
ABSTRACT SYMPOSIUM NAME: Materials Chemistry - Oral

CONTROL ID: 2211026

TITLE: [Adsorption of organic-based pesticides from aqueous solutions using lightweight carbon aerogels](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): A. B. Diciara¹, B. S. Litts¹, [R. E. Rogers](#)¹

INSTITUTIONS (ALL): 1. Chemical Engineering, Rochester Institute of Technology, Rochester, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Anthropogenic activities have increased the need to purify water from source to point of use. The use of highly porous, lightweight aerogels as adsorbents of high bonding affinity for a large variety of chemicals provide opportunities for enhanced separation processes. In this study, carbon aerogels (CA) were prepared from a single step process based on the dehydration of aqueous solutions of sucrose containing well dispersed nanostructures by sulfuric acid. The effect of preparation on the aerogel structure, density, and its adsorption properties for the removal of different pesticides from aqueous solutions was investigated. In particular, the nature and the amount of nanostructures (graphene, multi-walled or single-walled carbon nanotubes) along with their dispersion state throughout the carbonaceous matrix strongly influence the adsorption properties of the aerogel. Adsorption kinetics and isotherms were examined and results show that the aerogels with a content in nanomaterials as low as 2 wt.% exhibit faster uptakes at comparable or higher capacities than previously reported data for activated carbon and carbon nanotube papers. This makes carbon aerogels extremely compelling for environmental remediation and separation applications.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Bio-based Materials and Processes - Oral - INVITED ONLY

CONTROL ID: 2211365

TITLE: [The acetylation landscape of the H4 Histone Tail](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [G. Papoian](#)¹, D. Winogradoff¹, I. Echeverria¹

INSTITUTIONS (ALL): 1. Chemistry and Biochemistry, University of Maryland at College Park, College Park, MD, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Histones tails, the intrinsically disordered terminal regions of histone proteins, are key modulators of the structure and dynamics of chromatin, and consequently, are central to many template directed processes including DNA replication, repair and transcription. Acetylation of histone tails is a major post-translational modification (PTM) involved in regulating the structure of chromatin, yet it remains unclear how acetylation modifies the disordered state of histones tails to, in turn, affect their function. In this work, we investigated the consequences of gradually increasing the acetylation level of the H4 histone tail by characterizing the conformational ensembles of un-acetylated, mono-, di-, tri-, and tetra-acetylated H4 histone tails. We found that progressive acetylation has a cumulative effect on the H4 tail, however, specific effects are also found for the biologically important K16 mono-acetylated H4 histone tail. We have determined molecular mechanisms behind both cumulative and specific effects of various acetylation patterns. In addition, we explore the mechanisms by which different acetylation patterns may result in specific

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recognition of the H4 histone tails by protein or DNA binding partners.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Oral

CONTROL ID: 2212021

TITLE: [Facilitating chemistry education collaborations across borders and between cultures in the Middle East: The Malta Conferences](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. Z. Hoffman](#)^{1, 2}, Z. M. Lerman²

INSTITUTIONS (ALL): 1. Department of Chemistry, Boston University, Boston, MA, United States.
2. Malta Conferences Foundation, Washington, DC, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Conflicts among nations, as exemplified by the Middle East, have serious consequences to the entire world and place barriers to the free exchange of ideas, the establishment of collaborations, and the development of innovations in science, technology, and education. Science diplomacy, in the form of contacts among scientists from all sides of the international conflicts, could provide the bridges to peace that are important to everyone. The issues that involve science education are the same across national boundaries: increasing the interests of students to study science, utilizing technology and pedagogy for better teaching and learning, encouraging the education of women, and understanding the effects of cultural differences on education. Building on the fact that science is an international language, major international meetings known as the "Malta Conferences" (formally "*Frontiers of Science: Research and Education in the Middle East - A Bridge to Peace*") have been held biennially since 2003, at which scientists and educators from Middle East nations gather with Nobel Laureates and other eminent individuals to discuss potential solutions to the problems of the region in the areas of environmental air and water quality, renewable energy sources, nanotechnology and material science, chemistry safety and security, and science education at all levels. Among the collaborations that originated at the Malta Conferences are efforts to improve drinking water quality and alleviate its scarcity, to foster graduate studies and faculty sabbaticals across the boundaries, and to develop electronic collaborations among science educators and students in the form of on-line periodicals and courses. It is hoped these collaborations will yield results that will be the cornerstones for future innovations and a bridge to peace.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Food Chemistry - Oral

CONTROL ID: 2212253

TITLE: [Nutraceutical and phytochemical profile of the aerial parts of the Jamaican blackberry \(*Rubus jamaicensis*\)](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [R. E. Williams](#)¹

INSTITUTIONS (ALL): 1. Chemistry, The University of the West Indies, Kingston 7, Mona, Jamaica.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract:

“Nutraceutical and phytochemical profile of aerial parts of the Jamaican blackberry (*Rubus jamaicensis*)”
Williams, Ruth; Bowen-Forbes, Camille; Goldson-Barnaby, Andrea
Department of Chemistry, The University of the West Indies.

The *Rubus* genus acts as a reservoir of numerous species which show nutraceutical properties including anticancer, anti-diabetic and antihypertensive activity. Nutraceutical properties listed above are linked to the noteworthy antioxidant capacity of the *Rubus* genus. This study seeks to further unlock the intrinsic value of the aerial parts of the *Rubus jamaicensis* (Jamaican blackberry) by exploring numerous bioassays. Antioxidant capacity was determined based on redox potential (Total polyphenol assay, TPA) and radical scavenging activity (Trolox equivalence antioxidant capacity, TEAC and 2, 2-Diphenyl-1-picrylhydrazyl assay, DPPH). Fatty acid analysis of the ethyl acetate extract showed the presence of high levels of omega-3 fatty acids which impart potential health benefits. The overall fat content of the dried leaves was found to be $1.86 \pm 0.12\%$. Purification of the ethyl acetate extract resulted in the isolation of compounds characterized by GC-MS and NMR. Compounds characterized thus far may be classified as terpenoids, fatty acids and flavonoids. Well diffusion antimicrobial assay shows marked antimicrobial activities of water extracts obtained.

CONTACT (COUNTRY ONLY): Jamaica

DECISION STATUS: Accept

ABSTRACT STATUS: decisioned_accepted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: News from Carbon World - Oral - INVITED ONLY

CONTROL ID: 2212366

TITLE: [Site-specific functionalization of Buckybowls: Tailoring properties and structures](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [C. Dubceac](#)¹, A. S. Filatov¹, A. Zabula¹, M. A. Petrukhina¹

INSTITUTIONS (ALL): 1. Chemistry, University at Albany, SUNY, Albany, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Functionalization of corannulene, a polycyclic aromatic hydrocarbon (PAH) with a bowl-shaped sp^2 hybridized carbon framework, is of great importance for assisting in activation of non-planar carbon surfaces, altering their properties and reactivity, and setting the ground for the development of novel carbonaceous compounds. Derivatives of corannulene ($C_{20}H_{10}$) have been shown to exhibit unique chemical and physical properties, making them promising candidates for a variety of emerging materials chemistry applications. Significant efforts have been directed towards the development of controlled functionalization routes with the purpose of tuning the properties and reactivity of the carbon bowl. Exterior derivatization of corannulene by various substituents has been broadly studied, while the interior surface functionalization is limited to only two examples: spoke cycloaddition of dihalocarbenes and covalent bond formation at the hub carbon atom of corannulene through the addition of external carbocations under Friedel-Crafts reaction conditions. In both cases, the preparation of the functionalized bowl-shaped products as solid crystalline materials and their structural analysis have been lacking. We therefore focused on product crystallization that allowed us to accomplish the first structural characterization of interior functionalized corannulene using single crystal X-ray diffraction. A family of corannulene-based cations with different tails bound to the surface has provided a unique set for evaluating the geometry transformation and solid state packing with various anions. For the recently characterized corannulene adducts with dichlorocarbene, the effect of cyclopropanation on the carbon core is revealed, including changes in bowl depth, bond lengths, and bonding angles. Interesting variations in the solid state packing of mono- *versus* bis-adduct are also discovered.

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Furthermore, the solid state aggregation patterns of these polar bowls have been correlated to their properties. These studies should facilitate the design of functionalized non-planar PAHs with structures and properties tailored for further development of novel carbonaceous materials.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Inorganic Chemistry - Poster

CONTROL ID: 2226113

TITLE: [Charging fragments of fullerenes and nanotubes with multiple electrons: X-ray structural highlights](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): S. N. Spisak¹, C. Dubceac¹, N. J. O'Neil¹, Z. Zhou¹, A. S. Filatov¹, A. Zabula¹, M. A. Petrukhnina¹

INSTITUTIONS (ALL): 1. Chemistry, University at Albany, SUNY, Albany, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Open geodesic polyarenes that map onto the surface of fullerenes and represent the caps of nanotubes gain special attention due to their unique balance of strain and aromaticity. They also exhibit excellent electron accepting abilities in stepwise reduction reactions. For example, the smallest bowl-shaped polyarene corannulene (C₂₀H₁₀) is known to accept up to 4 electrons upon reduction with alkali metals. We have been able to isolate crystalline products of various reduced states of corannulene and accomplished their first X-ray crystallographic characterization. This allowed us to provide the first structural details of corannulene anions and to evaluate the effects of adding multiple electrons to its curved core. Moreover, the resulting carbanions were shown to serve as unique π -ligands able to provide convex and concave faces as well as multiple binding sites for metal coordination. From corannulene, we have moved to larger curved polyarenes having extended π -surfaces and comprised of several bowl-shaped moieties fused by different linkers. We have investigated the addition of multiple electrons to a fragment of armchair carbon nanotube and followed its severe structural deformation by X-ray crystallography. We have used controlled derivatization of the bowl core both at the periphery and interior surface to further tune the properties of bowl-shaped polyarenes. The recent highlights of our X-ray crystallographic investigations of a broad class of charged curved carbon-rich aromatic systems will be presented.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Green Labs - Oral - INVITED ONLY

CONTROL ID: 2215282

TITLE: [Supporting safe, sustainable laboratories in the 21st century](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): R. Stuart¹

INSTITUTIONS (ALL): 1. Environmental Health and Safety, Keene State College, Keene, NH, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

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Abstract: Laboratories account for a disproportionate share of the carbon footprint on a college campus. This is driven by the high energy use by equipment and ventilation, heavy materials uses, and unusual wastes associated with laboratory work. In response to this challenge, many campuses are developing "Green Laboratories" programs that seek to find opportunities to conserve energy use while protecting laboratory workers' health and safety. This presentation will discuss the opportunities we've discovered in this work and opportunities for expanding this into the chemistry education practices.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials for Energy - Oral

CONTROL ID: 2212742

TITLE: [Determination of optoelectronic and transport properties of sandwich type structures based on organic semiconductors](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. Huerta Francos](#)¹, [M. Espinosa](#)², [M. Sanchez](#)³, [M. Menéndez](#)⁴

INSTITUTIONS (ALL): 1. Anahuac University, Mexico, Mexico.
2. Universidad Anahuac Mexico Norte, Queretaro, Queretaro, Mexico.
3. Universidad Anahuac Norte, Huixquilucan, Estado de Mexico, Mexico.
4. Universidad Anahuac Norte, Puebla, Puebla, Mexico.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: The discovery of organic light emitting diodes (OLED) based on organic molecules lead to the study and understanding of optical transport properties of organic semiconductors (OS). As OS thin films are constituted of individual molecules held together by weak van der Waals forces, many of the physical properties of the solid are strongly influenced by the degree of intermolecular orbital overlap. Phthalocyanines (Pc) are a type of highly stable OS, which are classified as p-type semiconductors characterized by low mobility and low carrier concentration as well as absorption bands that extend from the ultraviolet to the infrared region.

Throughout our project, we have accomplished to create a sandwich-type ITO/nylon 11/MPc (M = Zn, Mn)/Ag structure. This structure was fabricated by vacuum thermal evaporation. Next, the effect of thermal relaxation technique and annealing on structural, morphological, optical and electrical properties of thin films were examined by scanning electron microscopy (SEM), Energy Dispersive X-Ray Spectrometry (EDS) and FT-IR spectroscopy measurements. By a Uv-Vis spectroscopy, optical parameters were determined, and subsequently the Tauc model was applied to those parameters in order to determine the types of transitions presented in the different films. In this case, the found transitions were indirect for both Zn and Mg films. Also, transport characteristics of sandwich organic devices and their junction properties, such as the diode ideality factor and barrier height, were studied by measuring current-voltage characteristics in dark and under illumination conditions. Due to the obtained results, these materials may have strong potential as organic semiconductors, which soon after may be used in optoelectronic devices.

CONTACT (COUNTRY ONLY): Mexico

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

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ABSTRACT SYMPOSIUM NAME: Materials for Energy - Oral

CONTROL ID: 2212715

TITLE: [Preparation of composite films of metal phthalocyanines for optoelectronic applications](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. Espinosa](#)², M. Menendez³, M. Huerta Francos¹, M. Sanchez⁴

INSTITUTIONS (ALL): 1. Anahuac University, Mexico, Mexico.
2. Universidad Anahuac Mexico Norte, Queretaro, Queretaro, Mexico.
3. Universidad Anahuac Norte, Puebla, Puebla, Mexico.
4. Universidad Anahuac Mexico Norte, Mexico City, Mexico City, Mexico.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Metallophthalocyanines have been recently subject of considerable interest because of their electrical properties that give them a semiconducting behaviour, which is useful in solar cells. The objective of this work is to prepare MPC-polymer composite films for the creation of organic semiconductors. The films were produced by thermal evaporation of Fe, Ni and Co metallophthalocyanines on a nylon 11 surface which was previously deposited on different substrates, in order to perform the structural characterization of the cells and determine their optical parameters involved. The thin films were heated up to 100 °C for 10 minutes, and then to 120 °C for an hour. This procedure helped the metallophthalocyanine penetrate into the nylon 11 surface. Film characterization was performed through Fourier-transform infrared (FT-IR) spectroscopy, scanning electron microscopy (SEM), Profilometry, and Energy Dispersive Spectroscopy (EDS). The optical parameters were determined by an UV-vis spectroscopy and by applying the Tauc model in order to determine the band gaps. The Tauc optical band gap values of the thin films were calculated from the absorption coefficient and were found to be of around 1.8 eV, arising from non-direct transitions. After the film characterization, the electrical current of the films was measured in three different ways; at room temperature with no influence of light, with the influence of a UV shortwave and a UV longwave. The three previously mentioned films (Fe, Ni and Co) showed the best results when they were under the influence of the UV shortwave, followed by the ones of the UV longwave, and at last, the ones measured with no influence of light. Given the results shown previously, these materials may have potential use in solar cells and/or electronic device fabrication.

CONTACT (COUNTRY ONLY): Mexico

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Environmental Chemistry - Oral

CONTROL ID: 2213145

TITLE: [A new method to measure aerosol particle bounce and estimating the phase state of atmospheric aerosols](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [S. Jain](#)², G. Petrucci¹

INSTITUTIONS (ALL): 1. Chemistry, University of Vermont, Burlington, VT, United States.
2. Chemistry, University Of Vermont, Burlington, VT, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Organic aerosol (OA) is a ubiquitous component of atmospheric particulate that influences both human health and global climate. A large fraction of OA is secondary in nature (SOA), being produced by oxidation of volatile organic compounds (VOCs) emitted by biogenic and anthropogenic sources. Atmospheric SOA could be liquid or solid in phase and can affect the global climate in multiple and complex ways through its interactions with radiation and clouds. SOA can either scatter or absorb solar radiation,

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thereby modifying the Earth's radiative balance. Such scattering or absorbing largely depends on aerosol physical properties and environmental conditions. SOA particles can also act as cloud and ice condensation nuclei, impacting atmospheric albedo, cloud formation and lifetime. Moreover, the physical state of particles can affect particulate phase chemical reactions, and thus the growth rates of newly formed atmospheric particles. Hence understanding the phase state of aerosol is a key to understanding the global climate change.

In the present work, we describe a simplified method to measure the phase state (liquid or non-liquid) of organic by estimating the bounce factor of polydisperse SOA using only a multi-stage cascade electrical low pressure impactor. The method eliminates the need for an independent measure of the particle size distribution (for example, as with an SMPS) and relies on comparison of absolute ion currents at each impactor stage under conditions that favor or reduce particle bounce. We validated the proposed method with solid, liquid and transition aerosols (aerosol which transitions from liquid to non-liquid state upon ozonolysis), namely ammonium sulfate (AS), dioctyl sebacate (DOS) and oleic acid (OA), and present bounce factor evolution of aging α -pinene-derived SOA. This method allows for the real-time determination of SOA phase state for polydisperse aerosols, permitting studies of the relationship between SOA phase, oxidative formation and chemical aging. The proposed method allowed us to evaluate the impact that various parameters, such as SOA precursor, relative humidity, oxidation type and mixing ratio, can have on the phase of atmospheric organic particulate.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Biochemistry - Oral

CONTROL ID: 2213214

TITLE: [Constrained peptides for metal binding and catalysis](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. R. Aldous](#)¹, J. Kritzer²

INSTITUTIONS (ALL): 1. Chemistry, Tufts University, Avon, MA, United States.

