



ACS
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AMERICAN CHEMICAL SOCIETY

2022 Rochester Collegiate Research Symposium

April • 9 • 2022

Event Program

8:30am – 8:50am

Check-in

8:50am – 9:00am

Welcome Address by David McCamant

Associate Professor of Chemistry, University of Rochester

Green Carpet Lounge

9:00am – 10:15am

Poster Presentations

Green Carpet Lounge

10:15am – 11:30am

Speaker Presentations

(See page 8 for individual titles and times)

Lander Auditorium (Hutch 140)

11:30am – 12:30pm

Keynote Speaker, Kathryn Knowles

“Synthesis and Photophysics of First-Row Transition Metal Oxide
Nanomaterials”

Lander Auditorium (Hutch 140)

12:30pm – 1:00pm

Student Awards Presented by Colin Wright

Chair, ACS Rochester Section

Organizing Committee:

Brittney Beidelman

(Chairperson)

Melissa Koch

(Co-Chairperson)

James Stair

Amber Charlebois

Maryann Mendel

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Keynote Speaker: Kathryn Knowles

“Synthesis and Photophysics of First-Row Transition Metal Oxide Nanomaterials”



Biography: Kathryn Knowles completed undergraduate studies in chemistry and mathematics at the University of Rochester and earned a Ph.D. in chemistry from Northwestern University under the direction of Professor Emily Weiss with the support of a graduate research fellowship from the U.S. Department of Energy's Office of Science. She worked as a postdoctoral research associate in Prof. Daniel Gamelin's group at the University of Washington before returning to Rochester as an Assistant Professor of Chemistry in 2016. Throughout her career, Prof. Knowles's research

has focused on studying inorganic nanomaterials that can convert light to energy in the form of electricity or fuels and characterizing structure-function relationships that influence the fundamental mechanisms that underpin these energy conversion processes. Her work has been supported by a DOE Energy Efficiency and Renewable Energy (EERE) Postdoctoral Research Award, an ACS Petroleum Research Fund Doctoral New Investigator Award, and a National Science Foundation early CAREER award. She is also a Scialog Fellow for Negative Emissions Sciences.

Winners of the Rochester ACS Undergraduate Award in Chemistry

Awards to be presented by Colin Wright, Chair of ACS Rochester Section

Emily Benton; SUNY Geneseo

Emily Benton is originally from a working farm in Carlisle NY. She is currently a Chemistry and Art History double major at SUNY Geneseo. In addition to academic excellence in the classroom, Emily has participated in a wide variety of undergraduate research. She worked with Dr. Kazu Yokoyama in the Chem Dept studying the adsorption of SARS-CoV-2 alpha spike protein on gold nanoparticles, she worked with Dr. Stephen Padalino in the Physics Dept studying xylene coatings to optimize scintillation detectors in Geneseo's particle accelerator, and she has presented on the work of Johannes Vermeer at local art history conference. Emily will graduate in May 2022 and plans to attend graduate school studying conservation of books and works of art on paper. One of her professors said, 'Emily represents the very best of a liberal arts education and she is a joy to work with' and she is highly deserving of the Rochester ACS Undergraduate Award.

Kendra Watson; University of Rochester Chemical Engineering Dept.

Kendra Watson is the Department of Chemical Engineering's 2022 ACS Award winner. Top of her class, Kendra holds a 3.92 in a very rigorous program. She has done applied chemistry research work in Professor Astrid Mueller's lab, both as an Eisenberg Fellow and through independent research. She is the is a co-inventor on a provisional patent application ("Acid-free solution process for structurally intact carbon fiber paper with long-lasting hydrophilicity") and also a co-author on a research article that is in review in a Nature Portfolio Journal (<https://www.researchsquare.com/article/rs-1284564/v1>). Kendra plans to remain at the U of R next year for her Masters in Chemical Engineering.

Kaelyn McFarlane-Connelly; University of Rochester Chemistry Dept.

Kaelyn has maintained an outstanding GPA while completing the challenging BS degree in Chemistry from the University of Rochester this year before continuing her professional training in a PhD program in the fall. Kaelyn nearly completed her degree in 3 years and has spent an enormous amount of time in the research lab, studying CdSe semiconductor nanocrystals with Professor Todd Krauss. Initially, she completed the synthesis of silver-doped CdSe quantum dots, then during the Covid lock-down, she completed a theoretical analysis of the band energies of CdSe/CdS core-shell quantum dots and, most recently, Kaelyn has assembled CdSe photoelectrodes for solar hydrogen production. On top of all this, Kaelyn has been an outstanding community member, having lead our Undergraduate Chemistry Council this year and been a Teaching Assistant in a big variety of courses. Congratulations, Kaelyn!

