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Symposium Program

- 3:30–4:00 PM: Participant Check-In
[PRE-REGISTER AT THIS LINK.](#)
- 4:00–4:45 PM: **Poster Session A**– Attend at the room # corresponding to the poster #
- 4:45–5:30 PM: **Poster Session B**– Attend at the room # corresponding to the poster #
- 5:30–6:00 PM: Awards and Announcements
- ACS Membership Service Awards
 - College Recognition Awards
 - High School Teacher Awards
 - Research Awards
- 6:00–7:00 PM: [The Unique World of Metallic Nanoparticles](#)
[Dr. Nasrin Hooshmand](#)
Senior Research Scientist
[Georgia Tech Laser Dynamics Laboratory](#)



The Unique World of Metallic Nanoparticles

Nasrin Hooshmand

Laser Dynamics Laboratory, School of Chemistry and
Biochemistry, Georgia Institute of Technology, Atlanta,
Georgia 30332, USA

Abstract

Metallic nanoparticles especially those made of silver and gold have fascinated scientists for decades due to their unique optical properties generated at the nanoscale when they are exposed to electromagnetic radiation. Today these materials can be synthesized and applied in a variety of applications including, biological sensing, drug delivery, solar cell, cancer treatment, etc. This talk will describe the theory and some applications of metallic nanoparticles and also discuss some of the Laser Dynamics Laboratory's activities, including plasmonic nanoparticles and their application in cancer diagnosis and treatment.

Biography

Dr. Nasrin Hooshmand is a Senior Research Scientist in the School of Chemistry & Biochemistry and Assistant Director of the Laser Dynamics Laboratory at Georgia Institute of Technology. She received her Ph.D. and M.Sc. degrees in physical chemistry. Her research interests center on light-matter interactions at the nanoscale. She has developed computational strategies and simulation protocols to analyze and model optical properties of plasmonic (noble metal) nanoparticles for imaging, sensing, and healthcare applications. She has won several awards including the Research Faculty Teaching Fellow award. Due to her mentorship, research, teaching, and leadership, she has been named in the 2020 Faces of Inclusive Excellence Publication at Georgia Tech. Dr. Hooshmand's publications possess a unique combination of expertise in computational physical chemistry, plasmonics, and nanoscience. She is an author and co-author of more than 40 publications in the most prestigious multidisciplinary scientific journals such as the Proceedings of the National Academy of Sciences (PNAS).

Poster Session A

Poster 1A

DESIGN AND CHARACTERIZATION OF AN IN VITRO CRISPR/CAS 9 MODEL SYSTEM

Danil Ratnikov, Swapan Jain*

Bard College

30 Campus Rd, Annandale-On-Hudson, NY 12504

sjain@bard.edu

CRISPR/Cas9 is a technique in molecular biology yielding effective DNA cleavage. For effective DNA cutting, CRISPR/Cas9 system requires appropriate single guide RNA (sgRNA) and a functional sgRNA binding site on Cas9 enzyme. The goal of this project is to design a functional CRISPR/Cas9 test tube model system for further research in the lab. The costs and inaccuracy associated with RNA synthesis constitute a limitation for CRISPR technology use. To this end, a truncated functional sgRNA is desired. In this study, we will also design a shortened sgRNA that is missing the trans-activating CRISPR RNA (tracrRNA) portion. The cleaving potential of sgRNA system composed entirely of shortened sgRNA is evaluated thermodynamically using isothermal titration calorimetry (ITC) and *in vitro* gel cleavage assays. The findings indicate cleavage ineffectiveness of the designed RNA, while full sgRNA is functioning normally. The ITC data suggests no noticeable difference in the thermodynamic interactions between the modified sgRNA cas9 system and the full sgRNA cas9 system.

Poster 2A

PROGRESS TOWARD THE BIOCHEMICAL CHARACTERIZATION OF A PROTEIN INVOLVED IN THE PRODUCTION OF MICROBIAL PLASTICS

Stella Rose Schneeberg, Atahualpa Pinto*

Bard College

30 Campus Road, Annandale-on-Hudson, NY 12504

apinto@bard.edu

Poly(3-hydroxyalkanoates) (PHAs) are biodegradable polymeric materials that are of interest due to their ability to serve as green alternatives to the less environmentally friendly petroleum-based plastics that populate our modern world. PHAs are produced by various microorganisms from sugar and fatty acid feedstocks, and they are degraded by microorganisms as well. The metabolic fundamentals of the production of PHAs can be investigated through studying the behavior of the protein PP_0763 from the soil bacterium *Pseudomonas putida* KT2440, which is involved in the metabolic redirection of intracellular fatty acids toward PHA biosynthesis. PP_0763 has been successfully expressed and purified, and insight can now be gained into the substrate specificity of this protein via biochemical assay. In order to move forward with assay design, in this study we demonstrate our progress towards the synthesis of a panel of enantiopure 3-hydroxyfatty acids via an asymmetric aldol strategy. Once complete, our assay will test the protein's affinity for 3-hydroxyfatty acids of varying hydrocarbon chain lengths, leading to clarification of the role the protein plays in PHA biosynthesis.