2. Dept. of Chemistry, Tufts University, Medford, MA, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: As we strive for more efficient and higher yielding syntheses, asymmetric catalysis by metalloenzymes has become important in the fields of energy and pharmaceuticals. Metal-peptide mimics hold immense potential for examining metalloenzyme mechanisms, as well as improving yield and selectivity while using less expensive catalysts. Our lab explores how constraining small peptide sequences can tune metal binding and activity. Cyclization via cysteine bisalkylation and incorporation of metal binding moieties are applied to discover new metal-peptide complexes. Our goal is to characterize and apply these complexes to asymmetric reactions including cyclopropanation and epoxidation, taking advantage of the chirality and modularity of peptides to control reactivity and enantioselectivity.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Green Polymers - Oral - INVITED ONLY

CONTROL ID: 2213336

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TITLE: [Development of new routes to benign polymeric materials](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [G. W. Coates](#)¹

INSTITUTIONS (ALL): 1. Cornell Univ, Ithaca, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Society depends on polymeric materials now more than at any other time in history. Although synthetic polymers are indispensable in a diverse array of applications, ranging from commodity packaging and structural materials to technologically complex biomedical and electronic devices, their synthesis and post-use fate pose important environmental challenges. The focus of our research is the development of new routes to polymers with reduced environmental impact. In this work, we aim to transition from fossil fuels to renewable resources, and are developing synthetic methods that limit energy and raw-material consumption. In addition, we are designing materials that will eventually degrade into non-toxic materials, and have properties comparable to current commodity plastics. In this lecture, the development of new methods for the synthesis of sustainable polymers will be presented.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Organic Chemistry - Poster

CONTROL ID: 2223197

TITLE: [Synthetic Studies on Small-Molecule SHIP1 Agonists](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [B. Duffy](#)², J. D. Chisholm¹

INSTITUTIONS (ALL): 1. Syracuse University, Syracuse, NY, United States.

2. Chemistry, Syracuse University, Syracuse, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: The SH2-containing inositol 5'-phosphatase SHIP1 plays an important role in modulating cellular signaling that occurs through the PI3K axis. SHIP1 agonists are currently under investigation for a number of disease states, particularly allergic inflammation and cancer. Synthetic studies leading towards an efficient and concise total synthesis of SHIP1 agonists will be described.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS: Accept

ABSTRACT STATUS: decisioned_accepted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Oral

CONTROL ID: 2213588

TITLE: [Implementation of a one credit chemical safety course](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [K. I. Gublo](#)¹

INSTITUTIONS (ALL): 1. Chemistry, SUNY Oswego, Liverpool, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

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Abstract: This session will discuss the proposal and implementation of a one credit chemical safety course for undergraduate science majors at SUNY Oswego. Some of the topics covered in this course include personal protective equipment, fire safety, corrosives, incompatibles, and chemical management. The course outline, syllabus and assessment tools will be provided. With more students performing independent research often unsupervised, the need for a formal lab safety course was apparent. Learn how to implement a course like this at your university.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Intersections of Chemistry and Art - Oral - INVITED ONLY

CONTROL ID: 2215755

TITLE: [Degradation of polymers used to make art: origins, measurement, and prevention](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [C. H. Stephens](#)¹

INSTITUTIONS (ALL): 1. Institute for the Preservation of Cultural Heritage, Yale University, West Haven, CT, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: The long term degradation behavior of cotton, linen, wood, and kozo paper-based artifacts, all artificially-aged at 90°C and 50% relative humidity to promote hydrolytic breakdown, was examined in order better preserve paper-based objects found in libraries and museums. Degradation was monitored using gel permeation chromatography (GPC), pH and Yellowness Index measurements, uniaxial tensile testing, moisture content, and carbonyl content assays. The cellulose component of all four papers dominated measured changes to the molecular weight while the presence of hemicellulose in the linen, wood, and kozo papers led to unique measured moisture contents, carbonyl group, and YI values relative to cotton after the same amount of degradation had occurred. Acid generation during hydrolysis was the inspiration for three art conservation-based projects, one to identify where acid groups are located in cellulose fiber using fluorescent tagging, one to prevent acid migration between paper-based artifacts in storage, and one to understand degradation in cellulose acetate.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: resubmitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Organic Chemistry - Oral

CONTROL ID: 2216492

TITLE: [Anion abstraction catalysis: Mechanistic studies and development of dimeric thiourea catalysts](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [D. Lehnher](#)¹, D. D. Ford¹, N. S. Rajapaksa¹, E. N. Jacobsen¹

INSTITUTIONS (ALL): 1. Chemistry and Chemical Biology, Harvard University, Cambridge, MA, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

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Abstract: Hydrogen bond (H-bond) donors, such as chiral thiourea derivatives, are an emerging class of catalysts that can promote a range of highly enantioselective transformations. In some of these reactions, it has been postulated that the H-bond donor catalyst abstracts an anion from a neutral organic precursor to generate a cationic electrophile. This reactive ion pair intermediate can then undergo enantioselective attack by a nucleophile to afford the enantioenriched product. While this mode of activation has been proposed for a number of transformations, little is known about the mechanistic details. A mechanistic study of a prototypical anion-abstraction reaction catalyzed by H-bond donors will be presented that sheds light onto this topic and reveals unanticipated complexities.

Our study revealed three key features of the reaction: 1) two molecules of catalyst work cooperatively to activate the electrophile, 2) the catalyst resting state under typical reaction conditions is a non-productive dimeric aggregate and 3) the catalyst exists as a mixture of *E*- and *Z*-amide rotamers, thus there are potentially three different combinations of pairwise rotamers that could exist in the key transition- and ground-state structures. These results provide insight for structural modifications of the catalyst towards improving catalyst activity, a long-standing problem in thiourea-catalysis in which high catalyst loadings (ca. 15 to 20 mol%) and long reaction times (up to several days) are typical.

The mechanistically guided catalyst design for improved catalysis includes: 1) covalently linking two thioureas to both enhance cooperative activation of the electrophile and prevent deactivation of the catalyst resulting from aggregation and 2) conformationally biasing the amide fragment of the catalyst into the rotamer associated with the higher enantioselective pathway. Application of these design elements allowed for the development of highly active catalysts able to operate with loadings below 1 mol% while maintaining high levels of enantioselectivity. These results illustrate the feasibility of highly active catalysis based on H-bonding from thioureas, and suggest that dimeric thiourea catalysts may provide a general strategy for achieving highly active catalysts in the field of anion-abstraction catalysis.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials Chemistry - Oral

CONTROL ID: 2251061

TITLE: [Cycloaddition strategies to polyhalogenated carbon-rich architectures: *ortho*-arylene foldamers, polycyclic aromatics, and graphene nanoribbons](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [D. Lehnherr](#)¹, J. M. Alzola¹, W. Dichtel¹

INSTITUTIONS (ALL): 1. Chemistry and Chemical Biology, Cornell University, Ithaca, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Polycyclic aromatic hydrocarbons (PAHs) are conceptually the building blocks of many carbon-rich based materials, such as graphene, fullerenes, and carbon nanotubes. Our interest in developing bottom-up synthetic approaches to subunits of these materials, such as graphene nanoribbons, has led us to develop new synthetic strategies to form carbocycles, including benzannulation strategies for the formation of PAHs. These strategies will be presented with a particular focus on unique methods of incorporating halides into aromatic frameworks. A catalyzed reaction of a haloalkyne with a halogenated benzaldehyde provides a rapid, convergent assembly of polyheterohalogenated naphthalenes with each halide substituent potentially being unique (X = F, Cl, Br, I).

This synthetic method can be used either for the formation of truly unique monomers for polymer synthesis, or for the conversion of acetylene-based architectures into complex polyhalogenated polycyclic aromatic

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structures. For example, *ortho*-arylethylenes can be transformed to *ortho*-arylenes, both in oligomeric and polymeric settings, enabling the exploration of hydrocarbon-based foldamers and their polyhalogenated analogs. X-ray crystallography of the defined-length *ortho*-arylene oligomers confirms their ability to adopt helical structures with intramolecular pi-stacking. Traditional cross-couplings methods are typically ineffective for the formation of such *ortho*-arylenes due to the sterically congested architecture, in contrast our method does not suffer from this limitation and enables access to uniquely substituted precursors to graphene nanoribbons towards controlling edge functionality, including unsymmetrical edge-substitutions with unique halogenation patterns.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: The Legacy of Minority Institution - Oral

CONTROL ID: 2223728

TITLE: [A community-based learning archetype for science : Native American health and medicine](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [D. G. Hilmey](#)¹

INSTITUTIONS (ALL): 1. Chemistry, St. Bonaventure University, Allegany, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: A general education college course was developed and implemented, bringing together Native American leaders, undergraduates, an Iroquois medicine man, high school students, and concepts of chemistry and science. The resulting class was profound in both student and community learning. Science students experienced, firsthand, the teaching of the Seneca Nation of Indians and learned of their traditional medicines and culture. The students then investigated the chemical and biological science in some of the Seneca medicinal sources and presented them to the Seneca community leaders and high school students in Salamanca, NY. The class was envisioned to be a part of the Seneca mission to validate their traditions, but it evolved into something far more profound. The group experienced the Seneca people in a powerful and intense series of events.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Biochemistry - Poster

CONTROL ID: 2216740

TITLE: [The prevalence of batrachochytrium dendrobatidis in Oswego County, NY](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [L. Muok](#)¹

INSTITUTIONS (ALL): 1. Syracuse Academy of Science Charter School, Syracuse, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: The fungus *Batrachochytrium dendrobatidis* is a causal agent that has played a part in global amphibian declines. In this study, we documented its prevalence in Oswego County, NY. With an aim toward an increased understanding of *B. dendrobatidis* prevalence locally, we collected amphibians in April, May,

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June, and July 2014 at different locations in Oswego County, NY, and took swabs of the ventral surfaces of all individuals caught. We then performed Polymerase chain reactions on DNA extracted from the swabs and compared them with *B. dendrobatidis* control DNA. Our data showed that 6.3% of amphibians sampled carried the fungus, with prevalence ranging between 6.4–28.6% for *Eurycea bislineata* (Two-lined Salamanders), *Notophthalmus viridescens* (Eastern Newts) *Lithobates catesbeianus* (Bull Frogs), *Lithobates clamitans* (Green Frogs), and *Rana sylvatica* (Wood Frogs). The documented commonness levels in different species, combined with the lack of observed mass amphibian declines suggest that the fungus may be endemic in local amphibian populations, but additional research is needed to establish the relative importance of this data for the health of amphibian populations in Oswego County and NYS.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Analytical Chemistry - Poster

CONTROL ID: 2216719

TITLE: [GC-MS volatile organic compound analysis in drinking water samples](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): C. Muok¹, F. Mahmoud¹

INSTITUTIONS (ALL): 1. Syracuse Academy of Science Charter School, Syracuse, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Abstract

Volatile Organic Compounds (VOC) are organic compounds that have a high vapor pressure at ordinary room temperature. In this study the VOC's that used were benzene, toluene, ethylbenzene, and xylene. These chemicals can pose as a threat to our health. These risks can include cancer, irritation to the skin, respiratory infections, and neurological effects. In this research, we aimed to analyze the bottle water samples and water samples from our school and common public area (Destiny USA) for VOC samples by Gas chromatography–mass spectrometry (GC-MS). For this purpose, each sample of water was first measured with a 10 mL volumetric pipette then put into a 10 mL vial and stirred for 5 min at 600 rpm to make sure that the VOC's are distributed evenly throughout the vial. The possible VOC samples were collected by Solid Phase Micro Extractor (SPME) and inserted into the GC-MS to determine the VOC presence and concentration in the water samples. The high-grade water bottles, Voss and Aquafina had lower concentrations of VOC than Nirvana, Syracuse Academy Of Science, and Destiny USA.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: resubmitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Biochemistry - Poster

CONTROL ID: 2268200

TITLE: [Bactericidal Effect of Hexamethylenetetramine](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): L. Rowser-Groh², N. N. Dingra¹, K. McCue¹

INSTITUTIONS (ALL): 1. Chemistry Department, SUNY Oswego, Oswego, NY, United States.

2. Syracuse Academy of Science Charter School, Syracuse, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Escherichia coli lives in the intestines of animals and humans and most of E. coli are harmless and important to the human intestinal tract. Some E. coli are pathogenic, they can cause illness which includes diarrhea which can come from contaminated water and food or through contact with other organisms¹.

Hexamethylenetetramine (HMTA) is an organic compound with the formula (CH₂)₆N₄. HMTA can be toxic at high levels of dosage and it can be harmful to the skin and eyes. It is usually found in a crystal form, it is hazardous with carbon monoxide, carbon dioxide and nitrogen oxides and highly flammable.

In this experiment we tested the bactericidal effect of HMTA on the bacteria *E. coli*. HMTA is known to hydrolyze to formaldehyde and ammonia,² which negatively affects *E. coli* bacteria growth. HMTA has been used as a medicine for treating urinary tract infections.

References

1. www.cdc.gov/ecoli/general/
2. <http://www.epa.gov/opprd001/inerts/hexamethyl.pdf>

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Food Chemistry - Poster

CONTROL ID: 2217746

TITLE: [Non-chemical treatment to extend fruit shelf life](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [C. E. Garcia Maso](#)¹, [R. Alquraishi](#)¹

INSTITUTIONS (ALL): 1. Syracuse Academy of Science Charter School, Syracuse, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Abstract

Knowing that fruits are part of our daily lives, and learning we can possibly increase the shelf life by stopping ripening appealed to our interest. In order to increase fruit shelf life, different non-chemical methods were used. The fruits underwent different procedures with UV-C treatment, dry heat, conventional microwave, and pulse microwave. DNA and protein were extracted from tomatoes and made into gels. The gels were run through the Bio Rad Power Pac basic in order to get the results. None of the protein and DNA of sample tomatoes were damaged during the process of non-chemical treatments and the browning enzyme turned off and shelf life was possibly preserved.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Physical Chemistry - Oral

CONTROL ID: 2217816

TITLE: [A quasi-atomic perspective of three-center-two-electron Zr-H-Si interactions](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [J. Duchimaza Heredia](#)¹, [K. Yan](#)¹, [A. D. Sadow](#)³, [M. S. Gordon](#)²

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INSTITUTIONS (ALL): 1. Iowa State University, Ames, IA, United States.
2. Ames Lab US DOE, Iowa State University, Ames, IA, United States.
3. Department of Chemistry, Iowa State University, Ames, IA, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: The cationic disilazido zirconocene complex $[\text{Cp}_2\text{ZrN}(\text{SiHMe}_2)_2]^+$ exhibits spectroscopic and structural features analogous to intramolecular 3-center-2-electron metal-H-C agostic interactions. These interactions facilitate hydrogen migration between the metal center and the disilazido ligand, leading to unexpected reactivity between the cation and Lewis bases. Ab initio calculations verify the agostic-like Zr-H-Si interaction. A novel quantitative orbital localization scheme generates quasi-atomic molecular orbitals. The quasi-atomic orbital localization is applied for more comprehensive analysis of the individual atomic contributions to the intramolecular interaction between zirconium and β -hydrogen atoms. As a result, this study provides key insights into the mechanistic importance of agostic-like interactions in early transition metal chemistry.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Oral

CONTROL ID: 2218598

TITLE: [Chemical Jokes facilitate learning of important chemistry concepts](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [K. Zaman](#)¹

INSTITUTIONS (ALL): 1. Science, The Community College of Baltimore County, Essex, MD, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: It is accepted by most that a large number of students perceive chemistry as a boring and difficult discipline. Many students are of the opinion that they took chemistry only because chemistry was one of their program requirements, not realizing that it is one of the most important scientific disciplines. They do not understand the importance of chemistry. They attend chemistry classes because they have to do it. Some students lose their interest in chemistry after a few weeks into the semester irrespective of the greatness or otherwise of the instructor. The author of this presentation decided to motivate his students by sharing chemical jokes during lectures. For example, while explaining the idea of atoms the author made the students laugh by saying "do not trust the atoms, they make up everything". It also gave the students a clear message that all matter is made up of tiny particles called atoms. Chemical jokes have increased retention in his classes, and improved the overall performance of his students. In this presentation the author will share with the audiences some of the chemical jokes that were used by him during his lectures and that facilitated learning of difficult chemical concepts.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Advances in Colloid and Surface Chemistry - Oral - INVITED ONLY

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CONTROL ID: 2219752

TITLE: [Semiconductor nanocrystals for robust and efficient solar hydrogen production](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): T. Krauss¹, F. Qiu¹, R. Eisenberg¹, Z. Han¹, P. L. Holland², C. Liu¹, J. Peterson¹