Abby Manning; Nazareth College

Abby is a senior Biochemistry Major who is graduating in May after only three years at Naz. She was very active in the department where she contributed to two research projects, "The Interactions of Cresyl Violet with Nucleic Acids" and "The Development of a Microwave Assisted Synthesis of Amides". She has presented her research in many forums including several virtual poster sessions throughout Covid. We are excited to celebrate her with this Rochester Local Section Outstanding Senior Chemistry Award. She will be heading over to the University of Rochester Biophysics Department!

Jack Russo; Hobart and William Smith Colleges

Jack Russo is a senior chemistry major from Hobart and William Smith Colleges. Jack has done organic chemistry research with Erin Pelkey for the past two years which includes both summers and during the past four semesters in the academic school year. He has investigated Friedel-Crafts alkylation reactions involving indole and he discovered a novel ring opening reaction between indole and simple azetidines which led to homotryptamines in one-step. Jack has spearheaded a methodology study around this discovery involving himself and two of his peers and he is currently writing this work up for submission to a peer-reviewed journal. Jack is also doing an independent study where he is developing new "organic chemistry 2" problems that are anchored in the primary literature. After graduation, Jack will pursue a Ph.D. in chemistry at an institution to be determined (very soon).

Hunter Czajkowski; SUNY Brockport

With a 3.88/4.00 College/Biochemistry major overall GPA, it is evident that Hunter has achieved an exceptionally high level of academic success. However, what really distinguishes her from her peers is her unprecedented scholarly success in addition to her wide faceted involvement of service and enrichment activities outside the classroom. She managed to arrange several internships that included research work where her analysis contributions were so valuable that she is co-author on a stunning seven peer-reviewed articles submitted to the primary medical literature, five of which are already published by the time of writing this nomination letter. This is simply unprecedented for an undergraduate student! Her service and enrichment activities include being part of the track team, where she is active as pole vaulter and does pentathlon (hurdles, high jump, long jump, shot put and 800m), and taking on leadership roles in the Rotary Club and the Pre-Professional Health Club. Hunter clearly exemplifies the spirit of the Rochester Section ACS Chemistry Achievement award.

Shao Demyttenaere; Rochester Institute of Technology

Shao M. Demyttenaere is from Cazenovia, NY, and joined RIT in the fall of 2018 as a chemistry undergraduate major with the intent of pursuing a BS/MS degree in materials science. Shao has always been interested in environmental sustainability and materials science. She has also gained great interest and experience in analytical chemistry during her time at RIT. Already in her 2nd semester, she joined the research group of Dr. Matt Miri to work on the development of sustainable polymers. Dr. Miri was immediately impressed by her quick adaptation of the characterization techniques. She was not only highly productive, but also devoted much of her time reproducing measurements and increasing their precision and accuracy. In addition, Shao trained several junior students and proved herself as a great team player within the research group. She maintained these outstanding manners in research over the entire four years. Shao has also done great in her course work, as indicated by her GPA of 4.00. This spring semester she is completing her MS degree with a capstone project isolating bacteria, which preferentially degrade commercial biodegradable plastic bags with Dr. Jeffrey Lodge as her advisor.

Rebekah Phelan; Roberts Wesleyan College

Rebekah has been unanimously selected for this award by the chemistry faculty at our institution. She has outstanding academic capabilities and maintains a 3.800 GPA, while being a part of the Honors Program at Roberts Wesleyan College. Throughout her time here, Rebekah has worked for the Department of Biological and Chemical Sciences as a Teaching Assistant, Chemistry Stockroom Assistant, and a grader. Rebekah has also been an active member of our Adopt-A-School program outreach to School #3 in Rochester. Rebekah currently part of a research group isolating unknown bacteria from various soil samples and then analyzing the chemical composition of the soil where these bacteria thrive by atomic spectroscopy, mass spectroscopy, and liquid chromatography. In addition to her work within the department, Rebekah is very active on campus. She currently serves as Student Body Vice President, serves on the Social Life Committee, and participates in various intramural teams throughout the year. Rebekah has excelled as an undergraduate student and plans to pursue her Ph.D. in Chemistry after finishing her degree at Roberts.

Jared Jorolemon; St. John Fisher College

Jared Jorolemon, an Honors scholar, will earn a BS Chemistry degree (minor in mathematics) from St. John Fisher College in three years with a GPA of 3.86. He recently presented his summer science fellows independent research (mentor: Dr. Alexey Ignatchenko) at the ACS Spring conference in San Diego, CA with the support of a Rochester ACS undergraduate travel award. After graduation, Jared will enter the doctoral program at the University of Notre Dame in Fall 2022.

Jacob Willower; St. John Fisher College

Jacob Willower will earn a BS Biochemistry degree from St. John Fisher College in Spring 2022 with a GPA of 3.97. He was a summer science fellow completing independent research on the construction of hyperbolic surfaces using carbon heptagons with Dr. Alexey Ignatchenko. After graduation, Jacob will take a gap year and apply to medical school.