Poster 3A

EXPLORING THE BIOTIC AND ABIOTIC ENVIRONMENTAL INTERACTIONS OF SOIL CHEMISTRY AND NOVEL *BACILLUS* SPP. ISOLATES

Mia Sheshova, Brooke A. Jude*, and Emily C. McLaughlin*

Bard College
Annandale-on-Hudson, NY 12504

mclaughl@bard.edu

The complex heterogeneity of soil makes it challenging to study the biological and chemical processes involved in its biotic environment. Nevertheless, the interaction between the biotic and abiotic environment can explain the symbiotic and antagonistic relationship between the soil and its surroundings. In fact, soil microbiota plays an essential role in the decomposition, nutrient cycling, and fertilization of the soil, which exemplifies the importance of bacteria in affecting the soil's chemistry. Bacteria are the messengers of chemical diversity in the soil. Therefore, measuring the distribution of inorganic matter while trying to unravel the bioactive compounds secreted by the bacterial secondary metabolism highlights the differences between soil locations. To better understand the presence of certain bacteria and their metabolites, this study aims to compare the soil chemistry of locations with artificial or natural turf in order to correlate their distinction with the production of bioactive compounds that elicit antimicrobial activity against the ESKAPE pathogens, species known for virulence and antibiotic resistance. This study focuses on the characterization of phenotypic and genomic identities from three novel *Bacillus* strains isolated from natural and artificial turf. Our goal is to examine the relationship between the three bacterial strains and the soil's chemical composition through digestion/extraction and analysis techniques using NMR, GC/MS, and ICP/OES.

Poster 4A

STEREOSELECTIVE OXIDATION ADDITION TO PLATINUM(II)

Juliette Knapp, Craig M. Anderson*

BARD COLLEGE

30 Campus Road, Annandale-on-Hudson, NY, 12504

canderso@bard.edu

Oxidative addition is a fundamental organometallic reaction that is often observed in catalytic reactions. In this study, diimine, thiophene-derived ligands containing two stereocenters were reacted with a tetramethyl platinum dimer to give platinum(IV) or platinum(II) complexes through oxidative addition reaction and reductive elimination. These platinacycles were reacted with alkyl halides to explore the stereochemical consequences of oxidative addition reactions.

Poster 5A

SYNTHESIS, CHARACTERIZATION, AND PHOTOPHYSICAL PROPERTIES OF CYCLOMETALATED PLATINUM(II) COMPLEXES CONTAINING A SECOND CHELATE LIGAND

Belle Coffey, Craig M. Anderson*

BARD COLLEGE

30 Campus Road, Annandale-on-Hudson, NY, 12504

canderso@bard.edu

Cyclometalated platinum(II) compounds with cheating phosphine ligands were synthesized, characterized, and their photophysical properties were measured. The compounds were characterized by multi-nuclear NMR spectroscopy. Absorbance spectra, emission spectra, lifetime of excited states, and quantum yields were determined in solution, solid state, and in PMMA (poly(methyl methacrylate)) films. When doped in PMMA films, our cyclometalated platinum(II) compounds' quantum yield doubled, if not tripled, when compared to samples in other states.

Poster 6A

CHEMICAL ANALYSIS OF HISTORIC ALTAR IN THE HUDSON VALLEY

Liri Ronen and Christopher N. LaFratta*

Bard College

30 Campus Rd. Annandale-on-Hudson, NY 12504

clafratt@bard.edu

Through the 18th and 19th century, the parsonage site in Germantown, NY housed the Calvinist minister of Germantown, as well several individuals of African-American descent, both free and in bondage. An etching of a traditional Bakongo Cosmogram found next to the hearth in the basement of the Parsonage, which served as the slave quarters, had, along with other material evidence, raised interest in the strong possibility of the fireplace's use as an altar. Through extraction, microscopy, and spectroscopy of trace chemical and botanical evidence, I hope to reveal more about the practices and habits of the parsonage dwellers, and provide further proof of the spiritual activity that might have taken place there.

Poster 7A

LOW ONE-PHOTON ABSORPTION POLYMERIZATION FOR 3D MICROFABRICATION

Cecily Rosenbaum and Christopher N. LaFratta*

**Bard College
30 Campus Rd. Annandale-on-Hudson, NY 12504**

clafratt@bard.edu

Direct Laser Writing (DLW) opened the doors for the efficient and customizable fabrication of both 2D and 3D micro- and nanostructures. Currently, Two-Photon Polymerization (TPP) is the ubiquitous DLW method; however, its use is cost inhibitive. Low One-Photon Absorption (LOPA) provides a cheap avenue for DLW and yields comparable 2D and 3D structures in their size and complexity. The underlying mechanistic components of LOPA are largely unknown, and thus require further investigation in order to optimize low one-photon polymerization methods. This work seeks to elucidate these underlying components, as well as demonstrate LOPA's use as an alternative to TPP.

Poster 8A

PAPER-BASED 3D-UPAD DEVICE FOR A COLORIMETRIC SANDWICH IMMUNOASSAY

Frank Rybicki and Christopher N. LaFratta*

**Bard College
30 Campus Rd. Annandale-on-Hudson, NY 12504**

clafratt@bard.edu

This project describes the novel fabrication of a paper-based 3D- μ PAD using a colorimetric sandwich ELISA assay to detect C-reactive protein (CRP), an inflammatory biomarker, in a blood sample. Unique patterns were screen printed on to chromatography paper using a highly hydrophobic plastisol ink to create different layers with three specific channels in the device, which hold stored reagents. The patterned layers are stacked on top of one another using a paper-tape-paper sandwich to create three fluidic channels in the device. A sliding strip is fabricated with a nitrocellulose sensing zone loaded with the CRP capture antibody. This sliding strip is pulled through the device and completes each microfluidic channel when the sample or a buffered solution is added to each well, culminating in a colorimetric read out. One example where such device would hold important clinical relevance is to detect different cytokines in a blood sample to predict the severity of a COVID cytokine storm.