INSTITUTIONS (ALL): 1. Dept of Chem, Univ of Rochester, Rochester, NY, United States.
2. Chemistry, Yale University, New Haven, CT, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Homogeneous molecular-based systems for light-driven reduction of protons to H₂ typically suffer from short lifetimes because of decomposition of the light-absorbing molecule, such as an organic dye. A complementary approach to entirely molecular systems would be to incorporate nanoscale based systems, such as semiconductor nanocrystals, into an artificial photosynthesis system. Nanocrystals offer several potential advantages including durability, electronic states and redox potentials that are size tunable, and the ability to store and deliver multiple electrons. We will present studies of a robust and highly active system for solar hydrogen generation in water that uses CdSe nanocrystals capped with dihydrolipoic acid (DHLLA) as the solar energy harvester and a soluble Ni²⁺-DHLLA catalyst for proton reduction. With ascorbic acid as a sacrificial electron donor at pH 4.5, the system gives over 600,000 turnovers with respect to catalyst. Under appropriate conditions, the nanocrystal based system has undiminished activity for at least 360 hours under illumination at 520 nm, and achieves quantum yields in water of over 36%. We will also present measurements of the efficiency and robustness of photo-hydrogen production for core CdSe nanocrystals compared to other more highly engineered nanoparticle systems such as core-shell CdSe-CdS nanocrystals and CdSe-CdS dot-in-rod nanoparticles.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS: Accept

ABSTRACT STATUS: decisioned_accepted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials Chemistry - Poster

CONTROL ID: 2277927

TITLE: [A comparative study on the preparation and pH dependent durability of nanoparticles loaded on nanomembranes for water treatment applications](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): N. K. Trejo¹, M. Frey²

INSTITUTIONS (ALL): 1. Fiber Science and Apparel Design, Cornell University, Ithaca, NY, United States.
2. Fiber Science and Apparel Design, Cornell University, Ithaca, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: In this study carboxylic acid coated iron oxide nanoparticles (CA-Fe₃O₄ NPs) were applied to Nylon 6 nanomembranes by three different techniques: 1) simultaneous electrospinning/electrospraying, 2) layer-by-layer (LbL) assembly, and 3) chemical grafting. The purpose of this research was to evaluate the nanoparticle treatment uniformity and durability by each method. CIELAB spectrophotometry, which evaluated the color difference on the membranes revealed that electrospin/spraying and chemical grafting methods produced a uniform NP dispersion. Inductively coupled plasma atomic emission spectroscopy (ICP-AES) results indicated that all methods released particles, however, a substantial amount of particles remained on the membranes. Furthermore, the durability of the treatments is pH dependent, and driven by electrostatic interactions. At the highest release conditions, LbL membranes retained 97.6%, the grafted membranes maintained 98.3%, and the electrospun/electrosprayed membranes maintained 99.2% of the total NP loads after 60 minutes. Potential applications for these membranes can be for assisting with the clean-up

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of polluted rivers based on the adsorption and magnetic properties of the nanoparticles. Ultimately, few studies have yet to evaluate the durability of NP treatments on fibers for end-use applications although it is currently an issue of high concern.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Inorganic Chemistry - Oral

CONTROL ID: 2222118

TITLE: [Competition between ligation and solvation in heavy alkaline earth metal tetraarylborates](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [C. M. Lavin](#)¹, A. G. Goos¹, D. G. Allis¹, K. Ruhlandt-Senge¹

INSTITUTIONS (ALL): 1. Department of Chemistry, Syracuse University, Syracuse, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: One of the challenges in heavy alkaline earth metal chemistry is the limited ability to accurately predict the structures of these compounds due to the significant influence of numerous factors responsible for achieving steric saturation for the large metal centers. Recent work has aptly demonstrated the impact of non-covalent interactions in controlling the structural chemistry of the target compounds. Thus, considering the close correlation between structure and function, non-covalent interactions play a unique role in providing the physical properties needed for particular applications.

This project is based on tetraarylborates due to their various substitution patterns and their ability to provide metal- π interactions to investigate the structure determining factors in heavy alkaline earth metal complexes. These novel compounds demonstrate the importance of ligand and solvent choice to achieve the desired structures along with the competition between ligation and solvation, thus providing insight into the critical role of secondary interactions on structural pattern and ion association modes.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: News from Carbon World - Oral - INVITED ONLY

CONTROL ID: 2223687

TITLE: [Novel aromatic architectures derived from the benzannulation of alkynes](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [W. Dichtel](#)¹

INSTITUTIONS (ALL): 1. Chemistry and Chemical Biology, Cornell University, Ithaca, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Congested aromatic systems, such as *ortho*-arylenes, are more difficult to access than their *meta*- or *para*-linked counterparts because their steric hindrance poses a challenge for transition metal-catalyzed cross-coupling reactions. We have explored a new entry into such systems, which is based on the Asao-

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Yamamoto benzannulation of aryl acetylenes. This reaction is highly efficient, enabling its application for modifying conjugated polymers, tolerant of extreme steric hindrance, and is regioselective for many substrates. The application of this reaction to access new molecular and polymeric aromatic systems, such as contorted aromatic systems and extended graphene nanoribbons, will be presented.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Organic Chemistry - Poster

CONTROL ID: 2224847

TITLE: [A study of hydrophobic vs. hydrophilic componets of molecules in C3 to C10 acyclic imide synthesis: An undergraduate research project](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [K. S. Marshall](#)¹

INSTITUTIONS (ALL): 1. Mail Drop BC SCI, Quinnipiac Univ, Hamden, CT, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: The original approach to the synthesis of N-vanillyl-di-(8-methyl-6-nonen)imide **1** involved the N-alkylation of a symmetrical acyclic imide **2**. When the R group was 2 carbons the preparation of imide **2** went very smoothly. However, increasing the R group to 9 carbons [the desired size] the process completely failed. This approach was then abandoned and an alternate approach was attempted. Large acyclic imides have been synthetic challenges with only a few mthods reported for their construction. This project was based on the procedure of Davidson and Shovronek¹ which involved a one pot reaction between 1 eq. of amide, 1.1 eq. of acid anhydride and 1 eq. of acid chloride to prevent nitrile formation. The current project was to study the relationship between the hydrophobic side chain and the hydrophilic carbonyl moiety during imide formation .At what carbon size does the hyrophobic portion override the hydrophilic portion resulting in no or very little imide product formation. Experiments involved going from C-3 to C-10. Reaction % yields (of recrystallized imides) were used to access the comparison. Preliminary results were C-3 30%; C-4 35.8%; C-5 37.3%; C-6 33.8%; C-7 9.11%; C-8 15%; C-9 10.3% and C-10 2.2%. A marked decrease occurred at C-7.

¹D. Davison and H. Skovronek, *J. Amer. Chem. Soc.*, **80**, 376 (1958).

CONTACT (COUNTRY ONLY): United States

DECISION STATUS: Accept

ABSTRACT STATUS: decisioned_accepted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Green Labs - Oral - INVITED ONLY

CONTROL ID: 2225924

TITLE: [Green chemistry & chemical hygiene, a marriage made in an undergraduate program?](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. Charlton-Smith](#)¹

INSTITUTIONS (ALL): 1. WVWC-1734, West Virginia Wesleyan College, Buckhannon, WV, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Chemical Hygiene and Green Chemistry truly go hand in hand. Chemical Hygiene Officers are the

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purveyors of chemical hygiene and green chemistry standards in laboratories. Since 1990 the Occupational Safety and Health Administration's lab standard has required a Chemical Hygiene Officer (CHO) in laboratories working with chemicals, however, formal education in the profession has never been standardized. West Virginia Wesleyan College is the first institution of higher education to offer a Chemical Hygiene and Safety (CHS) major specifically designed to produce certifiable CHO's with a firm grasp of chemistry, chemical safety and green chemistry practices. Key program elements include a traditional background comparable to a chemistry BS degree with additional coursework in chemical hygiene, industrial hygiene, HAZWOPER and Toxicology. This presentation will discuss the motivation behind this original program, implementation and how the program emphasizes, utilizes and integrates the twelve principles of green chemistry.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: author_withdrawn [Unwithdraw](#)

ABSTRACT SYMPOSIUM NAME: Green Labs - Oral - INVITED ONLY

CONTROL ID: 2225973

TITLE: [A strategy with lab ventilation management to enhance sustainability](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): E. Sweet¹

INSTITUTIONS (ALL): 1. Environmental Health and Safety, Cornell University, Aurora, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Incorporating operational strategies in laboratories that reinforce the long term ability for organizations to support science is a challenge that is often seen to compete with health and safety. A balanced approach to managing energy usage through proper chemical management and reducing heat generation allows the organization to lower ventilation rates and maintain the health of occupants of the laboratory. This presentation will discuss this approach to sustainability through the development of a Green Labs program.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials for Energy - Oral

CONTROL ID: 2227508

TITLE: [Soft chemistry approach to the synthesis of energy related materials](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): E. Dikarev¹

INSTITUTIONS (ALL): 1. Univ of Albany Suny, Albany, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: The major focus of this work is the development of an effective low-temperature approach for the preparation of energy-related materials. Our group is involved in the synthesis of volatile single-source precursors – molecules containing all the necessary elements in the proper ratio and decomposable in a

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controlled manner under mild conditions to afford target phase-pure products. Mixed-ligand approach to the design of heterometallic precursors with discrete molecular structures, while maintaining the proper metal:metal ratio for the target material, will be presented. Combination of two different diketonate ligands with electron-withdrawing and electron-donating substituents brings about changes in the connectivity pattern within heterometallic assembly and yields precursor with molecular structure, even in the cases when both homoleptic counterparts either form coordination polymers, do not exist, or produce complex with a different M:M' ratio. The applicability of the above approach to the synthesis of single-source precursors for multiferroic oxides, oxygen evolution reaction catalysts, and prospective cathode materials will be demonstrated.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Green Chemistry - Oral - INVITED ONLY

CONTROL ID: 2228067

TITLE: [Recyclable organocatalysis for organofluorination and other asymmetric synthesis](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): W. Zhang¹, X. Hung¹, W. Yi²

INSTITUTIONS (ALL): 1. University of MA Boston, Dorchester, MA, United States.

2. Nanjing university of Science and Technology, Nanjing, Jiangsu, China.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Organocatalysis has advantages such as free of toxic heavy metals, mild reaction conditions, novel mood of activation, and good structural amenability. It is a new technology for asymmetric synthesis and green chemistry applications. However, organocatalysis requires high catalyst loading and separation/recycling of organocatalysts is not an easy task. The development of fluorous organocatalysis provides an efficient way to address the issue. In addition to phase tag separation, the stereoelectronic effect of the fluorous chain can be used to modify the reactivity and selectivity of the catalysts. This presentation highlights our recent effort on the development of recyclable organocatalyst-promoted fluorination, Michael addition, Robinson annulation, and one-pot addition/cyclization for asymmetric synthesis of biologically interested molecules.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Green Chemistry - Oral - INVITED ONLY

CONTROL ID: 2229645

TITLE: [Planetary boundaries that we MUST all live by: opportunities for innovative interdisciplinary research and education in sustainable technologies](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): M. C. Cann¹

INSTITUTIONS (ALL): 1. Dept of Chemistry, University of Scranton, Scranton, PA, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

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Abstract: In 2009 planetary boundaries were proposed that define a “safe operating space for humanity.” The nine boundaries are climate change, chemical pollution, stratospheric ozone depletion, aerosol loading, ocean acidification, nitrogen and phosphorus cycles, freshwater use, land use changes, and biodiversity loss. Any one (or combinations thereof) of these offers a plethora of interdisciplinary opportunities in education and research in sustainable technologies with chemistry as a central theme. The challenge is to ask yourself: how can I, through collaboration with my colleagues in academia and industry, employing education and research, contribute to the effort to stay within these boundaries?

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Medicinal Chemistry - Poster

CONTROL ID: 2228298

TITLE: [Antibiotic activity of 5-substituted 1H-tetrazoles](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. Coca](#)¹, E. Roberts², J. Dudley¹, L. A. Feinn¹

INSTITUTIONS (ALL): 1. Chemistry, Southern CT State University, New Haven, CT, United States.
2. Biology, Southern Connecticut State University, New Haven, CT, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Several tetrazole derivatives were evaluated for antibacterial activity against *Staphylococcus aureus*, *Escherichia coli*, and *Pseudomonas aeruginosa*. Most derivatives showed significant antibacterial activity and many derivatives exhibited a minimum inhibitory concentration below 250 µg/mL.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Organic Chemistry - Oral

CONTROL ID: 2228308

TITLE: [Synthesis of 5-Substituted 1H-Tetrazoles Catalyzed by Post-Transitional Metals](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): J. Dudley¹, L. A. Feinn¹, [A. Coca](#)¹

INSTITUTIONS (ALL): 1. Chemistry, Southern CT State University, New Haven, CT, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Several 5-substituted 1H-tetrazoles were synthesized in water using microwave heating in high yield. The cycloaddition between organonitriles and sodium azide was catalyzed by indium chloride and bismuth chloride.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS: Accept

ABSTRACT STATUS: decisioned_accepted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Progressive Methodology for Organic Synthesis - Oral - INVITED ONLY

CONTROL ID: 2228356

TITLE: [From strained carbocycles to heterocycles](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [P. Wipf](#)¹

INSTITUTIONS (ALL): 1. Univ of Pittsburgh, Pittsburgh, PA, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Cyclopropanes and cyclobutanes are commonly used building blocks in organic synthesis. A few natural products also contain these scaffolds, and a considerable number of organic methods have focused on their preparations and synthetic transformations. In contrast, applications of bicyclo[1.1.0]butanes and methylene cyclopropanes in organic synthesis have been much more limited. Our group has been able to extend bicyclobutane and methylene cyclopropane chemistry for the preparation of fused and bridged pyrrolidines, some of which represent completely novel architectures. We are also applying this methodology toward the total synthesis of polycyclic alkaloids.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Bio-based Materials and Processes - Oral - INVITED ONLY

CONTROL ID: 2228555

TITLE: [Engineered biocatalysts for solar fuels](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [K. Bren](#)¹

INSTITUTIONS (ALL): 1. Chem Dept, Univ of Rochester, Rochester, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Molecular hydrogen (H₂) is an energy-dense alternative to fossil fuels, and many synthetic molecular catalysts capable of assembling protons and electrons into H₂ have been developed. This presentation describes a complementary approach in which biomolecules are being engineered as catalysts for the reduction of water to H₂. In particular, semisynthetic metalloproteins and metallopeptides that are water soluble and oxygen tolerant are being prepared. These artificial hydrogenases are readily synthesized and modified using standard peptide synthesis and protein engineering techniques. Derivatives with enhanced stability, activity, and efficiency have been prepared by altering protein or peptide amino acid sequence. To store light energy as the solar fuel H₂, biological chromophores capable of photoinduced charge transfer to catalysts are being developed. This work is part of a multidisciplinary effort at the University of Rochester to engineer assemblies for photocatalytic hydrogen generation, drawing on approaches from biochemistry, synthetic chemistry, and nanotechnology.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Organic Chemistry - Poster

CONTROL ID: 2228819

TITLE: [Converting primary amines into alcohols via N-nitrosodichloroacetamides](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [C. E. Jakobsche](#)¹, L. Wang¹, B. G. McCarthy¹, N. S. MacArthur¹

INSTITUTIONS (ALL): 1. Chemistry Dept, Clark University, Worcester, MA, United States.