Undergraduate Speaker Presentations

Ten-minute talks followed by five minutes Q&A

10:15 – 10:30

“Exploring the Interactions Between Cresyl Violet and Nucleic Acid Molecules”

Presenter: Abby Manning; Nazareth College

Collaborator: Megan Griffin

Advisor: Amber Charlebois

This research project examines the interactions that take place between cresyl violet (CV), an organic compound used for staining tissue and neurons, and nucleic acids. CV is a planar molecule that forms a complex with DNA and RNA and generates different colors. Running different sequences of DNA and RNA oligos, 15 bases in length, through gel electrophoresis and using CV as the stain produces the color differences. RNA tends to be stained more of a purple color while DNA stains as a bluer tone. To more precisely quantify these colors UV-Vis spectroscopy is used. In gel, a fiber optic UV-Vis is used to analyze the band on the gels, and a Cary 60 is used for the solution studies. The wavelength scans of the different oligos are unique with multiple peaks/forms present and therefore indicate that these nucleic acid-CV interactions may be base dependent. To further explore the CV local environment, we have experimented with different pHs around the pKas of the molecule. CV has been found to have distinctive spectra for each pH, similar to what is observed in the CV stained nucleic acids, providing insight into the local environments within the DNA and RNA oligos. PeakFit (Systat Software Inc.) continues to be used to identify and quantitate the peaks which represent the monomer, dimer and other unique forms.

10:30 – 10:45

“Direct Aminopropylation of Indoles via Lewis Acid Catalyzed Ring Opening of α -Unsubstituted Azetidines”

Presenter: Jack Russo; Hobart and William Smith Colleges

Collaborators: Rebecca Huss, Christina Mitrow

Advisor: Erin Pelkey

Herein is described a simple synthetic route to access homotryptamines in moderate yields via an In(OTf)₃ catalyzed SN₂-type ring opening of activated, α -unsubstituted azetidines with indoles. This methodology is the first direct C3 aminopropylation of indoles using unsubstituted azetidines, allowing for efficient access to the synthetically valuable homotryptamine scaffolding.

10:45 – 11:00

“Diastereoselective Carbo-Nazarov Electrocyclizations”

Presenter: Yahia Ali; University of Rochester

Advisor: Alison Frontier

A diastereoselective, cationic cyclization cascade reaction for the formation of functionalized cyclopentenes was developed featuring a novel carbo-Nazarov 4- π electrocyclization. The strategy is modular; joining an aldehyde and an enyne via a halo-prins reaction to furnish an adduct which is finally cross-coupled to a biaryl nucleophile to furnish the cyclization precursor. Ionization of this precursor with triflic acid initiates the electrocyclization which is followed by trapping of the resulting allyl cation by the biaryl moiety to form three contiguous stereocenters and two carbon-carbon bonds in one synthetic step. Additionally, an example of a rare 6- π cyclization brought upon by unique conformational properties of the substrate is also demonstrated.

11:00 – 11:15

“Improving Charge Transport in Quantum Dot Sensitized Photocathodes for Hydrogen Production”

Presenter: Kaelyn McFarlane-Connelly; University of Rochester

Collaborators: Emily Edwards

Advisor: Todd Krauss

The production of hydrogen from solar-driven water splitting is a promising route towards achieving alternative green energy solutions. While many processes have been studied, recent attention has been focused on light-absorbing nanomaterial electron sources to make use of their strong absorptivity and high photostability. In this work, the fabrication of CdSe quantum dot (QD)-sensitized photocathodes was adjusted to enhance charge transport characteristics. A reliable spin-coating process for producing a thin and conductive NiO layer on ITO covered glass slides was first developed. Then, in-situ and post-processing techniques for depositing quantum dots onto thin films were combined to utilize the favorable electrostatic interactions between thioglycolic acid (TGA)-capped CdSe and the NiO surface. Pre-synthesized TGA-capped CdSe ($\lambda_{\text{max}} = 530\text{nm}$) were left to dry on NiO electrodes, which allowed for increased coverage as compared to the normal spin-coating approach. Subsequently, improved charge transport was observed in photocurrent studies. Following irradiation from a 150 mW blue light source and a bias potential of -0.1 V, a photocurrent density of $\sim 138 \mu\text{A}\cdot\text{cm}^{-2}$ was achieved. Additionally, the pairing of these photoactive electrodes with Co-based biocatalysts was explored. In combination with a stable mini-protein, CoMC6*a, the photocathodes showed remarkable stability, producing current for over 60 hours and achieving a maximum photocurrent density of $68 \mu\text{A}\cdot\text{cm}^{-2}$. This study highlights the effect of fabrication methodologies on charge transport in QD-sensitized photocathodes and discusses a process for developing stable, high photocurrent devices.