Poster 9A

ALGINATE ENCAPSULATION PROTECTS XYLANASE FROM OXIDATIVE INACTIVATION

Esabelle D. Gervasio, Annemarie A. Lee, Elisa M. Woolridge*

Marist College
3399 North Road, Poughkeepsie, New York 12601

elisa.woolridge@marist.edu

A mixed system of hydrolytic and oxidative enzymes provides opportunity to facilitate lignocellulosic biomass utilization via deconstruction without chlorine-based reagents that would otherwise prevent lignin recovery and valorization. Xylanase and laccase have utility as hydrolytic and oxidative delignification agents, respectively, when applied in separate steps; however, these enzymes have limited use when applied simultaneously, as laccase, with its requisite redox mediator for oxidation of nonphenolics, promotes xylanase inactivation. Laccase is also susceptible to modification by the oxidized mediator. Our work has sought to identify methods to minimize enzyme inactivation, such as enzyme immobilization. In this study, xylanase was encapsulated with either Ca^{2+} - or Cu^{2+} -alginate, and then exposed to the laccase mediator system (LMS), with variations such as mediator type, mediator concentration, and treatment pH. Results demonstrate that alginate-encapsulated xylanase retains substantial activity when exposed to the LMS relative to non-encapsulated xylanase. This indicates potential to develop a mixed enzyme system with reduced enzyme damage for maximized biomass delignification.

Poster 10A

EFFECT OF *B. PAPYRIFERA* EXTRACT ON GROWTH OF *DROSOPHILA SPECIES*

Chris Civil, Lucia Speranza, Miles Wilklow-Marnell*

SUNY New Paltz
1 Hawk Dr, New Paltz, NY 12561

marnellm@newpaltz.edu

In our research we are investigating the use of birch bark extract; containing triterpenoids such as betulin, betulinic acid, and lupeol as its major components, in order to observe the effects it has on *Drosophila* species. In previous studies it has been shown that extracts from *Terminalia Arjuna* have similar triterpenoids and have been observed to be a deterrent in the growth and development of *D. Melanogaster* when incorporated into their diet. Dried bark of white birch (*Betula papyrifera*) was extracted by Soxhlet method using various solvents. The average yield of concentrated extracts was 19.35%. ¹H-NMR studies confirmed the presence of Betulinic triterpenoids when compared to known reference spectra. The relative content of betulin, betulinic acid, and lupeol is being investigated by GCMS analysis. Silylation was found to be necessary for elution of betulinic acid. Preliminary results have indicated that there is enhanced development of the larvae's life cycle when *B. papyrifera* extract is incorporated into their diet contrary to the extract obtained from *T. Arjuna*.

Poster 11A

PHYTOCHEMICAL AND INSECTICIDAL STUDIES OF *SAUSSUREA LAPPA*

Sery Pak, Aabir Aslam, Varsha Talanki, Aaron Haselton*, Preeti Dhar*

State University of New York at New Paltz
1 Hawk Drive, New Paltz, NY 12566

haseltoa@newpaltz.edu
dharp@newpaltz.edu

Saussurea lappa (*S. lappa*) is an herb that is indigenous to the Himalayan region (India, Pakistan, and China). The roots of this plant are used in agricultural fields and stored with woolen clothing due to its insecticidal properties. Literature studies have shown that two terpene derivatives found in this plant (costunolide and dehydrocostus lactone) are known to exhibit insecticidal activity. In the previous year, crude extracts of *S. lappa* using various solvents (water and ethanol), in addition to sequentially extracting *S. lappa* with solvents of increasing polarity (hexane, ether, ethyl acetate and ethanol) were concentrated and then evaluated for the presence of saponins, tannins, flavonoids, alkaloids, carbohydrates, and terpenoids using standard tests. In continuation of this study, the pesticidal effects associated with increasing concentrations of the ethanolic crude extract were investigated with *Drosophila melanogaster*. Within 12 hours of oviposition, *D. melanogaster* eggs were tested against 12.5, 25, and 50 mg/ml concentrations of the crude ethanolic extract to evaluate its effect on larvae growth over 2, 3, and 4 days post-oviposition. Following larval extraction, the resulting lengths were measured and analyzed. The results of the preliminary bioassays will be presented.

Poster 12A

GC-MS DETERMINATION OF POLYCYCLIC AROMATIC HYDROCARBON (PAH) CONTENT IN SOIL COLLECTED FROM HISTORIC LIME KILNS

Jeffrey Kitchen, Megan A. Ferguson*

**SUNY New Paltz
1 Hawk Drive
New Paltz, NY, 12561**

fergusom@newpaltz.edu

Following the recent acquisition by the Kingston Land Trust of a 5.9-acre parcel previously mined for limestone including historic lime kilns, surface soil samples were examined for elevated levels of chrysene, benzo(a)pyrene, benzo(a)anthracene, and other polycyclic aromatic hydrocarbons (PAHs). PAHs are a product of combustion and present a health risk that could determine future recreational use of the land. PAH extractions involving sonication in cyclohexane, followed by Gas Chromatography Mass Spectrometry (GC-MS), were used to identify and quantify PAHs in soil samples collected from locations throughout the parcel. Results will be considered in relation of concentration to distribution, proximity to extant structures, and soil composition. Effectiveness of extraction and GC-MS techniques will also be considered.

Poster 13A

BARIUM CONCENTRATION AT THE KINGSTON LAND TRUST

Julia Mei Hanzl, Megan A. Ferguson*

**SUNY New Paltz
1 Hawk Drive
New Paltz, NY, 12561**

fergusom@newpaltz.edu

Soil samples from land recently acquired by the Kingston Land Trust were tested for trace elements that could be harmful to humans if overexposed. The main focus of this paper is to determine the concentration of barium, which can be sourced back to the historic lime kilns on the property. Soil was collected at various locations including old lime kilns, an abandoned limestone quarry, and a primitive parking lot made from moving onsite rock waste. It was then digested using HNO_3 , H_2O_2 , HCl and various heating periods. The elements and their concentrations within the mixtures were determined by ICP-AES. Establishing the concentration of barium within the soil can help those working at the Kingston Land Trust make decisions about how best to ensure safe public access to the land.