PRESENTATION TYPE: Poster Preferred

ABSTRACT BODY:

Abstract: N-Nitrosoacetamides undergo thermal rearrangements into acetates, and the relative ease and efficiency of these transformations is affected by the chemical nature of the acetamide. Following a detailed comparison of various acetamide structures we have identified dichloroacetamides as optimal substrates for this rearrangement sequence, which can be used to easily convert primary amines into alcohols through a 4-step, 1-purification sequence. After evaluating the substrate scope on simple amine substrates, we are currently applying this methodology to the synthesis of higher complexity chemical structures with biological relevance.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Environmental Chemistry - Oral

CONTROL ID: 2229078

TITLE: [Hydroxyl radical formation from bacteria-assisted Fenton Chemistry at neutral pH](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [J. Grossman](#)¹, T. F. Kahan¹

INSTITUTIONS (ALL): 1. Chemistry, Syracuse University, Syracuse, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Fenton chemistry is one of the primary sources of hydroxyl radicals (OH) in natural waters in the absence of sunlight. Dark Fenton chemistry is thought to occur only in acidic waters, due primarily to solubility limitations of iron at higher pH. We have investigated the effects of the iron-reducing bacteria *Shewanella oneidensis* (SO) on dark Fenton chemistry at neutral pH. We show that SO significantly increases OH production rates at neutral pH; OH production rates increased by a factor of 1.5 when iron was in the form of Fe(II), and by a factor of six when iron was in the form of Fe(III). Hydroxyl radical production rates depended linearly on SO cell density and on H₂O₂ concentration. Our results suggest that bacteria-assisted Fenton chemistry could greatly increase dark radical production in natural waters, especially at near-neutral pH.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

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ABSTRACT SYMPOSIUM NAME: Recent Advances in Food Chemistry and Nutritional Biochemistry - Oral - INVITED ONLY

CONTROL ID: 2229177

TITLE: [Covalent adduct chemical ionization \(CACI\) and molecular ion tandem mass spectrometry for characterization of unusual fatty acids in foods and oils](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): J. Brenna¹

INSTITUTIONS (ALL): 1. Nutrition, Cornell University, Ithaca, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Conventional lipidomics approaches by mass spectrometry typically deliver molecular information about carbon and double bond number on specific, intact molecular species of phospholipids, triacylglycerols, and other molecules that carry unsaturated fatty radical (acyl or alkenyl groups) but ignore double bond positions and chain branching. For several years, we developed methods for identification of double bond position or chain branching in minor fatty acids found in foods. For localization of double bonds we use an approach termed “covalent adduct chemical ionization (CACI)” tandem mass spectrometry capable of determination of double bond position in fatty acid methyl esters (FAME). A gas phase ion-molecule reaction ionizes and derivatizes the analyte. Collisional activation results in two specific diagnostic ions that locate the double bonds. The method has been applied to fatty acids of unusual double bond structure up to pentaenes. Chain branching in saturates are a little appreciated feature of fatty acids originating primarily in milkfat and ruminant meats. Collisional activation of the molecular ion of electron impact ionized FAME yields a mass spectrum very different from the MS-1 spectrum. A rearrangement around the tertiary carbon at the branch point yields strong product ions very characteristic of structure. Basics of both methods and examples of applications in oils and foods will be presented.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Inorganic Chemistry - Oral

CONTROL ID: 2247191

TITLE: [Design of the first volatile precursors for low-temperature synthesis of up-conversion NaREF₄ materials.](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): M. C. Barry¹, E. Dikarev¹

INSTITUTIONS (ALL): 1. Univ of Albany Suny, Albany, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: A new approach to design single-source precursors for the most efficient up- and down-conversion materials is reported. Heterobimetallic fluorinated β -diketonates NaRE(β -dik)₄ (RE = rare earth) with a proper Na:RE ratio have been obtained with high yields through a simple, one-pot synthesis that utilizes commercially available reagents. Compounds were found to be highly volatile and to retain their heterometallic structure in the gas phase as well as in solution. Thermal decomposition of diketone precursors affords target fluoride materials in the form of α -cubic or β -hexagonal NaREF₄ phase under relatively mild conditions. Synthesis, characterization, and thermal decomposition of a new class of single-source precursors will be discussed.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

NERM April 6, 2015

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Bio-based Materials and Processes - Oral - INVITED ONLY

CONTROL ID: 2229772

TITLE: [Titanium minerals and biochemistry](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. Valentine](#)¹

INSTITUTIONS (ALL): 1. Temple University, Wynnwood, PA, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Titanium is the ninth most abundant element in the earth's crust, and titanium minerals are widespread, yet conventional wisdom holds that biology has very little to do with titanium. The element has a reputation for inertness that is belied by data from several experimental systems. This talk will address some interactions between titanium minerals and biology at the molecular level, and will examine cases in which organisms and/or biomolecules induce, bind, or dissolve titanium minerals.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Recent Advances in Food Chemistry and Nutritional Biochemistry - Oral - INVITED ONLY

CONTROL ID: 2230612

TITLE: [Analytical approaches for the determination of chemical residues on the surfaces of fruits and vegetables by mass spectrometry](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [J. D. Henion](#)¹, [D. Eikel](#)¹, [N. Sousou](#)¹, [C. Hao](#)¹

INSTITUTIONS (ALL): 1. Advion, Inc., Ithaca, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: An automated surface-sampling technique called liquid extraction surface analysis (LESA), coupled with infusion nano-electrospray high-resolution mass spectrometry and tandem mass spectrometry (MS/MS), will be described and applied to the qualitative determination of surface chemical residues resulting from the artificial spraying of selected fresh fruits and vegetables with representative pesticides. When the surface of a spinach leaf was analyzed by LESA, trace levels of diazinon were readily detected on the spinach purchased directly from a supermarket before they were sprayed with the five-pesticide mixture. A 30 s rinse under hot running tap water appeared to quantitatively remove all remaining residues of this pesticide. This report showed that representative pesticides on fruit and vegetable surfaces present at levels 20-fold below generally allowed EPA tolerance levels are readily detected and confirmed by the described technologies making LESA-MS as interesting screening method for food safety purposes.

Alternatively, the technique of ASAP (atmospheric sample analysis probe) installed on a compact single quadrupole mass spectrometer (Advion, Inc.) will be described which allows for screening surface chemical residues on fruits and vegetables. The work flow is a simple swipe of the glass capillary tip on the food sample with the wetted closed-end tip of glass melting point capillary followed by insertion of this glass capillary tip into a hot stream of nitrogen gas in an APCI source.

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Finally, representative over-the-counter dietary supplements which may be purported to contain potentially unhealthy additives will be described using the same ASAP-compact mass spectrometer system.

Advances in Food Chemistry and Nutritional Biochemistry Symposium.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Physical Chemistry - Oral

CONTROL ID: 2251530

TITLE: [Origin of Recombination Centers in Organo-Halide Perovskites for Solar Photoconversion](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [R. J. Stewart](#)¹, [J. B. Asbury](#)²

INSTITUTIONS (ALL): 1. Chemistry, Pennsylvania State University, State College, PA, United States.
2. Chemistry, Pennsylvania State University, State College, PA, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Photovoltaics based on organo-halide perovskite absorbers are an emerging technology due to the recent explosion in their solar to electric power conversion efficiencies. Unusually high open-circuit voltages, long charge carrier lifetimes, and long diffusion lengths have been observed in these materials, which suggest these films have low defect densities. However, experimental evidence for the electronic structure and the identity of defects has been lacking. We sought to systematically explore the chemical nature defects in organo-halide perovskite films and the resulting influence of these defects on the densities of mid-gap states that may act as recombination centers for photogenerated charge carriers. By systematically altering film composition and measuring the charge carrier lifetime with transient photoluminescence and absorbance spectroscopy, we identify defects that are deleterious to charge carrier recombination.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Advances in Colloid and Surface Chemistry - Oral - INVITED ONLY

CONTROL ID: 2231173

TITLE: [Materials design with layered biomimetic nanocomposites](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [N. Kotov](#)¹, [Y. Kim](#)², [S. O. Tung](#)¹, [B. Yeom](#)¹, [T. Shyu](#)¹

INSTITUTIONS (ALL): 1. University of Michigan, Ann Arbor, MI, United States.
2. Chemical Engineering, University of Michigan, Ann Arbor, MI, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Finding materials with combinations of several extreme properties is one of the key requirements for the successful engineering of adaptive systems. Successful realization of such materials requires new choices for materials components and new approaches for materials “assembly”. Layer-by-layer assembly (LBL) is materials manufacturing technique from nanomaterials that affords hierarchical multiscale

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engineering of nanocomposite materials (Figure 1) based on sequential adsorption of nanometer scale layers of polymers and inorganic particle, nanowires, nanotubes, sheets, etc. In this presentation we demonstrate that LBL and related techniques can lead to the materials with seemingly “impossible” combinations of properties encompassing mechanical, electrical, optical, and biological properties. We will make particular emphasis in this presentation on nanoparticles composites which consistently demonstrate exceptional performance and display the potential for scalability. Finding composites with high stiffness properties + high damping and as well as high stiffness + transparency will be demonstrated. The pathway toward successful realization of two, three, and four different properties based on the structural designs and computer simulations is possible and will be exemplified using nanocomposites used for biomedical applications, such as brain implants. A new type of nanoscale “building blocks” such as aramid nanofibers (ANFs) can also be incorporated in such composites combining several hard-to-reach properties with potential applications as ion conductors for lithium ion batteries will be described. The last part of the talk will describe our latest exploits in the area of composites from plasmonic nanoparticles and materials designs to achieve the combination of high conductivity and high stretchability.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS: Accept

ABSTRACT STATUS: decisioned_accepted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: The Legacy of Minority Institution - Oral

CONTROL ID: 2231673

TITLE: [Engaging and mentoring STEM-focused students transitioning from tribal colleges to universities](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [J. Lee](#)¹

INSTITUTIONS (ALL): 1. Department of Biomedical Sciences, University of Minnesota Med School Duluth, Duluth, MN, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Native American students who major in STEM-focused fields do not have the same access to advanced courses and research at tribal colleges. Tribal colleges offer AA and AS degrees in generic science fields due to the limitations of coursework. Students transferring from tribal college to universities encounter a different culture when moving to and living on college campuses. Native American students need institutional support, with community events, tutoring services and academic support to succeed. This session will introduce ways that faculty and administration can do to interact with students, their local community and home communities.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Biochemistry - Oral

CONTROL ID: 2232061

TITLE: [Factors influencing selective nitration of tyrosines in proteins](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. S. Bayden](#)¹, V. A. Yakovlev², R. B. Mikkelsen³, G. E. Kellogg⁴

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INSTITUTIONS (ALL): 1. CMBioscience, Inc., Hamden, CT, United States.
2. Division of Molecular Radiobiology, Department of Radiation Oncology, Virginia Commonwealth University, Richmond, VA, United States.
3. Department of Radiation Oncology, Virginia Commonwealth University, Richmond, VA, United States.
4. Department of Medicinal Chemistry and Institute for Structural Biology and Drug Discovery, Virginia Commonwealth University, Richmond, VA, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Nitration at tyrosine residues occurs both *in vitro* and *in vivo*. Generally, one of the two tyrosine aromatic hydrogens that are ortho with respect to the hydroxyl group is replaced by a nitro group. Tyrosine nitration has been detected under physiological conditions in most organ systems and in a number of cellular models. Accumulating data supports a strong link between protein tyrosine nitration and the activation of signaling pathways in a variety of cellular responses and pathological conditions. We have built predictive models for selectivity in both *in vitro* and *in vivo* tyrosine nitration based on 3D structural features of 20 proteins for which high resolution X-ray crystallographic or NMR data are available and for which nitration of 35 total tyrosines has been experimentally shown under oxidative stress.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: News from Carbon World - Oral - INVITED ONLY

CONTROL ID: 2233424

TITLE: [Contorted aromatics featuring non-traditional ring sizes](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. Whalley](#)¹

INSTITUTIONS (ALL): 1. Chemistry, University of Vermont, Burlington, VT, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Traditionally, contorted aromatics have been synthesized by incorporating 5-membered rings into structures composed primarily of fused hexagonal rings. The introduction of these smaller ring sizes induces strain in the molecule forcing it to bend away from its desired planar orientation, which results in the emergence of interesting properties. We are interested in synthesizing non-planar molecules that incorporate ring sizes other than 5- and 6-membered and observing how the properties of the molecules change with the introduction of these non-traditional rings. With this in mind, we have synthesized a stable derivative of [8]circulene – the largest member of the circulene family synthesized to date – using a Diels-Alder reaction and a palladium catalyzed arylation as the key synthetic steps. Although, the structure distorts significantly from planarity, x-ray data validates the presence of a fully benzenoid structure which explains the remarkable stability of this compound.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Physical Chemistry - Poster

NERM April 6, 2015

CONTROL ID: 2233563

TITLE: [Synthesis and Application of Squaraines Targeted for Organic Photovoltaics](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [P. Cost²](#), C. Collison¹, J. A. Cody¹, C. Zheng¹, I. Jalan¹, B. Cona¹

INSTITUTIONS (ALL): 1. School of Chemistry and Materials Science, Rochester Inst of Technology, Rochester, NY, United States.

2. Chemistry, Rochester Institute of Technology, Marcellus, NY, United States.

PRESENTATION TYPE: Poster Preferred

ABSTRACT BODY:

Abstract: Squaraines are a class of small molecules enthusiastically investigated for organic photovoltaics (OPV) along with other applications such as bio-imaging and photo dynamic therapy. The choice of side group has a surprising influence over the packing and aggregation of these molecules in the solid state active layer of a target device. Two new squaraine molecules with bulky aniline alkyl groups were synthesized with and without stabilizing hydroxyl groups hydrogen bonded to the central C4O2 group. The goal of the work was to understand the relative influence of the hydroxyl groups and R-groups towards the packing as it influences device efficiency. The molecules were characterized for UV-VIS absorption and fluorescence in a variety of blends with PCBM in a variety of different morphologies, controlled through annealing. Changes in device efficiencies were correlated with this spectroscopic data. We will present an overview of synthesis, characterization, experimental validation of modeling results and device data. We will put forward a description as to how the functionalization of the squaraine influences the efficiency of the device through mechanistic interpretations.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Recent Advances in Food Chemistry and Nutritional Biochemistry - Oral - INVITED ONLY

CONTROL ID: 2234330

TITLE: [Choline supplementation during pregnancy and perinatal health](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [X. Jiang¹](#)

INSTITUTIONS (ALL): 1. Health and Nutrition Sciences, Brooklyn College , Brooklyn, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Choline is an essential nutrient often grouped with the B vitamins. Choline biomolecules participate in various biological processes including growth and development, cellular membrane formation, neurotransmission and one-carbon metabolism. The demand for choline increases substantially during pregnancy. Dietary recommendation for choline has been established at 450 mg/d in the form of Adequate Intake for pregnant women, yet the actual requirement of this nutrient is unknown. Supplementing third trimester pregnant women with extra choline (930mg/d versus 480 mg/d) beneficially influences maternal vasculature and fetal markers of stress. Choline supplementation improves maternal glucose tolerance and prevents fetal overgrowth in part by activating placental fat catabolism in mice with high-fat diet-induced gestational diabetes. Maternal choline supplementation may be an effective prophylaxis for the improvement of perinatal health.

(Advances in Food Chemistry and Nutritional Biochemistry Symposium)

CONTACT (COUNTRY ONLY):

NERM April 6, 2015

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Poster

CONTROL ID: 2265029

TITLE: [Nuclear Chemistry Under Western New York: A Lesson for General Chemistry](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [D. Ventura](#)¹, A. Poblocki¹

INSTITUTIONS (ALL): 1. D'Youville College, Buffalo, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: A major challenge that faces us as educators is igniting excitement in students about a certain topic. One method of obtaining the interest of students is by relating textbook topics to everyday life. Relating nuclear chemistry to Buffalo, NY and the surrounding Western New York area, in locations near to D'Youville College, has sparked an interest in this topic and has helped it become one of the favorites among the students. Although few realize it, Western New York has a strong past involved in nuclear chemistry, especially during World War II. We examine and investigate the use of this historic information to engage students in the undergraduate classroom. While this study may seem to only impact a small regional area, there are nearly 90 other locations of radioactive waste distributed across the United States, making similar lessons viable in nearly any region of the United States.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Green Polymers - Oral - INVITED ONLY

CONTROL ID: 2245913

TITLE: [Engineering bacteria for the production biodegradable plastics](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [C. T. Nomura](#)¹

INSTITUTIONS (ALL): 1. SUNY-ESF, Syracuse, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Poly-3-hydroxyalkanoates (PHAs) have attracted great interest as environmentally friendly replacements of petroleum-based plastics and have potential applications as bulk-commodity plastics and biomaterials for biomedical use. The physical properties of PHA polymers are dictated by their repeating unit composition and can be divided into three main classes: short-chain-length (SCL) PHA polymers are made up of repeating units of 3-5 carbons and exhibit thermoplastic properties, medium-chain-length (MCL) PHA polymers are made up of repeating units of 6-14 carbons and exhibit elastomeric properties and SCL-MCL PHA copolymers that exhibit a range of physical properties dependent on the mol ratio of SCL to MCL repeating units in the polymer. Our lab is interested in understanding what metabolic pathways in bacteria are used to generate PHA polymers. In this presentation, I will discuss some of the new pathways and methods we have designed to produce PHAs in bacteria and explore some new applications.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

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ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Environmental Chemistry - Oral

CONTROL ID: 2246038

TITLE: [Photolysis of Aromatic Pollutants in Aqueous, Organic, and Mixed Phases: Implications for Reactivity in Aerosols, Natural Waters, and Ice](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): T. F. Kahan¹, J. Grossman¹, P. Malley¹

INSTITUTIONS (ALL): 1. Syracuse University, Syracuse, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Condensed phases in the atmosphere such as cloud droplets, aerosols, and snow often contain both water and organic matter (OM). Reactivity can differ significantly between aqueous and organic phases. We have measured photolysis kinetics of the polycyclic aromatic hydrocarbons (PAHs) anthracene and pyrene in several organic solvents and in water, as well as in miscible and phase-separated aqueous-organic mixtures at atmospherically-relevant wavelengths. Photolysis rate constants generally increased with increasing solvent dielectric constant, with photolysis of both PAHs occurring more than ten times faster in water than in octanol. Local polarity had a much greater effect on PAH photolysis kinetics than changes in PAH absorptivity or singlet oxygen concentrations. Photolysis kinetics in homogeneous aqueous-organic mixtures varied monotonically with OM volume fraction. Kinetics in immiscible (phase-separated) solutions were more complex. In stagnant solutions, kinetics were well-described by equilibrium partitioning, but in turbulent solutions, kinetics were faster than predicted based on the amount of OM present. In frozen aqueous-organic samples, photolysis was substantially suppressed at OM concentrations well below those corresponding to a formal monolayer at a water surface, likely due to freeze-concentration effects. Chromophoric OM (that absorbs sunlight) such as fulvic acid suppressed anthracene photolysis primarily by blocking photons. Effects were greater in frozen samples, again likely due to freeze exclusion. Our results suggest that OM could greatly affect the photochemical lifetimes of PAHs in condensed phases in the environment such as aerosols and ice, even if the OM does not itself absorb photons.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials for Energy - Oral

CONTROL ID: 2247382

TITLE: [Nanocarbon Electrocatalysts for Sustainable Electrochemical Energy Storage and Conversion](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): G. Wu¹

INSTITUTIONS (ALL): 1. Chemical and Biological Engineering, University at Buffalo, SUNY, Buffalo, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract:

The oxygen reduction reaction (ORR) is one of the most technologically important electrochemical reactions for a variety of electrochemical energy storage and conversion technologies (*e.g.*, fuel cells, metal-air

batteries and water splitting). However, due to inherently sluggish kinetics, a large amount of expensive and supply-limited precious metals such as Pt is required as the catalysts for the ORR, greatly hindering the widespread applications of these clean energy technologies. Hence, it is desperately needed to design and develop advanced catalysts from earth-abundant elements, capable of facilitating the ORR at sufficient rates for practical applications. To this end, highly graphitized nanocarbons (e.g., carbon nanotube, graphene sheets, onion-like carbon) with proper heteroatom doping (e.g., nitrogen) has been developed as the most promising nonprecious metal catalysts to replace Pt. Importantly, there is increasing evidence showing that transition metal cations (M) such as Fe and Co are able to bond with nitrogen in various M-N coordinations embedded into the nanocarbon lattices. These complex moieties are furthermore capable of providing significantly improved activity compared to metal-free nitrogen-doped carbon materials.