11:15 – 11:30

“Synthesis of Bismuth Nanoparticles for Applications in Oncology”

Presenters: Mary Elizabeth Kane, Molly Roesch; Rochester Institute of Technology

Advisor: Kenneth Reed

Current methods to treat cancer result in large amounts of healthy cell death (low selectivity ratios) relative to the amount of cancer cells killed. D112 is a spectral sensitizing dye originally synthesized by Kodak that has a high selectivity ratio but was found to be hepatotoxic in mice. To alleviate this effect, it is theorized that conjugating the dye to a magnetically steerable nanoparticle would allow specific targeting of cancer cells as well as safe removal of the dye from the body. Bismuth metal is inert in biologicals and a highly diamagnetic metal, so the synthesis of bismuth nanoparticles has been explored. The goal has been to synthesize and stabilize a 2-5 nm particle. Proper solvent systems, stabilizers, and reducing agents are explored. Obstacles in the synthesis include reducing the bismuth to the zero valent state, controlling the size and self-aggregation of the particle, and solubilizing the bismuth (III) hydroxide feedstock.

Undergraduate Poster Presentations

Biological/Biochemical Posters

1- “Composition of Volatile Compounds from Rare and Endangered *Illicium Ekmanii*, a Species Endemic to Hispaniola”

Presenter: Sreya Gomes; Rochester Institute of Technology
 Collaborators: Morgan Bida, Angela Guerrero, Pepsi Homquist
 Advisor: Todd Pagano

Illicium ekmanii Smith is a rare and endangered plant species endemic to the mountainous areas of Hispaniola. Little is known about the volatile oil composition of this species, and it is currently under threat of habitat destruction by mining and agricultural practices. There are 37 known species in the *Illicium* genus, the most well-known of which is *I. verum* or star anise which has been used for thousands of years as a traditional medicine and flavor ingredient. The purpose of this study is to identify volatile oil compounds in the leaf essential oil of *I. ekmanii* Smith and examine how the results compare in relation to other *Illicium* species, such as *I. verum*. Samples of separate *I. ekmani* populations were tested from different mountain ranges on Hispaniola, Cordillera Central (CC) and Cordillera Septentrional (CS). The leaves of each sample were extracted to collect the oils by hydro-distillation before using gas chromatography with mass spectrometry (GC-MS) for identification of the compounds and flame ionization detection (GC-FID) for relative quantification. CC samples were dominated by the sesquiterpenes: α -copanene, trans-caryophyllene, and bornyl acetate, while CS samples had an abundance of phenylpropenes, including methyleugenol, elemicin, and safrole. *I. ekmani* samples from CS were the most similar to the results previously reported for *I. verum*, where an abundance of phenylpropenes was reported. This project represents the first known analysis of the essential oils found in this species, *I. ekmanii* from two distinct mountain ranges on Hispaniola. The results from this study will add knowledge about *I. ekmanii* and bring awareness to the conservation efforts underway to protect this rare plant and its habitat in Hispaniola.

2- “Essential Oils Antimicrobial Activity”

Presenter: Juan Giner, Rocío Pilán; Nazareth College
 Advisor: Amber Charlebois

The antimicrobial effect of essential oils has been tested in *E. coli*, *S. epidermidis*, *C. albicans* and *B. cereus* using the standard, pure composition of different oils, and extracting oils from spices. Peppermint, Eucalyptus, Clove and Cinnamon along with their standards eugenol and 1,8-cineole proved that essential oils killed bacteria with various success depending on their characteristics. The Kirby-Bauer method together with antibiotic discs (vancomycin and gentamicin) as a positive control were used to determine the sensitivity or resistance of pathogenic bacteria. Results indicate that clove is effective towards the four microorganisms and the other spices are effective to a

varying degree. Further research is being done to study the bactericide effectiveness of lower concentrations of these oils.

3- “Bone Fracture Repair: Testing Porous Properties of Calcium Phosphate Bioactive Cement and How it Compares to Pig Bone”

Presenters: Matthew Chudy, Jack Donaldson, Nobah Islam, Dean Ivanovski, Emily Rennells;
SUNY Geneseo

Collaborator: Nosheib Jadoon

Advisor: Barnabas Gikonyo

Autografting is the most effective method used for supplementing and replacing bone. Autografting is a risky procedure because of its invasive nature. When performing the procedure of autografting, one needs to remove small sections of bone to use as a stimulant at the fracture site. This study is made to design an alternative method to replace autografting. In our study, we used pig fibula as a model to compare the properties of our novel cement which is Calcium Phosphate based. Calcium Phosphate Cement (CPC) is ideal because it is a biocompatible bone substitute composed of Hydroxyapatite (HA), which constitutes a major component of human bone. The Hydroxyapatite will serve as the base ingredient for the cement. The cement allows for the successful osseointegration and the initiation of bone growth. We focus our efforts into understanding and finding a consistent porosity size between the bone and the cement. This will be done by using different concentrations of chitosan and sodium bicarbonate. Results of the experiment show that the sample most similar to the bone sample was the chitosan.