Poster 14A

ATOMIC FORCE MICROSCOPY OF PYROLYZED CHICKEN FEATHERS

Arlinda Durmishaj, Megan A. Ferguson*

**SUNY New Paltz
1 Hawk Drive
New Paltz, NY, 12561**

fergusom@newpaltz.edu

In the United States alone over 3 million pounds of chicken feathers are produced as a waste product each year. Chicken feathers could potentially be used as a feedstock for different applications including energy storage, water filters, electromagnetic shields and more due to the absorbency of keratin in the feathers and the tubular carbon-based structure of the feather fibers. In this study, chicken feathers were pyrolyzed under a N₂ atmosphere at temperatures ranging from 600-900 degrees C. The products were imaged using atomic force microscopy to observe the surface of the pyrolyzed feather material. Comparisons of product between different temperatures will be discussed.

Poster 15A

ROLE OF LIPID A PHOSPHORYLATION IN IDENTIFICATION OF PREY BY *BDELLOVIBRIO BACTERIOVORUS*

Julio Aguilar, Nelson Aguilar, Kristyn Gessner, Megan A. Ferguson*

SUNY New Paltz
1 Hawk Drive
New Paltz, NY, 12561

fergusom@newpaltz.edu

Bdellovibrio bacteriovorus is a Gram-negative bacterium that preys on nearly all other Gram-negative bacteria except itself, but the mechanism of prey identification remains unknown. Since the vast majority of Gram-negative cells have lipopolysaccharide (LPS) molecules composing their outer membrane and the lipid A region of LPS is highly conserved across species, the chemical composition of lipid A could be a target. *B. bacteriovorus* itself has highly unusual lipid A structure in which both phosphate residues present in typical lipid A are substituted by mannose. Here, *B. bacteriovorus* was grown both in liquid buffer and on agar with three strains of potential prey cells: K-12 *E. coli*, which has conventional lipid A, and two other K-12 strains that produce mono- or non-phosphorylated lipid A. In addition, the liquid predator/prey suspension was pipetted onto filtration membranes and the membranes were imaged as a time series using AFM. In liquid buffer, *B. bacteriovorus* preys on all types of *E. coli*, although LPS phosphorylation level may impact how quickly predation occurs. In double layer agar plates, a clear preference for dephosphorylated over mono- or nonphosphorylated LPS is established, but under certain conditions *B. bacteriovorus* is still able to consume mono- and nonphosphorylated prey. Since *B. bacteriovorus* cells are significantly smaller than *E. coli* cells and do not efficiently scatter visible light, clearing of liquid suspension (measured by optical density at 600 nm) or agar was indicative of successful predation by *B. bacteriovorus*.

Poster 16A

RETENTION OF DEUTERATED BPA DURING PLANARIAN REGENERATION

Brianna M. Flood, Natalia Kurek, Spencer Mass, and

Pamela M. St. John*

**SUNY New Paltz
1 Hawk Drive
New Paltz, NY 12561**

stjohnp@newpaltz.edu

Bisphenol-A (BPA) is a xenoestrogenic environmental pollutant produced in large quantities by industry, including plastic manufacturing and packaging for consumer goods, health and beauty products and thermal printing. Due to its common use, ecological exposure is nearly unavoidable therefore, it is important to understand the effects of these compounds on the environment. Freshwater planaria (*G. tigrina*) are a species of flatworms known for their ability to regenerate. Prior work in our lab has demonstrated that exposure to bisphenol compounds severely affects planarian behavior and regenerative capacity however, it is often difficult to relate controlled exposure with the amount retained in an organism because of the variable BPA concentrations found in the environment. We exposed planaria to deuterated BPA (d8-BPA) in order to differentiate it from the more ubiquitous form. During a 14-day exposure, regenerating planaria were imaged optically to understand the effect d8-BPA had on their growth. The area of the regenerated blastema was ratioed to the area of the whole worm to generate a growth curve and the phenotypic changes were correlated with the amount of d8-BPA retained.

Poster Session B

Poster 1B

Cp* IRIDIUM COMPLEXES BEARING PHENYLIMINO- QUINONE-BASED LIGANDS

Ashleigh Arrington, Joseph Spiconardi, Miles Wilklow-Marnell*

**State University of New York at New Paltz
1 Hawk Drive
New Paltz, NY 12561**

marnellm@newpaltz.edu

A set of N,O binding, quinone-based ligands including 1,4-dihydroxy-benzylidene-phenylimine ($^{\text{Ph}}\text{NHQ}$) and other variations with substitutions on the phenyl ring were prepared. Half-sandwich iridium complexes of the general formula $^{\text{Ph}}\text{NHQIrCp}^*\text{Cl}$ were synthesized using $[\text{Cp}^*\text{IrCl}_2]_2$ as the iridium source, and characterized via X-ray diffraction and NMR spectroscopy. The complexes have been assessed as catalysts in several reactions, including the Guerbet upgrading of ethanol to higher alcohols. Coordinatively unsaturated cationic derivatives of the $^{\text{Ph}}\text{NHQ}$ complex were prepared with triflate and tetrafluoroborate counterions by reaction with their corresponding silver salts, and characterized by ^1H and ^{19}F -NMR spectroscopy. Ligand addition studies of these complexes has been conducted with a series of nitrile-based ligands, CO, and triphenylphosphine, monitored by ^1H -NMR spectroscopy. The formation of iridium hydride complexes by activation of H_2 was observed after reaction of $[\text{Cp}^*\text{Ir}(\text{NHQ})][\text{Otf}]$ with sodium ethoxide followed by exposure to 1 atm H_2 .