In our recent effort, cost-effective nitrogen-doped graphene composites have been prepared *via* the graphitization of inexpensive carbon-nitrogen precursors (e.g., polyaniline), combined with transition metals (Co or Fe) as catalysts, and unique metal-organic frames (MOFs) as templates. As a result, new types of graphene-rich composite catalysts were developed and exhibited substantially improved activity for the ORR in various electrolytes including aqueous and nonaqueous. The synthesis-structure-activity correlations for the carbon nanostructures were further established by tuning their synthetic chemistry (supports, nitrogen precursors, heating temperature, and transition metal types and contents). This allows us to investigate how the resulting morphology and nitrogen-doping functionalities influence the catalyst activity. This unique *in situ* formation of nitrogen-doped nanocarbon electrocatalysts directly from heteroatom polymers provides a new route for preparation of advanced nonprecious metal catalysts for sustainable electrochemical energy storage and conversion applications.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: resubmitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Poster

CONTROL ID: 2248457

TITLE: [Educational experience: Training high school teachers in the field of "Clean energy: Hydrogen/fuel cells"](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. Bailey](#)¹, X. Li¹, M. Toro¹, B. Mastrangelo¹, G. A. Takacs¹

INSTITUTIONS (ALL): 1. Rochester Inst of Techlgy, Rochester, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Meeting energy needs in a sustainable and environmentally responsible way is currently a major global challenge. The purpose of this educational project was to prepare high school teachers to understand the sources of clean and renewable energy, issue of Global Warming, and fuel cells application for electricity generation using hydrogen as an incredible fuel and clean energy carrier. The program included: (1) designing and offering a lecture/training course during four Saturdays for high school Chemistry and Earth Science teachers in order to help them teach material associated with "Clean Energy/Hydrogen/Fuel Cells"; (2) assisting the teachers with incorporating the educational material as a unit into their high school program; and (3) designing and organizing two lab experiments in "Hydrogen-Oxygen Fuel Cell Construction", and "Measuring the Amount of Hydrogen Stored in Chemical Compounds and Using the Hydrogen for Electricity Generation with Fuel Cells". The lecture/training course also included: Green House Effect, Hydrogen Properties, Production and Storage of Hydrogen, Hydrogen Infrastructure, Fundamentals of Electrochemistry, Batteries, and Fuel Cell Applications. A Summer Camp for 9 - 12 grade students entitled: "The Science of Fuel Cells" is scheduled during Summer, 2015.

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CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Advances in Colloid and Surface Chemistry - Oral - INVITED ONLY

CONTROL ID: 2248371

TITLE: [Water adsorption and oxidation on anatase TiO₂](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. Selloni](#)¹

INSTITUTIONS (ALL): 1. Princeton Univ, Princeton, NJ, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Semiconductor-based photocatalysis for the degradation of pollutants and the decomposition of water into H₂ and O₂ has been an important area of research for decades. Due to its abundance, non-toxicity, high stability under a variety of conditions, as well as proper band alignment relative to the water redox potentials, the most widely used material in heterogeneous photocatalysis is titanium dioxide (TiO₂). I shall discuss recent applications of first principles electronic structure calculations and molecular dynamics simulations to understand materials properties and reaction mechanisms relevant to TiO₂-based photocatalysis, with focus on water adsorption and the mechanism of water oxidation at the surface of anataseTiO₂.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials for Energy - Oral

CONTROL ID: 2284891

TITLE: [Controlling composition, asymmetry, and internal microstructure of nanomaterials using a core/alloy approach](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. M. Maye](#)¹

INSTITUTIONS (ALL): 1. Department of Chemistry, Syracuse University, Syracuse, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: This presentation focuses on our recent nanoparticle synthesis strategy that employs atomic interdiffusion at a core/shell interface to produce alloy-terminated nanocrystals. These core/alloy nanoparticles have alloy compositions that are determined by shell thickness, processing temperature, initial core diameter, and surface capping ligand. As a proof of principle, we have fabricated an assortment of noble metal alloy heterostructures. The alloying is preceded by the layer-by-layer deposition of the shell material (i.e., Ag, Pd, Pt), followed by a microwave mediated hydrothermal annealing step, which induces core/shell inter diffusion and alloying. We show the extension of this approach by using alloy phase behavior to drive asymmetric growth of heterostructures with janus-like interfaces. Using these structures, a second novel galvanic replacement reaction step can be used to alter plasmonic properties, structure, and catalytic activity. We thank the NSF for support of this project (DMR-1410569).

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

NERM April 6, 2015

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Oral

CONTROL ID: 2250543

TITLE: [Establishing regional student-faculty collaborations in green chemistry teaching, research and outreach education: Project GreenLab](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [E. J. Brush](#)¹

INSTITUTIONS (ALL): 1. Department of Chemistry, Bridgewater State University, Bridgewater, MA, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: The Project GreenLab initiative is focused on Green Chemistry teaching, research and outreach education, and is being developed and coordinated by faculty and students from Bridgewater State University (BSU). The overarching goal is to build regional professional expertise in green chemistry education, and a workforce trained and educated with the knowledge and skills to enter new career opportunities in green and sustainable chemistry. This presentation will provide an introduction to the GreenLab project, and discussion on our approach to engaging students and educators from BSU and community colleges, high schools and middle schools through: (1) community outreach education; (2) hands-on activities & programs; (3) high school professional development; (4) research applying the 12 principles of green chemistry to solve problems; and (5) participatory action research with middle school students. Funding for Project GreenLab was provided by a BSU Presidential Fellowship award, the BSU Center for the Advancement of STEM Education, and an EPA P3 Phase I grant (SU835696).

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Inorganic Chemistry - Oral

CONTROL ID: 2252753

TITLE: [Electrically Conductive 2D Metal–Organic Frameworks for Chemiresistive Sensing](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. G. Campbell](#)³, [D. Sheberla](#)³, [S. Liu](#)³, [T. M. Swager](#)¹, [M. Dinca](#)²

INSTITUTIONS (ALL): 1. MIT, Cambridge, MA, United States.

2. Building 2-321, MIT, Cambridge, MA, United States.

3. Chemistry, MIT, Cambridge, MA, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: There has been significant interest in using metal–organic frameworks (MOFs) as next-generation functional materials in electronic devices. Due to their high surface area and robust chemical tunability based on a “bottom-up” synthetic approach, MOFs have been especially targeted for use in sensors. An ongoing challenge, however, has been a lack of efficient signal transduction due in large part to the fact that the vast majority of MOFs are insulators. Here we describe the first successful use of conductive MOFs in chemiresistive sensors, enabled by a new family of 2D MOFs with high electrical conductivity. Sensors fabricated from the 2D MOF $\text{Cu}_3(\text{HITP})_2$ (HITP = 2,3,6,7,10,11-hexaiminotriphenylene) exhibit reversible, quantitative detection of ammonia vapor at sub-ppm levels. This sensitivity is competitive with values

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reported for sensors based on carbon nanotubes (CNTs), conductive organic polymers, and metal chalcogenides (*e.g.* MoS₂). Rational synthetic variation of the 2D MOF structure can be used to tune the chemiresistive response to various analytes, allowing for selective detection and/or analyte identification. Finally, data pertaining to sensing mechanism with 2D MOFs will be discussed.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Bio-based Materials and Processes - Oral - INVITED ONLY

CONTROL ID: 2254913

TITLE:

[Biom mineralization Proteins: Controlling Pre- and Post-nucleation Aspects of Mineral Formation](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [J. S. Evans](#)¹

INSTITUTIONS (ALL): 1. New York University, New York, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract:

The formation of the mollusk shell and sea urchin spines represent events in calcium carbonate crystal engineering that are controlled by proteins. One of the major steps in this engineering process is the formation of protein phases or hydrogels which control pre- and post-nucleation events in the calcium carbonate mineralization process. To explore this phenomenon further, we will present studies of nacre (aragonite) mollusk shell proteins and a sea urchin spicule matrix (calcite) protein and show that both organisms utilize similar protein hydrogel - based strategies to assemble and organize mineral nanoparticles, and in the case of the nacre proteins, introduce nanoporosities within calcium carbonate crystals. These protein-based processes not only provide insights into the formation of natural biominerals but also represent novel building strategies for creating inorganic-based materials under ambient conditions.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Advances in Colloid and Surface Chemistry - Oral - INVITED ONLY

CONTROL ID: 2254937

TITLE: [Energy and dipole dependence of electron transfer at surfaces](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [L. Gundlach](#)¹, J. Nieto-Pescador¹, B. Abraham¹

INSTITUTIONS (ALL): 1. Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Electron transfer at interfaces is a critical process in surface catalysis, novel electronic applications and solar energy conversion. The fast kinetics (below 100 fs) and the inhomogeneous environment complicate identifying the parameters that dominate the reaction. I will present ultrafast spectroscopic studies of model systems with well-defined variations in excess energy and dipole moment.

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In the first part excited state dynamics of a phlorin macrocycle attached to TiO₂ nanoparticles will be discussed. The dynamics was measured after excitation to the S₁ and the S₂ state. On the electrode, heterogeneous electron transfer (HET) times from both states were very similar and around 50 fs. Surprisingly, the large difference in the density of acceptor states that are resonant with the respective donor level of the molecule does not significantly influence HET dynamics.

In the second part I will present measurements of electron injection dynamics from a series of three Zn(II) tetraphenylporphyrins with alternating dipole moment. The influence of the dipole moment on the energy level alignment can be observed in the ultrafast injection dynamics of the chromophores bound to a metal oxide semiconductor. The three molecules show the expected dipole dependent HET dynamics in the S₂ state, while the S₁ does not show ultrafast HET.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Inorganic Chemistry - Oral

CONTROL ID: 2255304

TITLE: [Calcium arylphosphonates for bone therapy](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [V. Lopez](#)¹, M. D. Lijewski¹, V. N. Bampoh³, K. Ruhlandt-Senge²

INSTITUTIONS (ALL): 1. Chemistry, Syracuse University, Syracuse, NY, United States.

2. Department of Chemistry, Syracuse University, Syracuse, NY, United States.

3. University of Minnesota, Rochester, MN, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: The quest for bioactive and biocompatible materials for bone therapy is of growing importance, as currently used materials display significant limitations. Our work utilizes bisphosphonates, a chemical entity used in various common drugs to treat bone diseases, in conjunction with calcium to obtain biocompatible and bioactive metal organic frameworks (MOFs). These materials are expected to be mechanically strong, light-weight, and flexible. Different geometries for the resulting MOF can be tailored by using specific ligand topology. In addition, studies using aryl phosphonates have concluded that the substitution pattern has an effect on the dimensionality and pore size of the complexes. The understanding of this allows for the design of materials with a defined surface area and pattern that will ultimately allow optimal interaction with the bone tissue. This talk will discuss the effects of ligand topology on the structural properties.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Bio-based Materials and Processes - Oral - INVITED ONLY

CONTROL ID: 2255429

TITLE: [Virus Nanoreactors and the Hierarchical Assembly of Coupled Catalytic Materials](#)

NERM April 6, 2015

AUTHORS (FIRST NAME INITIAL, LAST NAME): T. Douglas¹

INSTITUTIONS (ALL): 1. Dept of Chemistry, Indiana University, Bloomington, IN, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: The virus like particle (VLP) derived from bacteriophage P22 presents a unique platform for constructing catalytically functional nanomaterials by directed encapsulation of enzymes into the interior volume of the icosahedral capsid. Enzyme encapsulation has been engineered to be genetically programmed allowing “one pot” biosynthesis and directed self-assembly of desired enzymes within the roughly 60 nm diameter P22 capsid. The resulting nano-reactors comprise multiple copies of the cargo enzymes, densely packaged within the capsid at local concentrations that mimic predicted high intracellular macromolecule concentrations. Using enzymes derived from many different organisms, we have encapsulated multi-enzyme pathways within the P22 capsid through a process of directed self-assembly. The resulting nanoreactors demonstrate the bioengineering of robust and complex coupled catalytic nanomaterials.

The system provides a platform with which to interrogate the effects of crowding on enzyme activity, the importance of catalyst adjacencies, the diffusion of intermediate species between partner catalysts in model synthetic metabolic pathways, and the effects of the capsid as a potential barrier limiting substrate access to the encapsulated enzymes. Aspects of the structure and kinetic behavior of these systems have been elucidated and a diffusion-based model for coupled cascade reactions has been developed. Using P22 nanoreactors as individual building blocks, with single or multi-enzyme systems encapsulated within them, we can extend the utility of the system towards the fabrication of long-range ordered materials that exhibit complex coupled catalytic behavior.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Organic Chemistry - Oral

CONTROL ID: 2257682

TITLE: [\[Lewis Acid\]⁺\[Co\(CO\)₄\]⁻ Catalysts for Enantio- and Regioselective Transformations of Epoxides](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): J. R. Lamb², G. W. Coates¹

INSTITUTIONS (ALL): 1. Cornell Univ, Ithaca, NY, United States.