4- “Investigating the Impact of Solvent on β -sheet Forming Peptide”

Presenter: Yahui Guo; University of Rochester

Collaborator: Francine E. Yanchik-Slade

Advisor: Bradley Nilsson

Amphipathic peptides with alternating hydrophobic/hydrophilic amino acid sequence patterns self-assemble into β -sheet nanofibrils. These β -sheet forming peptides self-assemble into β -sheet bilayers with the hydrophobic residues isolated from the solvent in the interior of the bilayer. These supramolecular fibrils have been used as biomaterials for drug delivery, tissue engineering, and regenerative medicine. Previous work has shown that the amphipathic L-Ac-(FKFE)₂-NH₂ peptide self-assembles in water initially into helical ribbons that evolve into nanotubes over time. In this project, we examine on the self-assembly of L-Ac-(FKFE)₂-NH₂ and the coassembly of L-Ac-(FKFE)₂-NH₂ with the D-Ac-(FKFE)₂-NH₂ enantiomer under three distinct solvent conditions to understand the impact of solvent environment on the self-assembly process. Specifically, the self-assembly of L-Ac-(FKFE)₂-NH₂ and coassembly of L/D-Ac-(FKFE)₂-NH₂ was monitored in 40% acetonitrile water with 0.1% TFA, water with 0.1% TFA, and water with 100 mM NaCl. The resulting assembly solutions were characterized using Fourier transform infrared spectroscopy (FT-IR) and transmission electron microscopy (TEM). While additional work is needed to gain further insight into solvent effects, preliminary findings indicate that self-

assembly occurs under all solvent conditions, although some polymorphism in assembly morphology may exist. Future work will focus on interrogation of the details of these effects.

5- “SERS for in Situ Investigation of Alzheimer Mouse Brain”

Presenters: Julia Malinchak, Joshua Thomas; SUNY Geneseo

Advisor: Kazushige Yokoyama

This is the first report on the amyloid fibril interacting with gold colloid nano- particles (diameter; $d \sim 80$ nm) monitored through the Surface Enhanced Raman Scattering (SERS). The Long Evan’s Cohen’s Alzheimer’s disease rat model was used and the hippocampus was extracted and processed with and without gold nano--particles. The middle section of the hippocampus was selected and examined for any sign of fibril that was confirmed of having amyloid beta ($A\beta_{1-40}$ or $A\beta_{1-42}$). The SERS imaging exhibited an existence of the formation of gold colloidal aggregates with enhanced Raman signal, thereby implying the significant interaction between amyloid oligomers and gold nano-particle hippocampal section surfaces. The detectable fiber-like segment from within the hippocampal sections seemed to have a high correlation with the location of the formation of gold colloid aggregates, indicating that the terminal form of a fibril may remain in the hippocampal section containing highly interactive portions (i.e., oligomeric conformations) to cause such aggregation of $A\beta_{1-40}$ or $A\beta_{1-42}$ es.

6- “Protein Corona Formation by SARS-CoV-2 Spike Protein Over Nano-Gold Colloids and Reversible Aggregation”

Presenters: Christopher Lembo, Zichao Lin, Alexander Seram; SUNY Geneseo

Advisor: Kazushige Yokoyama

The SARS-CoV-2 alpha spike protein over the nano-gold colloid was investigated under the pH change between $pH \sim 3$ and $pH \sim 11$. The acidic condition (i.e., $pH \sim 3$) exhibited a sign of aggregation through unfolded conformation of RBD (Receptor Binding Domain) segment of a spike protein. As the pH was repeatedly altered between acidic ($\sim pH 3$) and basic ($\sim pH 11$), the aggregation was quasi-reversibly formed at $\sim pH 3$ and deformed at $\sim pH 4$. However, a definite conformation and exact adsorption orientation was not assigned yet. The conformational change was examined and compared to the case by omicron-spike protein, and reversible conformational change was observed. The addition of ACE2 to the spike protein coated 50 nm gold colloid showed two stages of conformational change implying there was a sign of two different sets of conformational change before and after roughly 25 minutes once spike protein was exposed to pH 4 condition. This was followed by a conformational change forming an aggregate at basic condition. This work demonstrated that the aggregation process of nanoparticles with SARS-CoV-2 protein corona was controlled by an external pH change.

Environmental Posters

7- **“Increasing Biodiesel Algal Lipid Density by Manipulating Glycerol Levels in Algal Growth Mediums”**

Presenters: Alejandro Lazaro, Samantha Ross, Lauren Saggese, Aiden Williams; SUNY Geneseo
Advisor: Barnabas Gikonyo

To many, algae are the pesky product of eutrophication in local lakes and ponds. In the laboratory, algae is a promising competitor for renewable resources of biodiesel.

Algae is versatile in the way that it ingests a notable amount of carbon emissions from the atmosphere. These emissions are then converted into energy-dense lipids, which can be harvested and transformed into biofuel. Despite the advantages, the amount of lipid yield is not significant enough to be considered a worthwhile option. Before the fuel industry can accept algae farming as a worthy alternative to fossil fuels, the reason for harvesting must be maximized further. Our purpose aims to make algal lipid extraction more efficient by determining the ideal growing conditions of the algae species *Chlorella Vulgaris*. Our research explores ways to effectively quantify and compare the algal lipid yield to the various controlled algal growth media and environments. Particularly, testing involves a) the interconnectivity between different algal lipid density and growing mediums and b) the effects, if any, of glycerol. The algal media used were BG-11 (algal culture medium) and BBM (Bold’s basal medium). Initial data suggested that density growth was higher when grown in the glycerol and BBM mixture. The results obtained with further experimentation are presented hereafter.