Poster 2B

INVESTIGATING SOIL LEAD CONCENTRATION AND PROVENANCE IN POUGHKEEPSIE AND NEWBURGH PUBLIC PARKS

Eva Gómez, Alison Spodek Keimowitz*

**Vassar College, 124 Raymond Ave
Poughkeepsie, N.Y. 12604**

alspodek@vassar.edu

Pediatric Blood Lead Levels (BLLs) have been found to be elevated in Poughkeepsie and Newburgh, N.Y. as compared to surrounding areas. This is of concern as exposure to lead early in life leads to adverse health outcomes throughout one's lifetime. This study builds upon the existing body of literature, examining public park topsoil in both cities as a possible source of exposure to lead in early childhood. To do this, we utilized XRF and ICP-MS to examine net lead concentration and lead isotopic ratios. Isotopic analysis by ICP-MS provides insight into provenance of lead contamination, which is of interest as Newburgh's People's Park was the site of the Consolidated Iron and Metal smelter (Superfund ID NYD0002455756) until 1999. Preliminary results indicate that out of the parks sampled only Pulaski Park in Poughkeepsie was found to have a mean Pb concentration (467.011 ppm) exceeding the EPA soil lead hazard value of 400 ppm. Poughkeepsie parks were found to have higher topsoil lead concentrations and variability (i.e. soil sample heterogeneity) as indicated by larger standard deviations between samples. Of all parks sampled, People's Park had the lowest soil Pb concentration (29.667 ppm) and standard deviation (<10 ppm). This is fitting with recent site remediation. The remainder of our study will focus on isotopic analysis by ICPMS and produce final findings for interpretation.

Poster 3B

COMPARISON OF NONPOROUS AND POROUS SILICA NANOPARTICLES FOR BIOMEDICAL APPLICATIONS

Abigail Graham, Brooke Finnessy, Chi K. Nguyen*

Department of Chemistry and Life Science, United States Military Academy, 753 Cullum Road, West Point, NY 10996.

chi.nguyen@westpoint.edu

Silica nanoparticles have been widely researched for a number of biomedical applications, including use as a drug carrier, imaging agent, and procoagulant. To determine optimal properties for biomedical applications, nonporous and mesoporous silica nanoparticles were studied. Nonporous and mesoporous silica nanoparticles were synthesized using surfactant mediated templating processes in either basic or acidic aqueous solvent environment. Samples were characterized by scanning electron microscopy, transmission electron microscopy, dynamic light scattering, and electrophoretic light scattering to obtain data regarding their size, shape, polydispersity, and zeta potential, which are essential to the function and biocompatibility of the nanoparticles.

Poster 4B

SYNTHESIS OF ORGANOMETALLIC CHROMOPHORES TO INVESTIGATE NOVEL MATERIALS FOR REVERSE SATURABLE ABSORPTION

Nanki Verma,¹ Danielle Cross,¹ Jack Harrison,¹ Thomas N. Rohrabough Jr.,² Ryan M. O'Donnell,² William M. Shensky,² Victor A. Jaffett,¹ Chi K. Nguyen^{1*}

1. Department of Chemistry and Life Science, United States Military Academy, 753 Cullum Road, West Point, NY 10996.

2. United States Army Combat Capabilities Development Command Army Research Laboratory, 2800 Powder Mill Road, Adelphi, MD 20783.

chi.nguyen@westpoint.edu

Organometallic iridium(III) complexes have seen increased application in fields such as non-linear optics (NLO), photoredox catalysis, photodynamic therapy, and organic light-emitting diodes. Reverse saturable absorption (RSA), a sub class of NLO, is of particular interest due to its excited state absorbing more light than the ground state. The aim of this research is to synthesize novel organometallic chromophores with RSA properties throughout the visible spectrum. Iridium was chosen as the transition metal center for the organometallic chromophore because of its strong spin-orbit coupling, which allows for multiple excited states, thereby increasing the compound's ability to absorb light from a broad range of wavelengths. Herein, we present the synthesis and characterization of an iridium metallocyclic dimer, $[\text{Ir}(\text{bpb})_2(\text{Cl})]_2$, using the 2-(4-bromophenyl)benzothiazole (bpb) ligand. Without further purification, the intermediate was collected and washed for subsequent synthesis to form the iridium acetylacetonate (acac), $[\text{Ir}(\text{bpb})_2(\text{acac})]$, complex. The resulting product was purified by flash column chromatography using hexane:dichloromethane solvent eluent that exhibited an R_f of 0.70. The isolated product was affirmed to be the $[\text{Ir}(\text{bpb})_2(\text{acac})]$ complex by proton NMR in deuterated dimethyl sulfoxide. The overall yield of the bright orange $[\text{Ir}(\text{bpb})_2(\text{acac})]$ complex was 26%. Photophysical properties of this complex was also investigated for its RSA properties.

Poster 5B

CHARACTERIZATION OF CATALYZED POLYMER-CARBON COMPOSITE MATERIAL FOR THE DEVELOPMENT OF CHEMICALLY-POWERED ARTIFICIAL MUSCLE

Abigail Waldman,¹ Kristen Guiney,¹ Haval Kareem,² Alex Langrock,² Luther Mahoney,² David Mackie,² Chi K. Nguyen^{1*}

1. Department of Chemistry and Life Science, United States Military Academy, 753 Cullum Road, West Point, NY 10996.

2. United States Army Combat Capabilities Development Command Army Research Laboratory, 2800 Powder Mill Road, Adelphi, MD 20783.

chi.nguyen@westpoint.edu

Significant advances have been made in legged robotic design regarding movement and autonomy. However, these designs remain challenged by inefficient leg actuation and do not yet support sustained operations due to energy requirements. This research aims to address these issues through the synthesis, tuning, and characterization of chemically-powered artificial muscle that convert chemical to mechanical energy to generate muscle actuation. The component materials investigated are super-coiled structures composed of catalysts, ionomers, host polymers, carbon fiber, and carbon nanotube. The work presented here are characterization results of component materials. Scanning electron microscopy was used to study the morphology of the carbon and polymer-carbon composite fibers embedded with catalyst, while energy dispersive X-ray spectroscopy was used to study the amount and distribution of metal catalyst on the fibers. Inductively coupled plasma and flame atomic absorption spectroscopy were used to quantify the amount of nickel, cobalt, and platinum in the catalyst. By altering the mole ratio composition and concentration of the catalysts integrated into the fiber, muscle actuation can be optimized in the presence of select chemical environments. The work presented here serves to advance and inform the development of chemically-powered artificial muscle for application in self-sustaining, autonomous, legged robots.