2. Chemistry and Chemical Biology, Cornell University, Ithaca, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: This talk addresses recent advances in epoxide transformations using catalysts of the form [Lewis acid]⁺[Co(CO)₄]⁻. First, these catalysts were shown to effect enantioselective carbonylation to yield enantioenriched *trans*-β-lactones from *meso*-epoxides. Fine-tuning the electronic properties of the ligand further improved enantioselectivity while revealing an unexpected relationship between the substrate’s steric environment and the electronic nature of the optimal catalyst. Second, a known side reaction of carbonylation was investigated to selectively give methyl ketones from monosubstituted epoxides in excellent yields. This system showed good functional group tolerance under mild conditions and low catalyst loadings compared to previous methods.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Biochemistry - Poster

CONTROL ID: 2257841

TITLE: [NagD from *Yersinia pestis*, a homolog to NagD UMPase from *E. coli*](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [L. Dass](#)¹, I. Moreno¹, S. F. O'Handley¹

INSTITUTIONS (ALL): 1. Rochester Inst of Tech, Rochester, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: NagD UMPase from *E. coli* is a member of the p-nitrophenyl phosphatase family of the Haloacid Dehalogenase (HAD) superfamily. There is a NagD homolog in *Yersinia pestis* with >80% identical or similar amino acids and thus it is predicted to be an UMPase like NagD from *E. coli*. However, the only way to truly know the activity of a protein is to characterize the purified protein. We are in the process of cloning the gene. Once the gene is cloned, we will express, purify, and characterize the enzyme, and compare its specific activity, pH optimum, and metal ion requirements to those of NagD from *E. coli*. *Y. pestis* is the causative agent of "the plague", a disease of historical significance that is still prevalent today. Studying proteins from *Y. pestis* will help us to understand this pathogen better and may help us to discover potential novel antibiotic targets.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Biochemistry - Poster

CONTROL ID: 2258527

TITLE: [A phosphoglycolate phosphatase virulence factor from *Staphylococcus aureus*](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [I. Moreno](#)¹, L. Dass¹, S. A. Ramirez¹, J. Hill¹, K. Blake¹, J. Thomson¹, S. F. O'Handley¹

INSTITUTIONS (ALL): 1. Rochester Inst of Tech, Rochester, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: *Staphylococcus aureus* is a major cause of hospital-acquired infections. The multi-drug resistant nature of certain *S. aureus* strains makes the discovery of new *S. aureus* drug targets vital. A newly discovered virulence factor from *S. aureus* was described as a homolog of NagD from *E. coli*, a member of the nitrophenyl phosphatase family of the HAD (Haloacid Dehalogenase) superfamily. We cloned the gene, expressed and purified the protein, and determined its activity. This virulence factor is not an ortholog of NagD UMPase from *E. coli*, but rather a phosphoglycolate phosphatase (PGPase). If phosphoglycolate accumulates in the cell, it will inhibit the glycolytic enzyme triose phosphate isomerase (TPI). In *S. aureus*, TPI also serves as an adhesion molecule that can bind to host cells via sugar-side chains; phosphoglycolate would interfere with this adhesion process and thus make it harder for *S. aureus* to infect a new host cell. Thus, this *S. aureus* PGPase may act as a virulence factor by degrading the TPI inhibitor phosphoglycolate. We have subcloned this PGPase into a His-tag vector and purified the protein using nickel affinity and size exclusion chromatography. We are currently screening crystals for use in determining the xray crystal structure. This research was supported by an NIH AREA grant and RIT FEAD grant (SOH) and an RIT research and creativity grant (IM).

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CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Recent Advances in Food Chemistry and Nutritional Biochemistry - Oral - INVITED ONLY

CONTROL ID: 2258020

TITLE: [Pumping iron across gestation: Is all iron created equal?](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [K. O. O'Brien](#)¹

INSTITUTIONS (ALL): 1. Nutr Sci, Cornell University, Ithaca, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: At birth the human fetus contains roughly 300 mg of iron (Fe), the majority of which is accrued over the last 90 days of gestation. Fetal Fe demands can be met from existing maternal Fe stores, or from maternal dietary intake of heme Fe (from animal products) and non-heme Fe (from plant or animal products). Little attention has focused on placental utilization of heme Fe in spite of recent findings that the human placenta very richly expresses heme transport proteins. To assess placental use of heme vs. non-heme Fe, we intrinsically labeled a piglet with a stable isotope of Fe (⁵⁸Fe). During the third trimester of pregnancy, 18 women (age 16 – 32 y) were fed two test meals each containing 8 mg of Fe. One test meal was comprised of the labeled ⁵⁸Fe-pork fed as chili, and the other test dose was administered as ferrous sulfate (⁵⁷FeSO₄). Maternal blood was collected 2-weeks post-dosing and cord blood was obtained at delivery to measure enrichment of the heme or non-heme Fe. As expected, pregnant women had a significantly higher utilization of heme (⁵⁸Fe) compared to ⁵⁷Fe (non-heme Fe) (47.7 ± 14.4 vs. 40.0 ± 13.2%, p=0.04, n=18). Of interest, neonates at birth had a significantly greater percentage of maternally absorbed ⁵⁸Fe compared to ⁵⁷Fe (5.4 ± 2.4 vs. 4.0 ± 1.6%; p<0.0001) suggesting a preferential fetal use of maternally ingested Fe derived from a dietary, animal-based heme source. The net amount of ⁵⁷Fe (p=0.002) and ⁵⁸Fe (p=0.004) transferred to the fetus were both inversely correlated with maternal serum hepcidin. Maternal utilization of the non heme Fe was significantly associated with maternal Fe status as evidenced by a positive association with serum transferrin receptor concentration (p=0.003, r²=0.43). Further research on mechanisms of placental Fe uptake of dietary heme and non-heme Fe are warranted.

Advances in Food Chemistry and Nutritional Biochemistry Symposium

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Poster

CONTROL ID: 2258581

TITLE: [Parametric equations and images for a large set of hydrogen atomic orbitals](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [I. Rhile](#)¹

INSTITUTIONS (ALL): 1. Albright College, Reading, PA, United States.

PRESENTATION TYPE: Poster Preferred

ABSTRACT BODY:

Abstract: Described are new and extended sets of parametric equations that allow for the generation of images of isosurfaces and contour lines for a large set of hydrogen atomic orbitals. Three sets of parametric

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equations were used: 1) A new set of parametric equations were used for 2s, 2p, 3d, 4f, and 5g orbitals. This set uses the Lambert W function, and is the first set of parametric equations for the 4f and 5g orbital isosurfaces. 2) A new set of parametric equations were used for d_{xy} , d_{yz} , d_{xz} , and $d_{x^2-y^2}$ orbitals. 3) Extensions of literature parametric equations were used for p and d_{z^2} orbitals. These equations can be used to generate images, vector and rasterized, using many software platforms, including gnuplot and Microsoft Excel, and they can be used in advanced undergraduate orbital plotting exercises. Further use of this work includes direct integration of the $\psi^*\psi$ for the 2s and 2p orbitals with the limits of the isosurfaces and generation of physical models.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Green Chemistry - Oral - INVITED ONLY

CONTROL ID: 2258933

TITLE: [Physicochemical studies of the binary systems water – 1-alkyl-3-methylimidazolium methanesulfonates](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. M. Hoffmann](#)¹

INSTITUTIONS (ALL): 1. Department of Chemistry & Biochemistry, The College at Brockport, State University of New York, Brockport, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Ionic liquids (ILs) are salts with melting points below 100°C. They possess low vapor pressures, and especially halide-free ionic liquids have been considered as green solvents for chemical synthesis. It has been noted several times that water present in the ionic liquid solvent medium does not react with water-sensitive reagents. In collaboration with the Stark group this motivated a series of physical property measurements of binary system water – 1-ethyl-3-methylimidazolium methanesulfonate ($[C_2mim][MeSO_3]$) as a function of composition and temperature, which were interpreted within the context of structural IL organization into polar and nonpolar domains that persist to high water content.¹ This presentation will show follow-up results obtained in our lab for the related IL 1-butyl-3-methylimidazolium methanesulfonate in binary system with water.² While the concentration dependence of a number of measured physical properties is very similar to $[C_2mim][MeSO_3]$ the temperature dependence shows marked differences with respect to activation energies for a number of physical properties as well as T_1 -NMR relaxation times, which will be discussed.

Stark, A.; [Zidell, A.W.](#) Hoffmann, M.M. *J. Mol. Liq.*, **2011**, Vol. 160, 166-179.

Hoffmann, M.M.; [Sylvester, E.D.](#); [Russo, J.W.](#) *J. Mol. Liq.*, **2014**, Vol. 199, 175-183.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Environmental Chemistry - Oral

CONTROL ID: 2259218

TITLE: [Investigation of phytoremediation of volatile organic compounds in indoor environments](#)

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AUTHORS (FIRST NAME INITIAL, LAST NAME): G. Peterson¹, T. Jones², D. Rispoli², V. Niri²

INSTITUTIONS (ALL): 1. Chemistry, State University of New York at Oswego, Bridgeport, NY, United States.

2. Chemistry, State University of New York at Oswego, Oswego, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Poor indoor air quality has been connected with sick building syndrome (SBS) and reduced worker productivity and satisfaction within workplaces. Volatile organic compounds (VOCs) are important indoor contaminants released from different sources including building materials, furniture, and electronics. Newly constructed buildings are known to have high VOC concentrations due to the recent installation of many VOC-containing products that are used in building construction. A substantial proportion of VOCs are detrimental to human health with effects ranging from dizziness and nausea to central nervous system damage, various forms of cancer, and even death. Because of the serious nature of VOCs as a health hazard, many remediation techniques are being developed. Phytoremediation is an emerging technology that uses plants to clean up indoor air through degradation, extraction, or immobilization of contaminants.

Using solid phase microextraction (SPME) coupled with gas chromatography-mass spectrometry (GC/MS), this project aimed to monitor the removal of airborne volatile organic compounds (VOC's) by common indoor plants. Five plants were selected for study based on previous phytoremediation research and alternative gas uptake mechanisms. The plants selected included three CAM plants; *Guzmania lingulata*, *Cassula argentea*, *Consolea facata*, and two C3 plants; *Chlorophytum comosum* and *Dracaena fragrans*. Three treatment conditions were applied to each plant to isolate active VOC uptake mechanisms; covering the base of the plant in foil, no foil, and the use of a light. Of the five plants; *Guzmania lingulata* showed the greatest overall VOC uptake in Light treatment conditions with more than 80% removal of six of the eight target VOC compounds over a twelve-hour sampling period. All tested plants showed less than 50% removal of dichloromethane or trichloromethane over the twelve-hour sampling period.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials Chemistry - Poster

CONTROL ID: 2259385

TITLE: [Synthesis and electrospinning of block copolymers](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): E. Gonzalez¹, L. Buttaro¹, M. Frey¹

INSTITUTIONS (ALL): 1. Fiber Science, Cornell University, Ithaca, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Electrospun polymeric nanofibers are attractive candidates for their use as biosensors due to their small pore size, high porosity and large surface area to volume ratio. When using nanofibers to construct biosensors, fibers with hydrophilic surfaces that are also non-water soluble are desirable. In this work, poly(lactic acid)-*block*-poly(ethylene glycol) block copolymers are synthesized and electrospun together with poly(lactic acid) homopolymer. Phase separation of the block copolymers during electrospinning process leads to the formation of biocompatible, biodegradable, hydrophilic yet non-water soluble fibers suitable for stable and efficient bioanalysis. Nanofibers are characterized by Scanning Electron Microscopy (SEM), Differential Scanning Calorimetry (DSC) and wettability test. Preliminary results on the synthesis of biotin end-functionalized poly(lactic acid)-*block*-poly(ethylene glycol) block copolymers are also present with the final goal to obtain biotin surface functionalized nanofibers.

CONTACT (COUNTRY ONLY): United States

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DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Physical Chemistry - Oral

CONTROL ID: 2260780

TITLE: [Photoswitchable spiropyran: Computational study of its photochromic reaction](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. D. Mayes](#)¹

INSTITUTIONS (ALL): 1. Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth, North Dartmouth, MA, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Photoswitchable materials, such as spiropyrans, have been vigorously studied for construction of novel dynamic materials. Spiropyrans are photochromic molecules which can be switched reversibly between colorless spiropyran (closed form) to colorful merocyanine (open form) by light of appropriate radiation. These structural isomers have completely different physical and chemical properties. The light induced changes have been harnessed for applications in discovering innovative materials in optical switching, sunglasses, optical data storage, optical nanoparticles, photonic crystal, and sensors. We study the photoresponsive nitro-substituted spiropyran and different conformations of merocyanine using a variety of electronic structure methods. The solvent effects on these systems are also studied.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Progressive Methodology for Organic Synthesis - Oral - INVITED ONLY

CONTROL ID: 2260926

TITLE: [The use of amphoteric reagents in drug discovery: from small molecules to peptide macrocycles](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. K. Yudin](#)¹

INSTITUTIONS (ALL): 1. Dept of Chem Univ of Toronto, Toronto, ON, Canada.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Contemporary approaches to drug discovery emphasize the need to access diverse and underexplored chemistry space. In this regard, peptides represent a particularly relevant therapeutic modality that has received renewed interest over the past several years. Macrocyclic topology allows one to minimize polar surface area of peptides by increasing the propensity to form intramolecular hydrogen bonds while shielding amide bonds from solvation. In this area, we have developed several enabling methods based on amphoteric aziridine aldehydes and alpha-boryl aldehydes. These methods allow us to synthesize peptide macrocycles and evaluate them as therapeutic candidates. In this talk, I will present the progress we have made in the area of inflammatory bowel disease, where our lead molecule recently showed positive efficacy data in a 12-day colitis study.

Another area of our research aimed at bioactive compounds pursues a “bottom-up” approach to underexplored molecules. Here, we start with a simple building block that can be readily elaborated into a relatively small drug-like molecule. To be relevant in drug discovery, this strategy relies on heteroaromatics,

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a well-established modality that is known to deliver drug candidates. Due to their favourable pharmacokinetic properties, small heterocycles belong to a rather overcrowded patent space with little possibility to maneuver. To address this challenge, we have pursued synthetic tools to rapidly build novel chemotypes. Our approaches have their origin in readily accessible amphoteric building blocks, employ simple starting materials, and deliver privileged structural endpoints while simultaneously facilitating access to hitherto unexplored chemotypes. Our long-term goal in this area is to develop heterocyclic inhibitors of protein domains that are known to recognize methylated lysine residues. I will discuss our recent structural biology findings that hinge on the novel heterocycles created in our lab. It is our expectation that amphoteric molecule-driven strategies will be heavily used in fragment screening and lead development campaigns.

CONTACT (COUNTRY ONLY): Canada

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Biochemistry - Oral

CONTROL ID: 2261861

TITLE: [Biomimetic Catalytic Complexes Organized by DNA Nanoscaffolds](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): J. Fu¹

INSTITUTIONS (ALL): 1. Chemistry Department, Science Building 306A, Rutgers University-Camden, Camden, NJ, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Living systems have evolved complex macromolecular nanostructure networks to mediate a range of cellular activities with high efficiency and specificity, including metabolic pathways, signaling transduction, gene expression and regulation. Many of these macromolecular systems are spatially organized with precisely controlled position and orientation of biomolecule components. If these systems can be mimicked and constructed artificially, they could be applied to the realization of smart nanobioreactors and devices that have utility in the production of high-value chemicals, the conversion of a variety of energy forms, and the development of new bio-diagnostics. Recently, DNA has emerged as promising molecular scaffolds to organize macromolecule structures on the nanoscale with controlled geometries and nanomechanical capabilities. In **Fig.1A**, GOx and HRP are organized with inter-enzyme distances ranging from 10 to 65 nm, confirmed by AFM imaging. The measured reaction rates decreased nonlinearly as the inter-enzyme distance increased. The result directly demonstrates the ability of DNA nanostructures to arrange multiple proteins with control over their number, relative distance, and spatial pattern, mediating the intermediate transport and activities. In **Fig.5B**, a tweezer-like DNA nanodevice is used to regulate the activity of an enzyme/cofactor pair. G6PDH and NAD cofactor were attached to different arms of the DNA tweezers. The actuation of enzymatic function was achieved by switching the tweezers between opened and closed states. **Fig.5C** shows the assembly of multienzyme complexes on DNA nanoscaffolds capable of substrate channeling with an artificial NAD swinging arm. The activity of the G6pDH-MDH complex was enhanced more than 90-fold with channeled NAD swinging arms. Further adjusting the relative ratios of enzymes can yield an additional ~ 2 – 3-fold increase in activity.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Biochemistry - Poster

CONTROL ID: 2262624

TITLE: [Biochemical investigation of the determinants of NicC binding affinity](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): J. Kraai¹, C. Christie¹, K. Hicks²

INSTITUTIONS (ALL): 1. SUNY Cortland, Marcellus, NY, United States.

2. Chemistry, SUNY Cortland, Cortland, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: This work involves examining 6-hydroxynicotinate 3-monooxygenase (NicC), an enzyme present in strains of the bacteria *Pseudomonas putida*. NicC catalyzes a decarboxylative hydroxylation reaction in which 6-hydroxynicotinic acid (the natural substrate) is converted to 2,5-dihydroxypyridine (product). Our ultimate goal of this project is to broaden the substrate specificity of NicC such that it can readily bind to polycyclic aromatic hydrocarbons (PAHs), a class of environmental pollutants that are commonly produced during industrial processes, and catalyze the turnover of monocyclic aromatic hydrocarbons. Toward this goal, our work involved measuring the binding affinity of NicC for various substrates that have different functional groups at the 6-position of the substrate in order to determine the physical parameters underlying substrate specificity. Specifically, we studied the binding affinities of the substrate analogs, 6-methylnicotinic acid and benzoic acid, for NicC using a fluorescence resonance energy transfer (FRET)-based affinity assay. Experimental results suggest that 6-methylnicotinic acid has a K_d value of approximately 7.5 ± 0.1 μ M, similar to the natural substrate which has a K_d of 11.2 ± 1.5 μ M. Thus, our studies indicate that the presence of a methyl group at the 6-position of the substrate has minimal effects on binding affinity. Initial studies with benzoic acid suggest this analog has 6-fold lower binding affinity for NicC than the natural substrate. Together, these data suggest that NicC substrate specificity is relatively narrow. Further experiments will involve measuring catalytic turnover with these analogs in order to determine if NicC substrate specificity is determined by reactivity or binding affinity.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: resubmitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials for Energy - Oral

CONTROL ID: 2263116

TITLE: [Aligned Multiwalled Carbon Nanotubes based Polymer Nanocomposites via in-Situ Polymerization](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): N. C. Das¹, S. Ganguly²

INSTITUTIONS (ALL): 1. Rubber Technology Centre, Indian Institute of Technology, Kharagpur, WB, India.

