learning consistently outperforms generic methods, achieving ARI scores of 0.8823 on Karate Club and 0.7565 on Political Books. Ablation studies confirm both cycle reasoning components are essential. We are extending experiments to larger-scale networks to demonstrate scalability.
This work recognizes that effective community detection requires domain-specific reasoning, and in meaningful cycle-rich domains, the cycles we overlook may be the very patterns that matter most for revealing hidden community structures.

We gratefully acknowledge these funding sources for generous support of student research:

National Science Foundation, including the following grants:
- REU : CHE-2150091, DMS-2349593
- DUE-2221277, MCB-2322867, MCB-2024182, MCB-2216956, DMR-2216346, PHY-2209421, DBI-2214633, DBI-2334070

National Institutes of Health, including the following grant:
- R15-GM148890

The Department of Energy, including the following grant:
- DE-SC0025690

4-VA
ACS Petroleum Research Fund, including the following grant: 59504-UR4
American Society of Plant Biologists
Argonne National Lab
Camille and Henry Dreyfus Foundation
Department of Defense – ASSURE
Department of Energy – Office of Science
International Society for Chemical Ecology
Jeffress Memorial Trust
JMU Second Century Scholarship
JMU/CSM Summer Scholarship Stimulus Program
NASA/XGS grant 80NSSC23K1021
Merck
Research Corporation for Scientific Advancement
Thomas F. Jeffress and Kate Miller Jeffress Memorial Trust
Tickle Summer Research Scholarship

JMU College of Science and Mathematics
JMU Center for Genome and Metagenome Studies
JMU Center for Materials Science
JMU Department of Chemistry and Biochemistry
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JMU Department of Physics and Astronomy
James Madison Innovations, Inc.
The Madison Trust—Fostering Innovation and Strategic Philanthropy
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