Poster 6B

COMPOSITE CNT-ALGINATE/DNA CAPACITIVE FIBERS

Felita Zhang, Alexa Zammit, Edward Tang, Paul Trackey, Mason Remondelli, Enoch A. Nagelli, F. John Burpo*

**United States Military Academy
Bartlett Hall, Building 753, West Point, NY 10996**

john.burpo@westpoint.edu

To address the need for multifunctional textile fibers that serve as both electrochemically functional and mechanically durable fibers for energy storage and sensing, carbon nanotube (CNT)-alginate and/or DNA solutions were syringe needle extruded into high concentration salt solutions to induce coagulation. Composite solutions were also separately extruded into a chemical crosslinking solution of 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (EDC) and ethylenediamine to facilitate covalent amide linkages between the biopolymers and oxidized CNTs. Different needle gauges were used to control fiber diameter. After rinsing, fibers were either ambient or supercritical dried. Resulting composite fibers were characterized with Fourier transform-infrared spectroscopy (FTIR), scanning electron and optical microscopy, nitrogen gas adsorption, electrochemical impedance spectroscopy, and cyclic voltammetry.

Poster 7B

THE EFFECT OF MICROPLASTIC INGESTION ON MILLIPEDES

Mackey, Kristina; Rhymes, Blake; Davidson*, Silas; and Labare*, Michael

Unites States Military Academy
Dept. of Chemistry and Life Science, West Point, NY 10996

Michael.Labare@westpoint.edu

Microplastics are through physically abrading plastic waste and are generally <1-5 mm in diameter. Multiple studies have shown microplastics are ingested by organisms in the marine realm with negative effects. Few studies have been conducted on the impact of microplastics on terrestrial organisms. This study examined the effects of the microplastic ingestion by the millipede, *Narceus americanus*. Millipeds play an important decomposition role in forest ecosystems. Microplastic particles were generated from commercial polypropylene rope. The average particle size was $401.5 \pm 273.5 \mu\text{m}$ by $174.2 \pm 103.5 \mu\text{m}$. Most of the particles were irregularly shaped. The millipeds were housed in plastic containers 25°C and 100% humidity in the dark and fed a semi-synthetic food mixture of dried oak leaves (42% dry wt), rabbit food (25% dry wt), and potato flakes (33% dry wt) and water (4.25 ml/g dry wt). The experimental group received 4 or 40 mg microplastic/g food (dry weight). The millipedes were monitored for changes in body mass (g), responsivity (R scale), and lifespan. Over a 2 week period the control millipedes were nearly two times more responsive than those fed microplastic. The millipedes consuming plastics had a greater mass variance from inception to termination and were 2- times more likely to die within 2-3 weeks. Future studies will determine if the millipedes biomagnify plastic additives such as phthalates and the effects of microplastics with and without phthalates on the intestinal microbiome.

Poster 8B

MECHANISTIC INSIGHTS INTO THE INHIBITION OF SARS-CoV-2 M^{pro} BY A NATURAL PHENOLIC COMPOUND FROM *THEOBROMA CACAO* L.: *IN SILICO* STUDIES BY MOLECULAR DOCKING AND DYNAMICS SIMULATIONS

Naike Ye, Francesco Caruso, Miriam Rossi*

Department of Chemistry, Vassar College
124 Raymond Avenue, Poughkeepsie, NY 12604

rossi@vassar.edu

The SARS-CoV-2 main protease (M^{pro}) is an internally encoded protease which serves to hydrolyze the translated polyproteins at designated sites. It directly mediates viral replication hence a promising target for drug design. Plant-based natural products provide scaffold for many effective antiviral medications, and are recently shown to be able to inhibit the SARS-CoV-2 M^{pro}. Polyphenols and phenolic compounds are a major class of bioactive natural compounds that are known for their antiviral and pleiotropic effects, which are also reported to be effective in M^{pro} activity inhibitions. This work focuses on the inhibition processes of M^{pro} by *trans*-clovamide, a natural phenolic compound found in cacao. Clovamide is a naturally occurring caffeoyl conjugate that is found in the phenolic fraction of *Theobroma Cacao* L. Here, we propose inhibitory mechanisms by which clovamide acts as a M^{pro} inhibitor as it scavenges reactive oxygen species (ROS) in the body. We use molecular docking and annealing-based molecular dynamics simulations to study the interactions between M^{pro} catalytic site residues and clovamide along with its analogues. Our molecular modelling studies provide mechanistic insights of clovamide inhibition of M^{pro}, and indicate that clovamide may be a promising candidate as a drug lead molecule for COVID-19 treatments.

Poster 9B

SYNTHESIS OF NOVEL CHIRAL TITANIUM AND COPPER BOROHYDRIDE COMPLEXES

Kevin Horiszny, Joseph Tanski*

Vassar College

Department of Chemistry

124 Raymond Ave, Poughkeepsie, NY 12604

jotanski@vassar.edu

The importance of chiral amine chemistry, especially with respect to the pharmaceutical industry, is immense, with approximately 40-45% of pharmaceuticals containing chiral amine scaffolds in their structures. To date, several stereospecific synthetic methods have been devised; of particular interest are asymmetric hydride transfer reactions catalyzed by chiral transition metal complexes. Our research is focused on the synthesis of several such complexes based on copper and titanium borohydride systems. We selected ligands based on similar compounds found in the literature which we believed would facily bond to our target metal in conjunction with borohydride ions. To date, we have isolated and characterized, *via* X-ray crystallography, two target copper compounds: 2,2'-Bis(diphenylphosphino)-1,1'-binaphthalene copper(I) borohydride and (4*S*,5*S*)-4,5-Bis(diphenylphosphinomethyl)-2,2-dimethyl-1,3-dioxolane copper(I) borohydride. Both assume distorted tetrahedral geometry about the Cu center, with bidentate bonding to the borohydride ligand. Although purple Ti(III) has been observed upon the reduction of Ti(IV) with BH_4^- in the presence of chiral bisphosphine and diol ligands, no complexes have been isolated to date, which we largely attribute to the known thermal instability of titanium borohydride compounds.