2. Rubber Technology Centre, Indian Institute of Technology, Kharagpur, India.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Vertically aligned carbon nanotubes (VACNTs) have highly anisotropic properties comparing to random CNT powders like mechanical and electrical properties. Many applications require that VACNTs be mechanically stabilized by incorporating them into polymer matrix. Commonly used methods for preparation of CNT/polymer composites are solution process and in situ polymerization, in which monomers instead of polymers are used as starting materials. Here, we have synthesized CNT/polymer composites via situ polymerization of polystyrene (PS) with VACNTs. We have investigated morphology VACNTs and VACNTs/PS composites using small angle neutron scattering (SANS) and scanning electron microscopy. The morphology shows rather curved tubes near the substrate both neat VACNTs and composites. The alignment

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order increases with the distance from the substrate as illustrated in Fig. A. Quantitative alignment order is performed using SANS. 2D SANS pattern on both neat and composite VACNT arrays are shown in Fig 1b. Apparently MWNTs remain aligned in composites upon polymerization. We also used TEM, AFM and GPC to characterize VACNTs/PS composites in details. TEM (Fig. B) shows that MWNTs are well-dispersed in the polymer matrix and structural integrity of MWNTs remain intact as indicated by the neat hollow tube structures.

In summary, The order of the tube alignment is enhanced upon polymerization with the lateral confinement. The cause of enhanced alignment is possibly related to the accelerated polymerization among VACNT arrays.

REFERENCES

1. Wei, Chen.; Dai, L.M.; Roy, A.; Tolle, T. B. *J. Am. Chem. Soc.* **2006**, *128*, 1412-1413.
2. Qu, L. T.; Dai, L. M. *Chem. Commun.* **2007**, 3859-3861.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Poster

CONTROL ID: 2263553

TITLE: [A classroom-based activity designed to enhance student comprehension of enzyme catalysis of reaction rate.](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. U. Gehret](#)¹

INSTITUTIONS (ALL): 1. Science & Mathematics, National Technical Institute for the Deaf, Rochester Institute of Technology, Rochester, NY, United States.

PRESENTATION TYPE: Poster Preferred

ABSTRACT BODY:

Abstract: The concept of enzyme-catalyzed reaction rate requires a foundational understanding of reaction rate prior to an explanation of enzyme influence on those rates. It is predicted that the interchangeable use of these terms diminishes student understanding of these concepts. A classroom activity has been devised that allows students to visualize a reaction in both an un-catalyzed and enzyme-catalyzed setting. Students' hands play the role of an enzyme by catalyzing the conversion of two pop beads linked together (substrate) into two individual pop beads (products) in the catalyzed setting. Students record the number of products they make over short periods of time, calculate the reaction rate at each interval and plot their progress on a graph. By comparing their progress to the same reaction occurring without the aid of a student's hands (un-catalyzed setting), it is the intention that this role-playing exercise will allow students to better comprehend enzyme catalysis and its influence on reaction rate. Furthermore, this kinesthetic approach allows to students to experience first-hand the effect substrate depletion has on enzyme-catalyzed reaction rate. Students should thus take away an appreciation for why the initial reaction rate of an enzyme is the best measure of its influence. Students are also asked to extrapolate on their experience to predict how temperature would influence their enzyme-catalyzed reaction rates. Survey results will reveal the effectiveness of this classroom activity towards improving student understanding of these fundamental concepts.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

NERM April 6, 2015

ABSTRACT SYMPOSIUM NAME: Environmental Chemistry - Oral

CONTROL ID: 2263912

TITLE: [The Unexpected Reactivity of Marine Cl](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. C. Leri](#)¹

INSTITUTIONS (ALL): 1. Natural Sciences, Marymount Manhattan College, New York, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Chlorine has the highest electron affinity of any element. In nature, Cl exists mainly as the chloride anion, which was long considered to be unreactive under environmental conditions. In terrestrial soils, that assumption has proved unfounded, largely due to the revelation of various chlorinating enzymes in soil microbes. In seawater, however, there has been little evidence to change the enduring perception of the unreactivity of chloride. Halogenating enzymes in marine organisms are primarily bromoperoxidases that take advantage of abundant bromide with lower electron affinity. Known modes of natural marine chlorination produce volatile species such as methyl chloride, which is emitted by marine algae and likely forms through the action of methyl transferases.

We have found high concentrations of organochlorine in naturally degraded particulate organic matter from oceanic sediment traps, with heterogeneously distributed aliphatic and aromatic fractions illuminated via X-ray spectromicroscopy. The major precursor of sediment trap material is phytoplankton biomass, the detritus of which undergoes oxidative breakdown as part of the marine carbon cycle. We hypothesized that unsaturated lipid and protein moieties in phytoplankton detritus would be susceptible to chlorination through oxidative degradation. Using a series of model experiments and a novel X-ray spectroscopic technique, we have shown that algal particulates are readily chlorinated through various abiotic pathways, including photochemical and Fenton-like reactions. These processes produce organochlorine in particulate algal detritus at levels exceeding 0.1% by mass. We have also measured non-volatile natural organochlorine in several species of marine phytoplankton for the first time.

This discovery of abiotic pathways for large-scale chlorination of marine organic matter provides the first suggestion of a marine chlorine cycle involving chemical transformations of chloride. Chlorinated organic matter may represent a particularly stable component of marine organic carbon, with possible implications for preservation in sediments.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Biochemistry - Poster

CONTROL ID: 2265130

TITLE: [Phenotypic and Complementation studies of PHO13 activity in *Saccharomyces Cerevisiae*](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [C. Kellogg](#)¹, [K. Blake](#)¹, [S. F. O'Handley](#)¹, [A. U. Gehret](#)²

INSTITUTIONS (ALL): 1. School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY, United States.

2. Science & Mathematics, National Technical Institute for the Deaf, Rochester Institute of Technology, Rochester, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

NERM April 6, 2015

Abstract: *PHO13* in *Saccharomyces Cerevisiae* (bakers yeast) is a para-nitrophenylphosphatase (pNPPase) within the haloacid dehalogenase (HAD) superfamily. The natural substrate for *PHO13* is currently debated but the enzyme has been identified in our lab to possess specific activity to 2-phosphoglycolate, making it a phosphoglycolate phosphatase (PGPase). In photosynthetic organisms, 2-phosphoglycolate is generated by the oxygenation reaction of RuBisCO in the Calvin Cycle. To be recycled back into the general metabolism, a photosynthetic PGPase must convert 2-phosphoglycolate to glycolate. In non-photosynthetic yeast, 2-phosphoglycolate must be generated by some other mechanism, possibly by oxidative damage to DNA. Regardless of its origin, 2-phosphoglycolate must be catabolized due to its ability to inhibit triose phosphate isomerase (*TPI*). Yeast cells lacking functional Pho13p (*pho13D*) are being investigated for growth phenotypes that support *TPI* inhibition by elevated 2-phosphoglycolate. These include the ability of the mutant strain to grow in the presence of hyperosmotic media (1M NaCl) or in the absence of exogenous inositol.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: News from Carbon World - Oral - INVITED ONLY

CONTROL ID: 2266445

TITLE: [Electronic transport properties of selected \$\pi\$ -bowls with different size, curvature and solid state packing](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [E. Margine](#)¹

INSTITUTIONS (ALL): 1. Department of Physics, Binghamton University, Vestal, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: First-principles calculations combined with the Boltzmann transport theory are used to investigate the electronic transport properties of four members of the extended family of indenocorannulene molecular crystals. The results for the electrical conductivity suggest that all corannulene derivatives should exhibit transport characteristics significantly improved compared to the parent corannulene. The findings point to a large sensitivity of the charge-carrier conductivity to the size as well as stacking direction of the π -bowls and indicate that this class of corannulene derivatives can provide new structural motifs that can be further tuned to achieve high-performance materials for organic electronic devices.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Physical Chemistry - Oral

CONTROL ID: 2266651

TITLE: [Ionic Liquids as Solvents and Electrolytic Co-Solvent Additives for Proton Transfer and Protein Studies](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): L. Yu², [T. D. Vaden](#)¹

INSTITUTIONS (ALL): 1. Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.
2. Chemistry and Biochemistry, Rowan University, Glassboro, NJ, United States.

PRESENTATION TYPE: Oral Only

NERM April 6, 2015

ABSTRACT BODY:

Abstract: Ionic liquids (ILs) are room-temperature molten organic salts that have broad applications in chemistry and biochemistry. ILs can function as solvents and co-solvent additives for numerous solutions. Acidic ionic liquid (AIL) solutions can be prepared by dissolving Bronsted acids in ILs to create solutions with high proton conductivity for fuel cell and other electrochemical applications. Water soluble ILs can be used as additives in aqueous solution for biochemical and biomedical applications such as biomass preparation, enzyme modulation, and antibiotic enhancement. In both cases (electrochemical and biochemical), there are open questions regarding the nature of the solute-IL interactions. Acid-IL interactions in AIL solutions will be discussed using Raman and IR spectroscopy combined with DFT calculations to characterize the solvation structures of protons and acids solvated by IL molecular ions. Biomolecule-IL interactions in aqueous solution will be discussed using protein folding experiments combined by ESI-MS and hydrogen-deuterium exchange (HDX) measurements to identify protein.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Biochemistry - Oral

CONTROL ID: 2266660

TITLE: [Spore display as a tool for Protein Engineering and Optimization](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): H. Jia¹, E. T. Farinas¹

INSTITUTIONS (ALL): 1. Dept of Chemistry Environmental Sci, NJIT, Newark, NJ, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Protein libraries were displayed in the spore coat of *Bacillus subtilis*, and this method was demonstrated as a tool for directed evolution under extreme conditions. *Escherichia coli*, yeast, and phage display suffer from protein folding and viability issues. On the other hand, spores avoid folding concerns by the natural sporulation process, and they remain viable under harsh chemical and physical environments. Previously, we demonstrated that spore display can be used to improve substrate specificity. Now we take advantage of the inert properties of the spores and evolve CotA under conditions of high organic solvent concentrations. *E. coli* or yeast display methods are not suitable in these conditions: cell lysis would occur and the genotype/phenotype connection would be lost. CotA is a laccase, which is copper-containing oxidase enzyme. A random library of CotA was expressed on the spore coat and approximately 3000 clones were screened at 60% dimethyl sulfoxide (DMSO). A Thr480Ala variant (Thr480Ala-CotA) was identified that was 2.38 folds more active than the wild-type CotA. In addition, the Thr480Ala-CotA was more active with varying concentration of DMSO ranging from 0-70%. The mutant was also found to be more active compare to wild-type CotA in different concentrations methanol, ethanol and acetonitrile with either 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulphonic acid)(ABTS) or syringaldazine (SGZ) as substrate. Recent results will also be presented for increasing the half-life in acidic pH.

CONTACT (COUNTRY ONLY):

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Materials Chemistry - Poster

CONTROL ID: 2267076

NERM April 6, 2015

TITLE: [Synthesis of Ordered Nickel–Molybdenum Compounds for Hydrogen Evolution](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [P. Csernica](#)³, J. R. McKone³, H. D. Abruna¹, F. J. DiSalvo²

INSTITUTIONS (ALL): 1. Cornell Univ, Ithaca, NY, United States.

2. Cornell University, Ithaca, NY, United States.

3. Chemistry and Chemical Biology, Cornell University, Ithaca, NY, United States.

PRESENTATION TYPE: Poster Preferred

ABSTRACT BODY:

Abstract: Electrolysis of water is an attractive method for producing clean hydrogen for storing and transporting renewable energy. Although hydrogen production by this method is most effective using precious metal catalysts, non-noble metals are attractive alternatives because of their reduced cost. Among the many bimetallic materials that have been investigated as catalysts for the hydrogen evolution reaction (HER), nickel–molybdenum (Ni–Mo) compounds have been shown to be particularly active. Importantly, their high activity suggests synergy between the two metals, as the bimetallic compounds are substantially more active than either of their constituents.

Previous studies of Ni–Mo HER catalysts have focused primarily on disordered alloys, which can only incorporate up to 25 at. % molybdenum into the polycrystalline structure. Here, an established method for producing the alloy was modified to create ordered Ni–Mo compounds that, unlike the disordered alloys, can incorporate up to 50 at. % molybdenum. Both the ordering and the incorporation of more molybdenum suggest that these compounds may have superior HER catalytic properties relative to their disordered counterparts. Additionally, the synthetic conditions can be slightly modified to produce Ni–Mo nitrides and carbides, which may also be active for the HER.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Biochemistry - Poster

CONTROL ID: 2268535

TITLE: [Substrate Specificity of NicC: Determination of Dissociation Constants for Substrate Analogs](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [S. Lothridge](#)¹, G. Simone¹, K. Hicks¹

INSTITUTIONS (ALL): 1. Chemistry, SUNY Cortland, Lisle, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Our research goal was to determine dissociation constants (K_d) for substrate analogs of 6-hydroxynicotinate-3-monooxygenase (NicC). NicC catalyzes the oxidative decarboxylation of 6-hydroxynicotinic acid (6-HNA) to 2,5-dihydropyridine in an aerobic nicotinate degradation pathway. NicC is present in the gram negative bacteria *Pseudomonas putida*, which are antibiotic resistant bacteria that are able to survive in harsh environmental and cellular conditions. To determine the substrate specificity of NicC, the binding of the natural substrate, 6-HNA, and a series of substrate analogs, including 6-chloronicotinic acid and 2-hydroxy-1-naphthoic acid, were measured using fluorescence resonance energy transfer (FRET) based binding assays. Our data indicate that 6-chloronicotinic acid has a similar dissociation constant as the natural substrate. However, the bicyclic analog 2-hydroxy-1-naphthoic acid binds NicC ~10 fold weaker than the monocyclic substrates. These data provide strong preliminary data into the substrate specificity of NicC. Specifically, our data demonstrate that the identity of the substituent on carbon-6 has minimal effect on binding affinity suggesting that substrate specificity might be based on reactivity, rather than affinity.

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CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: resubmitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials Chemistry - Poster

CONTROL ID: 2268709

TITLE: [Autocatalytic self-polymerization of biorenewable monomers](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): B. J. Tiegs¹, G. W. Coates¹

INSTITUTIONS (ALL): 1. Cornell Univ, Ithaca, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Progress toward sustainable materials has encouraged the development polymers based on bio-derived substrates as well as energy-efficient, benign polymerization methods. We report a new polymerization method utilizing the inherent reactivity of functional groups built into self-polymerizable monomers. These monomers are derived from renewable resources and are prepared by ring-expansive carbonylation. Self-polymerization of these monomers is autocatalytic; rapidly produces high molecular weight polymer; and requires no catalyst, solvent, or strict stoichiometric control. The resulting polymers are degradable and also functional due to pendant groups formed during the polymerization. The synthesis, polymerization, characterization, and mechanistic study of a range of substrates will be presented.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Biochemistry - Poster

CONTROL ID: 2268900

TITLE: [Binding Affinity Characterization of NicC for its native Substrate and Nicotinic Acid Substrate Analog](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): W. Zhen¹, K. Hicks¹

INSTITUTIONS (ALL): 1. Chemistry, SUNY Cortland, Cortland, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Recently, a pathway for nicotinic acid (NA) degradation was determined in *Pseudomonas putida* KT2440. One of the enzymes in this pathway, NicC, catalyzes the conversion of 6-hydroxynicotinic acid (6-HNA) to 2,5-dihydroxypyridine (DHP). Here we describe the biochemical characterization of this enzyme. Specifically, we have measured the binding affinity of NicC for its substrate, 6-HNA, and a substrate analog, NA. Binding affinities were measured using a fluorescence resonance energy transfer (FRET) based assay. The resulting dissociation constants indicate that 6-HNA binds ~30-fold more tightly to the enzyme than NA indicating that a substituent at the 3-position of the substrate is necessary for efficient binding. Future work will involve measuring kinetic constants with these compounds with the goal of determining a catalytic mechanism for the NicC-catalyzed reaction.