8- **“Investigating the Promise of Lignocellulosic Biofuels: Rice Husks as a Non-Human Feedstock”**

Presenters: Dineen Vogler, Valerie Lepore, Gage Smith; SUNY Geneseo
Advisor: Barnabas Gikonyo

The Earth has endured years of damage caused by an overuse of fossil fuels. To combat the damage, biofuels have become of interest as an alternative energy source. Biofuels represent an economical and often overlooked alternative to fossil fuels. Efforts have been geared toward the use of food sources such as corn as a first generation biofuel. Although first generation biofuels aid in curbing greenhouse gas emissions, they lead to increasing food prices, which negatively impacts developing countries. This project focuses on the use of one of the most abundant and readily available biomass, rice husks as biofuel feedstock. Second generation biofuels are also relatively inexpensive. The outermost layer that is separated from the rice grains during the milling process is usually thrown away as a waste product. Rice husks are ideal as a biofuel feedstock, because they're cheap if not free, and they have the power to curb greenhouse gas emissions. One of the greatest challenges in conversion of feedstock into biofuel is how to break the biomass down; a process termed pretreatment. For this project, a unique class of solvents, ionic liquids, are employed in the pretreatment process. An ionic liquid (1-Butyl-3-methylimidazolium chloride) was used for the pretreatment of the rice husks to yield glucose. The amount of glucose obtained

is then quantified using refractometry, and DNS analyses. From this, it is then possible to determine how efficient rice husks are as second generation biofuel. The results are presented and discussed herewith.

Inorganic Posters

9- “Synthesis and Characterization of Actinide Pyridine Dipyrrolide Complexes”

Presenter: Lauren Lopez; University of Rochester

Advisor: Ellen Matson

The study of the accessibility of the f electrons and orbitals available in the actinide elements is of particular importance in advancing our basic understanding of the elements as well as applications towards energy focused research projects. The study of the availability of the f electrons and orbital is one that is currently underdeveloped and remains in its infancy. Millsman and coworkers at West Virginia University have demonstrated the role and accessibility of d electrons in the synthesis of zirconium bis-pyridine dipyrrolide (PDP) (Zr (PhPDPPH)₂) complexes with varying ligands within the class. These complexes showed wide electrochemical potentials with multiple redox events. Herein, we demonstrate the synthesis and characterization of U (PhPDPPH)₂ (derived from [2,6-bis(3,5- phenyl-1H-pyrrol-2-yl)pyridine] (H₂PhPDPPH)) along with U (Cl₂PhPDPPH)₂ (derived from 2,6-bis(5-(2,6-dichlorophenyl)-3-phenyl-1H-pyrrol-2-yl)pyridine (H₂Cl₂PhPDPPH, Cl₂Ph = 2,6-dichlorophenyl)) in an effort to study the exact role of the available f electrons in metal to ligand charge transfer processes and the compound’s electrochemical potential in comparison to the results obtained by Millsman and coworkers. Additionally, preliminary studies have been performed on the synthesis of Th (PhPDPPH)₂ and the accessibility of the f orbitals within the compound to allow for a comparison across the actinide series.

Organic Posters

10- “Lewis Acid Catalyzed Ring Opening of α -Unsubstituted Azetidines”

Presenter: Rebecca Huss; Hobart and William Smith Colleges

Collaborators: Christina Mitrow, Jack Russo

Advisor: Erin Pelkey

Using alpha-unsubstituted azetidines as an electrophile in Friedel-Crafts like chemistry has posed a challenge due to nitrogen not being a good leaving group. However, this reaction is important to study because azetidines are a potentially useful building block for drug design, though simple azetidines are rarely studied. Our focus has been on studying the ring opening of simple azetidines using various indoles as nucleophiles. We found the most success by using indium triflate, calcium hydride, and chlorobenzene at a temperature of 130°C reacting for 16 hours. These reaction conditions have been tested with eight various indoles which has resulted in oils. Though

successful, there has been complications with the azetidine as there is an impurity in the starting material. This has posed a challenge as it is overpowering the product in ¹H NMR. However, by purification of the crude azetidine by column chromatography we have overcome this challenge and has led to successful ring opening reactions of tosyl azetidine.