Poster 10B

STRAIN-ENGINEERED MN-DOPING TRANSITION METAL DICALCOGENIDES

Owen T. Fauth and Leah Isseroff Bendavid*

Department of Chemistry, Vassar College
124 Raymond Ave, Poughkeepsie, New York, 12604

lebendavid@vassar.edu

We investigate the individual and combined effects of substitutional Mn-doping and strain engineering in monolayers of MoS₂ and MoSe₂, using density functional theory (DFT) to examine the structural, optoelectronic, and magnetic properties. Doping with Mn is shown to introduce magnetic character by producing localized spin polarization in the region near the defect. The Mn dopants preferentially couple ferromagnetically due to an interaction that is described as double exchange. Additionally, doping with Mn changes the electronic structure by introducing defect states within the band gap, which according to one form of DFT, results in half-metallic character. Compressive and tensile strain both decrease the band gap in the pure transition metal dichalcogenides (TMDs), retaining the materials' semiconducting character. Strain has a multivaried effect on the optoelectronic properties in the Mn-doped TMDs. Tensile strain demonstrates potential to strengthen ferromagnetic coupling, offering new possibilities for strain-engineering dilute magnetic semiconductors with more enhanced stability at room temperature.

Poster 11B

X-RAY AND ANTIOXIDANT DETERMINATION OF BUTEIN AND 2',4'-DIHYDROXY-3,4-DIMETHOXYCHALCONE TO EXAMINE THEIR ANTIMALARIAL ACTIVITY BY BINDING TO FALCIPAIN-2 (PDB CODE: 3BPF).

Ijeoma Okoye, Miriam Rossi*, Francesco Caruso

**Department of Biochemistry, Vassar College
124 Raymond Avenue, Poughkeepsie, NY 12604**

rossi@vassar.edu

Malaria is a global health burden as about 1-3 million people worldwide die from malaria every year and the antimalarial drugs in use are becoming less effective as malaria parasites gain resistance to them. Previous studies have shown that the stem extract of *Erythrina abyssinica*, a tree that is native to Africa, contains two compounds, 5-prenylbutein and homobutein, that have moderate antiplasmodial activity. The objective of my project was to structurally characterize butein and 2',4'-dihydroxy-3,4-dimethoxychalcone (DHDM; similar to butein) to elucidate possible molecular mechanisms by which these compounds could clear malaria parasites. We hypothesized that both compounds would chemically interact with the cysteine residue in the catalytic site of Falcipain-2 (a cysteine protease demonstrated to be involved in hemoglobin degradation in malaria-infected red blood cells). Results from single X-ray diffraction analysis and subsequent docking simulations showed that both butein and DHDM are in the right orientation and distance to allow for strong binding to the cysteine residue of Falcipain-2. The results from Rotating Ring Disk Electrode Voltammetry experiments also demonstrated that butein and DHDM have high antioxidant activity. Thus, both compounds could serve as potential competitive inhibitors of Falcipain-2 and consequently, starting points for the development of novel antimalarial drugs.

Poster 12B

TRACE ELEMENTAL AND Pb ISOTOPIC INVESTIGATION OF BEE HONEY FROM THE HUDSON VALLEY

Vanessa Vazquez, Ilaria Coppola, Alison Spodek Keimowitz*

**Vassar College
124 Raymond Avenue, Poughkeepsie, NY 12604**

alspodek@vassar.edu

The aim of this study is to use honey as a biomonitor to determine the concentrations of heavy metals in the Hudson Valley and to determine the isotopic ratios of Pb in honey to help determine provenance of Pb. Honey was collected from several different beekeepers along the entire Hudson Valley. Samples were digested with nitric acid by digiPREP to prepare a homogenous sample to be analyzed by ICP-MS. Lead concentrations were found to vary between samples, however samples with higher concentrations were from urban environments. Zn, Mn, and Fe were found to be the most abundant trace metals while cobalt is the least abundant. The concentrations of the trace metals in the honey samples were not high enough to be considered pollutants. The Pb isotope data of the Hudson Valley honey samples do not allow for the precise determination of the Pb source, but are consistent with local soil and rock trends. The honey samples analyzed are representative of the Hudson Valley environment.

Poster 13B

CHEMILUMINESCENCE OF 6-AMINO-2,3-DIHYDROBENZO[G]PHTHALAZINE-1,4-DIONE AND LUMINOL ANALOGS

Linnea Martin, Dr. Sarjit Kaur*

Vassar College
124 Raymond Avenue, Poughkeepsie, NY 12604

sakaur@vassar.edu

Luminol is used in forensic investigations to detect trace amounts of blood at crime scenes. This project focuses on 6-amino-2,3-dihydrobenzo[g]phthalazine-1,4-dione (ADIP) as a possible alternative to luminol as ADIP has been reported to show chemiluminescence in the green region of the visible spectrum (Periyasami *et al.* “Strong Green Chemiluminescence from Naphthalene Analogues of Luminol” 2014). The synthesis of ADIP was adapted from the literature and carried out as follows: nitration of naphthalene-2,3-dicarboxylic acid using nitric acid and sulfuric acid, cyclization with acetic acid and hydrazine to get the phthalhydrazide group, and reduction of the nitro group using iron powder and ammonium chloride. The products were characterized by ^1H and ^{13}C NMR, and FTIR spectroscopy. Current efforts are directed at scale-up of reactions, optimization and purification of compounds and investigation of the chemiluminescence properties of ADIP and several related luminol compounds using spectrofluorimetry with excitation blocked. The impact of conjugation and intramolecular hydrogen bonding will be evaluated by comparing the chemiluminescence emissions of luminol, isoluminol, phthalhydrazide, and 5-hydroxy-2,3-dihydrophthalazine-1,4-dione. Future work will be towards more direct synthesis of several luminol analogs reported in the paper by Periyasami *et al.*