11- “Synthesis of PY-454-C as a Tubulin Polymerization Inhibitor”

Presenters: Taylor Coburn, Carolyn George; Hobart and William Smith Colleges

Advisor: Erin Pelkey

Previous studies performed by The Pelkey Research Group have shown that isomeric diarylfuranones exhibit anti-cancer activity through tubulin polymerization inhibition. We have developed complimentary methods for preparing various isomeric diarylfuranones using 3-aryltetronic acids as key building blocks. Computational studies have suggested a new synthetic target, PY-454-C, which is predicted to strongly bind to the Colchicine binding site of tubulin. PY-454-C, is a diarylfuranine contains an indole ring with a phenylpropyl substituent on the nitrogen atom. This work outlines the progress in the synthesis of PY-454-C mainly concerning the alkylation of indole acetic acid. Currently, alkylation methods are resulting in a mixture of mono and di-alkylated products.

12- “Total Synthesis of Sakenin F”

Presenter: Aidan Kropiwnicki; University of Rochester

Collaborators: Amanda Canfield, Kaitlyn Houghtling

Advisor: Shauna Paradine

In the Paradine lab, we seek to develop methodologies for creating oxygen-containing heterocycle motifs that also have emphasis on being greener, safer, cheaper, and more robust. A previous technique towards accessing these scaffolds is through a palladium and phosphine ligand mediated heteroannulation of bifunctional reagents and olefins. However, phosphine ligands are often expensive and highly sensitive to ambient conditions, not to mention toxic to the human CNS. These factors not only reduce the atom economy of the transformation, but reduce the synthetic utility of this technique as well. A proposed alternative uses a urea-ligand platform that is a highly tunable, low-cost, bench-stable alternative. Our group has recently developed a method that successfully synthesizes a diverse scope of dihydrobenzofurans via a palladium and urea-mediated heteroannulation. This method not only addresses the aforementioned challenges reported in previous literature, but is done using green solvents and reduced loading of reagents to address atom economy.

In the interest of continuing my past research from this year and the summer prior, I will be working on completing the total synthesis of Sakenin F (Figure 1, bottom left). My past work has focused on the expansion of the scope of our recently developed method by using it on a more complicated substrate which would lead to the desired final molecule, of Sakenin F. This would

be the first total synthesis of Sakenin F, and it would also demonstrate the ability of our urea-ligand platform to help catalyze heteroannulations under sterically and electronically complex conditions.

Physical Posters

13- “Investigation β 2-Microglobulin Networking over Gold-Nanoparticle Surfaces”

Presenters: Theresa Lam, Jennie Dworkin; SUNY Geneseo

Advisor: Kazushige Yokoyama

While there are strong concerns and interests about the impact of β 2-microglobulin (β 2m) amyloids in the human body, no detailed investigation of an initial networking process of β 2m has been fully characterized. Our group has established a schematic method to investigate the peptide-peptide networking by controlling the protein conformation through external pH condition change over nano-gold particle surfaces. The protein conformation change was indirectly monitored by the peak shift of the SPR (Surface Plasmon Resonance) absorption band of the gold colloids coated with β 2m. Particularly, the red-shift of the band peak indicates the formation of the gold colloid aggregates due to the interaction between the β 2m or a formation of an oligomer. By a gradual insertion of β 2m to the bare gold colloids under the acidic condition (pH \sim 4), the formation of the aggregates was monitored as a function of β 2m concentration. For the core diameter of the gold colloid $d = 10$ nm, a gradual increase of the aggregates was observed until it reached the asymptote value. On the other hand, for $d = 100$ nm, the asymptote was achieved at a much lower concentration exhibiting a step-function-like feature. The difference in the mechanism may be attributed to the contact range between gold colloids and free β 2m monomers. The gold colloid with a larger diameter could have a higher cross-section to adsorb β 2m resulting in the aggregation at the relatively lower concentration of β 2m.

14- “Investigation of the Nano-Size Dependent Affinity of the SARS-CoV-2 Spike Protein to the Gold-Colloid”

Presenter: Jack Santariello; SUNY Geneseo

Collaborators: Zi Chao Lin, Alex Seram, Joshua Thomas

Advisor: Kazushige Yokoyama

An initial stage of viral infection by SARS-CoV2 was induced by a conformational change of the spike protein (s-protein). In order to understand the behavior of the s-protein and its conformational change, a template to solely investigate the s-protein is required. Our group attempted to adsorb the s-protein to the gold nanoparticle surface, and to characterize the behavior as a function of core nano-particle size

(i.e., diameter; d). As the pH was externally decreased, the red shift of the gold colloid SPR (Surface Plasmon Resonance) absorption band peak position was observed. Compared to the case of bare gold colloids, the gold colloid with $d \geq 50$ nm exhibited a drastic red shift at relatively higher pH conditions. By hypothesizing that a red-shift was due to the formation of the gold colloid

aggregates through the interaction between s-protein, we concluded that higher affinity to the s-protein was found for gold colloids with $d \geq 50$ nm.