Poster 14B

DETERMINATION OF HEAVY METAL ION CONTAMINATION IN SEDIMENT SAMPLES COLLECTED NEAR THE WHEELABRATOR DUTCHESS COUNTY INCINERATOR

Kaitlyn Cunningham, Kathlyn Doroski, Alison Keimowitz*

**Vassar College
124 Raymond Avenue, Poughkeepsie NY, 12604**

alspodek@vassar.edu

Municipal Solid Waste Incinerators, while regularly monitored, release heavy metals into the atmosphere and potentially harm those nearby. This project examines the heavy metal release from the Wheelabrator Dutchess County Incinerator by analyzing sediment cores from upwind and downwind of the incinerator. Core sections are examined for metals using ICP-MS (Inductively Coupled Plasma Mass Spectrometer) after acid digestion and the DMA (Direct Mercury Analyzer). Cores downwind of the incinerator were taken from Casperkill Golf Club and samples upwind of the incinerator were taken from Cluett Schantz Memorial Park. The DMA data appears to show that the cores upwind from the incinerator have slightly higher concentrations of mercury near the core top, likely due to road pollution. Other heavy metal data from the ICP-MS shows a similar trend, except for chromium, which shows the downwind samples having a higher concentration. Chromium, a common indicator of incinerator pollution, had a maximum average concentration of 18 mg/kg for the downwind sample and 6 mg/kg for the upwind sample. Based on these findings, pollution from the incinerator is generally less significant than other ambient pollutant sources; however, the incinerator may still contribute to overall pollutant levels based on the trend from chromium.

Poster 15B

SYNTHESIS OF PROCHIRAL IMINES FOR ASYMMETRIC REDUCTIVE HYDROGENATION

Susanna Monroe, Joseph Tanski*

Vassar College

Department of Chemistry

124 Raymond Ave, Poughkeepsie, New York 12604

jotanski@vassar.edu

Chiral amines are one of the most common moieties found in pharmaceutical drugs on the market today. Therefore, the development of cost-effective and efficient methods of asymmetric chiral amine synthesis is an ever-evolving field of inquiry. One such method is asymmetric reductive hydrogenation of imines. In this work, novel imines with protecting substituents that aim to decrease the partial positive character of the imine carbon center to deactivate the imine towards hydrogenation except by only a very strong hydride source, such as a transition-metal complex with a chiral ligand and a coordinated borohydride ion, are investigated. We have successfully synthesized three novel prochiral imine compounds with various functional groups to manipulate partial positive character, and characterized the products *via* ^1H , ^{13}C , and ^{31}P NMR spectroscopy, X-ray crystallography, and GC-MS.

Poster 16B

TOWARDS THE EVALUATION AND IMPROVEMENT OF AN EI-MS PEPTIDE FINGERPRINTING MODEL

**Flood B. M., Pesce M. D., Toscano E. J., Varghese S. M., McBrayer
D. N.***

**SUNY New Paltz
1 Hawk Drive, New Paltz, NY, 12561**

mcbayed@newpaltz.edu

We have been developing a Python-based fragment prediction program which serves to match experimental peptide fragments from Electron Ionization (EI) mass spectra with a generated fragment “fingerprint” produced using known peptide fragmentation mechanisms during EI. EI Mass Spectrometry (EI-MS) has several limitations in regard to its use to analyze peptides. Peptide fragmentation can be helpful in determining a peptide’s initial sequence, but can make it difficult to differentiate between peaks from contaminants and peptides. The goal of this work is to eventually be able to confirm the identity of a synthetic peptide by comparing its mass spectrum with our program-generated “fingerprint”. To confirm current predictions and to identify additional fragmentation mechanisms to refine the prediction model, various dipeptides were synthesized using fluorenylmethyloxycarbonyl (Fmoc)-based solid-phase peptide synthesis (SPPS). They and single amino acids were analyzed using Direct Exposure Probe EI-MS (DEP-EI-MS) to help validate and improve our fragmentation prediction model. In addition to manual analysis of mass spectra and theoretical overlap comparison between predicted fragments, Upset plots were created from the mass spectra as a way to visualize and determine peak matches between spectra. This analysis can identify contaminant peaks and help direct further investigations to identify additional fragmentation mechanisms.

Poster 17B

UV CURING OF EVA POLYMER IN SOLAR PANELS

David Gandham, Nicholas Brinsmade, Sarjit Kaur*

Vassar College

124 Raymond Avenue, Poughkeepsie, NY 12604

sakaur@vassar.edu

As solar cell technologies continue to proliferate, a reliable encapsulation layer in photovoltaic (PV) modules is important for optimal performance and longevity of solar panels. To mitigate the breakdown of the encapsulation layer that is inevitable in the field due to the exposure of UV light, a new approach to extend the life of solar panels was explored. The UV curing of ethylene vinyl acetate (EVA) polymer, the dominant encapsulant in the PV market, was investigated, and the degree of cross-linking was followed using several methods (swelling, Soxhlet extraction, and Young's modulus tests). The photoinitiated crosslinking reaction of EVA was carried using benzophenone and triallyl isocyanurate as the photoinitiator and cross-linker, respectively. Test films of EVA were exposed to 350 nm UV light (intensity of 9200 microwatts/cm²) over 2-6 minutes. The laboratory studies showed increased cross-linking and less dissolution of the polymer in toluene with increasing curing time. The performance of the cured test EVA films was also studied using Young's modulus, which increased in the highly cured samples with no apparent evidence of polymer brittleness. Studies are currently in place to follow the curing of the EVA films when exposed to sunlight for extended periods in the environment.

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