15- “A Model for Nano-Scale Spherical Surface Coverage and Protein Corona Formation by Amyloidogenic Peptides”

Presenters: Stephanie Afonso, Emily Benton; SUNY Geneseo

Advisor: Kazushige Yokoyama

The conformation of three amyloidogenic peptides; amyloid beta 1–40 ($A\beta$ 1–40), alpha synuclein (α -syn), and beta-2-microglobulin (β 2m) are closely associated with the process of causing neurodegenerative diseases. Use of a peptide adsorbed gold nano-particle system allowed us to investigate the interactive segment of each peptide responsible for peptide-peptide networking, which is crucial to initiate the formation of an oligomer and leads to fibrillogenesis. The adsorption orientation of the amyloidogenic peptides on the nano-gold colloid spherical surface was explained by simulating how much area of the metal surface was covered by the peptides, i.e., coverage ratio, Θ . The empirically extracted Θ was explained by the summation of the 1st layer and the 2nd layer with a spiking-out orientation of the prolate. Of note, the involvement of the 2nd layer was peptide type dependent. The nano-size dependence of Θ was linearly correlated with available spacing between adjacent peptides, S_d , which were approximated as prolates, For $A\beta$ 1–40 and α -syn, the 2nd layer was more included as S_d increased. In contrast, β 2m was found to gyrate over the gold surface as S_d increased, creating a partially positive (δ^+) region and repelling the extra β 2m from the surface. Thus, as S_d decreased, it prohibited the gyration of β 2m resulting in less δ^+ region, and more β 2m monomers were adsorbed with δ^+ segment as the 2nd layer than the case where β 2m gyrates more under relatively larger S_d . Based on the trend found in an experimentally extracted Θ as a function of S_d , optimized charge distribution of $A\beta$ 1–40 and α -syn were concluded to be negative partial charge (δ^-) region that was covered by the positive partial charge (δ^+) region. However, β 2m may have a relatively large and/or distributed δ^+ region with a small portion of δ^- at the one end of a prolate. The characterization made in this work confirmed current understandings on the formation of the protein corona over nano-particles.

16- “A Computational Study of the γ -Butyrolactone Monomer and its Complexes with Water”

Presenter: Annabelle Carney; Nazareth College

Advisor: Josh Newby

The γ -butyrolactone (GBL):water complex was computed and analyzed through the study of the GBL monomer, electron density mapping of both GBL and water, and utilized Gaussian 16 to make inferences on how this specific complex would occur in nature, and measure the energies, optimizations and frequencies. Several input structures led to complexes to be found in natural GBL and water interactions. Hydrogen bonding was seen as the driving force of these interactions, between the water monomer and the GBL's oxygen atoms. Accounting for isotopologues and the identified transition state, further research would be required to experimentally confirm the

structures and their physical chemistries. The understanding and conclusions of this phenomena were seen through the identification of computed interactions with various electron density theories. The information gained from the GBL:water complex can be used to examine the energy and transition of GBL to GHB, γ -hydroxybutyrate, commonly known as liquid ecstasy.

17- “Solvation Dynamics in Glyceline Deep Eutectic Solvents”

Presenter: Christian Green; SUNY Brockport

Advisor: Mark Heitz

Deep eutectic solvents (DESs) are important, novel solvents with application toward replacing, or at least reducing the amount of, hazardous organic solvents that are widely used in chemical industry. DESs are typically viscous making the solvent more difficult to work with, so the addition of modifiers such as cosolvents can significantly improve solution fluidity. In this work we are determining the physical properties of DES + cosolvent binary solvent systems and the subsequent interactions in neat and cosolvent-modified DESs. The physical properties measured in this work are primarily based on density and viscosity. In addition to physical properties characterization, we used steady-state and picosecond time-resolved fluorescence spectroscopy to determine the solvation dynamics in the DES + cosolvent binary mixtures. The goal of this project is to describe the solvation behavior in DESs and contribute to the chemical literature on environmentally friendly alternative solvents.

18- “Molecular Interaction of Imidazolium-based Ionic Liquids with a DNA-Oligonucleotide”

Presenter: Derek McNeil; SUNY Brockport

Advisor: Mark Heitz

With the rise in popularity of Ionic Liquids (ILs) the viability of using ILs as a green solvent and potential storage medium for DNA was studied. A self-complimentary 14-mer (7-TA) double stranded DNA oligonucleotide and 1-hexadecyl-3-methyl-imidazolium chloride (C-16MIMCl) were used to study IL intercalation within the DNA. Steady-state and time-resolved fluorescence measurements were made using fluorescein, which was covalently attached to the DNA oligomer. A wide range of C-16MIMCl concentrations were added to the DNA/buffer solution and are compared to the results with no added IL. Shifts in the steady state excitation and emission spectra show that upon addition of C16MIMCl the spectral parameters undergo a dramatic change with the addition of as little as 1 mM IL, indicating strong interactions between the IL and DNA. By 30 mM, the IL appears to have saturated the DNA. Time-resolved data from excited-state fluorescence lifetimes and rotational dynamics provide further, more detailed evidence that substantiates IL/DNA interactions. While the IL associates with the DNA, we find no evidence for DNA deterioration or denaturation.



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