CONTACT (COUNTRY ONLY):

DECISION STATUS:

NERM April 6, 2015

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Oral

CONTROL ID: 2269651

TITLE: [A generalized approach to guided inquiry and discovery based experiments in General Chemistry](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. K. Sharma](#)¹

INSTITUTIONS (ALL): 1. Chemistry & Physics, Wagner College, Staten Island, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: We present a guided inquiry, and discovery oriented approach to conduct experiments in the General Chemistry laboratory. This approach can be used to transform existing experiments in the curriculum to discovery experiments. In this approach, students are provided with a set of guiding questions, leading them to design, and implement an experimental investigation in response to a scientific question. This mirrors the process of scientific experimental design and research. The role of the instructor in this paradigm is to engage in discussions and enable students to design and implement the experiment. A solubility product determination experiment is typically carried out in the second semester General Chemistry curriculum. We present transformation of this experiment into a discovery and guided-inquiry experiment. Students discover the common ion effect from the experimental data and calculations. The empirical discovery of this phenomenon provides a crucial teachable moment. This approach can be generalized to create a template for construction of guided inquiry experiments. A work sheet with guiding questions is provided as a supporting document for easy integration into an existing curriculum. Our experience of implementing this approach, and lessons learned at a small liberal arts College will be shared. Since this approach can be used to convert existing experiments into discovery oriented experiments, there is no significant burden to the laboratory budget.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Oral

CONTROL ID: 2270019

TITLE: [From your crystal to structure in ten minutes: Contemporary instruments transform undergraduate laboratory](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. Y. Nazarenko](#)¹

INSTITUTIONS (ALL): 1. Buffalo State Coll, Buffalo, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: No, it is not an exaggeration: it can take as little as ten minutes from the time you pick up a crystal from the microscope slide till you see on your display a correct molecular structure with all atoms appropriately positioned. Contemporary in-house X-ray diffractometer enables to collect enough data in 2-4 minutes time for reliable molecular structure with 0.9 -1 Å resolution. Very user-friendly and simple GUI of modern crystallographic software makes it possible to process all raw data in 1-2 minutes and solve and refine the structure in one more minute with very little user involvement (and yes, you need a professional

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for this involvement). With this approach, X-ray diffractometer becomes one of many tools in a chemical laboratory, in many aspects much simpler for an unexperienced (but strictly supervised!) user than NMR or even UV-vis spectroscopy. This methodology opens the doors for an attractive possibility: to show the beginners where the chemical structures are coming from - from the experimental data! A great number of chemicals in your lab (or in your grocery store) contain crystals directly suitable for such experiment: glucose hydrate (Sweet'n Low), sucralose, taurine (from energy drinks), saccharine, potassium hydrogen phthalate (KHP), to name the very few.

In advanced classes, crystallographic data can be naturally combined with results coming from spectroscopic techniques such as Raman, IR, NMR, XRF, and mass-spectroscopy. Thermogravimetric analysis and Karl Fischer titration are also available for solvent assay.

Several real-world examples will demonstrate application of our approach to General Chemistry, Forensic Chemistry and Art Conservation undergraduate and graduate programs at SUNY Buffalo State. Financial support for this project from SUNY IITG-2012 and IITG-2013 is gratefully appreciated. Our special thanks to Dr. Bruce Noll and Dr. Milan Gembicky (Bruker AXS Inc.) for their continuous support of our activities in crystallography education.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Advances in Organometallic Chemistry and Catalysis - Oral - INVITED ONLY

CONTROL ID: 2270628

TITLE: [Organometallic and coordination chemistry of new pyridine/thione and pyridine/selone mixed-donor ligands](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [D. Rabinovich](#)¹

INSTITUTIONS (ALL): 1. UNC Charlotte Chemistry, Charlotte, NC, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: We have been developing new bidentate ligands containing both pyridine and N-heterocyclic thione (NHT) or selone (NHSe) donor groups with the goal of preparing synthetic analogues of methanobactin (mb), a fascinating small protein that plays a key role in the acquisition and transport of copper ions in methane-oxidizing bacteria. This presentation will outline recent advances in the design and application of several new mixed-donor ligands to the synthesis of mononuclear and dinuclear copper(I) complexes that mimic the metal center in mb. In addition, the coordination chemistry of these new soft ligands towards other transition and main group metals, including molybdenum(0), manganese(I), rhenium(I), silver(I), zinc(II), cadmium(II), mercury(II), indium(III), tin(IV), antimony(III) and bismuth(III), will be described.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Intersections of Chemistry and Art - Oral - INVITED ONLY

CONTROL ID: 2270645

NERM April 6, 2015

TITLE: [The world of chemistry on postage stamps](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [D. Rabinovich](#)¹

INSTITUTIONS (ALL): 1. UNC Charlotte Chemistry, Charlotte, NC, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Postage stamps constitute a simple yet effective communication medium, often used by governments or postal authorities to inform or engage the general public on a variety of subjects. They are also unusual but appealing visual aids that can be used in the classroom to teach chemistry or in publications to illustrate interesting aspects of a specific topic. Although postage stamps featuring historical figures, flora and fauna, sports, and the arts are fairly common, a surprisingly large number of stamps have also been issued to commemorate scientific discoveries or to honor well-known scientists. This presentation will showcase a series of postage stamps pertaining to the history of chemistry, the discovery and sources of the elements, chemical structures, laboratory equipment, biochemistry, and various aspects of the chemical industry.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Environmental Chemistry - Oral - INVITED ONLY

CONTROL ID: 2270686

TITLE: [Evaluation of drinking water treatment combined filter backwash water\(CFBW\) recycling technology based on Comet and Micronucleus assay](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [T. Chen](#)¹

INSTITUTIONS (ALL): 1. Harbin institute of technology, Harbin, China.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Based on recycling CFBW directly to drink water treatment plant (WTP) is considered as a feasible method in enhancement of pollutants removal efficiency, it motives us to evaluate the genotoxicity of water samples employing two pilot-scale drink water treatment systems, one with recycling combined backwash water, the other one with conventional process. An integrated approach of the comet and micronucleus (MN) assay were used with zebrafish (*Danio rerio*) to investigate the water genotoxicity in this study. The measured parameters, such as TOC, DOC, and trihalomethane formation potential (THMFPs), of recycling process were lower than that of conventional process. All the results showed that there was no statistically significant difference ($p > 0.05$) between conventional and recycling process, and indicated that the genotoxicity of water sample from recycling process was not accumulated in the 15 days continuous recycle trial. It was worth nothing that there was relationship between the concentration of TOC, DOC, UV_{254} , THMFPs in water and DNA damage score, corresponding to the R^2 were 0.68, 0.63, 0.28, 0.64. Nevertheless, both of the DNA strand breaks and MN frequency of all water samples after disinfection were higher than that of water samples from the former treatment units, meant that the disinfection by-products (DBPs) formed by disinfection could increase the DNA damage. Both of the comet and MN tests suggest that recycling process did not increase the genotoxicity risk, contrasting to traditional process.

CONTACT (COUNTRY ONLY): China

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Poster

CONTROL ID: 2271609

TITLE: [Exploring case study pedagogy in a community college classroom: An application of Boyle's Law](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [G. Perkins](#)^{1,2}

INSTITUTIONS (ALL): 1. Science/Chemical Education, Arizona State University, Tempe, AZ, United States.

2. Chemistry, Maricopa Community College, Phoenix, AZ, United States.

PRESENTATION TYPE: Poster Preferred

ABSTRACT BODY:

Abstract: Case study serves as an interdisciplinary pedagogy tool. It enables to integrate relevance, student involvement, basic scientific concepts (Gas Laws) and science skills such as speculation. The proposed submission for a poster is an effort to examine case study pedagogy in a community college classroom. A sample of 13 students participated on a discussion board pertaining to Gas Laws. Student pairs were given a scenario in which they were asked to imagine that on a snorkeling trip, they observed the diving behavior of gannets. When the gannets swam upwards, student pairs were asked to apply Boyle's Law and craft a hypothesis on what was enabling gannets to hunt for food underwater more effectively. A qualitative analysis of the discussion board responses revealed active participation in the learning process (all posted to discussion board prior to due date), ability to apply Boyle's law to a real-life situation; and ability to speculate (a critical science process skill) in comparing gannet's diving behavior to that of a fictional creature, the Nessie. Screen shots of sample discussions will be provided on the poster. A future plan is to explore the feasibility of this pedagogy in a laboratory setting. A sample response, "This is interesting. If the gannet had not already captured and consumed its prey as it dived in to the water, the buoyancy of their air sacs would help them accelerate to a prey as the bird ascends to the surface. By diving, the pressure acts like a slingshot for the birds, in conjunction with their air sacs.

First off, Nessie is not real. There has been no hard, verifiable and plausible evidence of its existence and therefore no true scientific assessment of its underwater behaviors and capabilities. Everything about the legend is speculation driven by a romanticism of a "noble" and mysterious creature that somehow has eluded modern technology.

But lets say Nessie exists, what is to say that it is a mammal that needs to surface for air like whales? Whales use the air they breath in for buoyancy and balance the pressure when they have to dive deep and this also helps them surface quickly. If Nessie exists in that fashion, it wouldn't still be a legend. But if Nessie instead has gills, why would it ever surface in the first place? If it had gills, their underwater behavior would be vastly different from a gannet diving into the ocean for a brief time to eat. Nessie's behavior would be similar to maybe a shark."

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Green Chemistry - Oral - INVITED ONLY

CONTROL ID: 2274207

TITLE: [Green Chemistry In Practice at Sigma-Aldrich](#)

NERM April 6, 2015

AUTHORS (FIRST NAME INITIAL, LAST NAME): J. Whitford¹

INSTITUTIONS (ALL): 1. Sigma-Aldrich, Saint Louis, MO, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Sigma-Aldrich has a strong tradition of sound environmental (green chemistry), social and fiscal responsibility performance. Sigma-Aldrich is committed to sustainable growth, which is good for the environment, people and customers. Over the past five years, Sigma-Aldrich has focused on broadening its product portfolio to help its customers reduce chemical related impact on human health and eliminate/minimize contamination of the environment through its dedicated, sustainable prevention program. Sigma-Aldrich's scientists are also involved in this process by continuously searching for greener alternatives, and environmentally friendly reaction media to enable a more environmentally efficient manufacturing process. During this presentation, we will demonstrate the practical application of the 12 principles and how Sigma-Aldrich is translating them into tangible tools for the scientific community through real examples of our greener re-engineered processes/products.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Biochemistry - Poster

CONTROL ID: 2274559

TITLE: [A FRET-based Assay to Screen for Antagonists of Hedgehog Cholesterololysis](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): T. Owen¹, G. Ngoje¹, B. P. Callahan¹

INSTITUTIONS (ALL): 1. Chemistry, Binghamton University, Binghamton, NY, United States.

PRESENTATION TYPE: Poster Preferred

ABSTRACT BODY:

Abstract: Hedgehog proteins (Hh) constitute a family of secreted signaling ligands responsible for proper development of human embryos while also being linked to the progression of several types of cancer in adults. Here we focus on the autocatalytic cleavage and modification of Hh by cholesterol, called cholesterololysis. This transformation which is essential for Hh function and occurs before secretion remains relatively unexplored mechanistically due to the lack of an effective assay. By modifying an existing FRET-based assay for studying self-cleaving inteins, we have developed a robust activity assay to continuously monitor Hh cholesterololysis in multi-well plates. Using this assay, a library of 240 protease inhibitors was screened for cholesterololysis antagonists. The screen yielded a covalent inhibitor (compound ID, ST044643) of Hh cholesterololysis with an apparent IC₅₀ of 5X10⁻⁶ M. Based on a binding assay with point mutants of Hh, ST044643 appears to modify an essential cysteine residue of the Hh, possibly by a S_NAr mechanism. We plan to use ST044643 as a positive control in screens against larger more diverse libraries of small molecules. In conclusion, we have developed and applied an optical assay with the potential to identify a novel class of Hh inhibitors and that might serve to regulate aberrant Hh activity.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Oral

NERM April 6, 2015

CONTROL ID: 2274747

TITLE: [Meeting General Education Competencies in the Chemistry Lab with Lab-Simulation Technology](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [K. A. Baessler](#)¹

INSTITUTIONS (ALL): 1. Chemistry, Suffolk County Community College, Brentwood, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Computer-based technology and education are deeply intertwined. Lab-simulation technology is currently being used to meet general education competencies such as:

- >Information Technology Competency
- >Scientific Reasoning
- >Critical Thinking Skills
- >Problem solving

This workshop will provide you with an overview of the LateNiteLabs lab-simulation platform and how it is currently being used to enhance both the teaching and learning environments in a general chemistry course. How general education competencies are met and, assessed will be described.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Chemical Education - Oral

CONTROL ID: 2277692

TITLE: [Gaussian-based Laboratory Exercises in Physical Chemistry](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [S. M. Basu](#)¹

INSTITUTIONS (ALL): 1. Susquehanna Univ, Selinsgrove, PA, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: The laboratory component of the second-semester Physical Chemistry course at Susquehanna University incorporates a significant computational component. Four of the seven multi-week laboratory exercises are computational in nature. Students use the Gaussian program and Gaussview to calculate molecular properties and visualize concepts they are concurrently learning in lecture. Experiments include calculation of vibrational and rotational parameters based on the harmonic oscillator and rigid rotor models, respectively, visualization of bond vibrations and use of calculated spectra to assign experimentally-obtained infrared and Raman spectra, electronic spectroscopy and molecular orbital theory. Students learn the fundamentals of computational methods and basis sets, learn how to operate the program and extract results from both the visual interface and output (text) files. These exercises have helped students understand molecular properties that are difficult to obtain using experimental methods only.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Inorganic Chemistry - Poster

NERM April 6, 2015

CONTROL ID: 2277784

TITLE: [Manganese catalysts: Synthesis, structure, characterization and their application in homogeneous catalysis.](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): R. N. Egekenze¹

INSTITUTIONS (ALL): 1. Chemistry, Howard University, Washington, DC, United States.

PRESENTATION TYPE: Poster Preferred

ABSTRACT BODY:

Abstract:

Five tridentate Schiff-base ligands and their corresponding reduced Schiff base ligands were prepared from the reaction between 2-aminoethyl-2-pyridine with 5-methoxy-, 5-bromo-, 5-Chloro-, 5-Nitro-, and nonsubstituted-salicylaldehyde. After Characterization by FTIR, ¹HNMR and UV-Visible spectroscopy, the Ligands were used in making Mn catalysts. The catalysts were characterized by FT-IR, UV-Visible spectroscopy, LC-MS, cyclic voltammetry and thermal gravimetry. X-ray crystallographic structures showed six-coordinate ML₂ (L = tridentate Schiff base or reduced Schiff base) complexes. In their cyclic voltammetry in acetonitrile solution, the Mn(III) complexes of the Schiff bases each showed one reversible redox process while the reduced Schiff bases each showed two reversible redox process in the -1.5 to +1.5 V (vs Ag/AgCl) window (Mn(III) \rightleftharpoons Mn(II)). LCMS analysis shows the molecular mass of the dimerization products of the reduced Schiff-base complexes. Evaluation of the catalytic activity of the Mn catalysts for the epoxidation of olefins using Triethyl amine/ perchloric acid [triethylammonium (base)] buffer and acetic acid/Ammonium acetate (acidic) buffer at OOC and room temperature showed that the reduced Schiff-base complexes gave higher epoxide yield than the Schiff-base complexes. Higher yield of epoxides were recorded at OOC than at room temperature for all the complexes. UV-visible absorption studies of the reactions of the complexes with aqueous H₂O₂ at room temperature and in dichloromethane showed appearance of new peaks at 255 and [323-332] indicating the formation of Mn-peroxo and Mn-oxo complexes that are the oxygen atom transfer intermediates leading to catalysis of the olefin. We report the crystal structures, LC-MS result, cyclic voltammogram, Uv-visible absorption spectra, ¹HNMR and GC-MS results for the catalysis experiment.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: News from Carbon World - Oral - INVITED ONLY

CONTROL ID: 2278402

TITLE: [Highly-Reduced Corannulene Aggregates with Different Alkali Metals: Different Geometries within the Same Electronic Structure](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): A. Y. Rogachev¹

INSTITUTIONS (ALL): 1. Biological and Chemical Sciences, Illinois Institute of Technology, Oak Park, IL, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Recent experimental achievements in chemistry of reduced corannulene (C₂₀H₁₀, the smallest bucky bowl) revealed a tendency of highly reduced curved polyaromatic molecules to form sandwich-like aggregates. The latter contain five or six alkali metals as positive "electrostatic glue" between two negatively charged bowls in their convex-convex orientation and show remarkable stability in solution. The electronic structure of these systems was investigated in detail in the present study with help of modern tools of

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quantum chemistry. The influence of the nature and size of alkali metal on stability and dynamics of such systems was clearly established. Increase of size of the metal (from Li⁺ to Na⁺, K⁺, Rb⁺, and Cs⁺) leads to substantial lowering of stability of sandwich-like aggregates and increasing of mobility of metal cations between two polyaromatic sheets. Importantly, the electronic structure of all aggregates stays essentially the same albeit changes in geometry were found dramatic. For example, the distance between two bowls can vary from 3.42Å to 4.41Å without any significant changes in electronic structure.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Advances in Organometallic Chemistry and Catalysis - Oral - INVITED ONLY

CONTROL ID: 2278510

TITLE: [Mechanism Guided Improvement of Pd\(II\) Precatalysts for Cross-Coupling](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [N. Hazari](#)¹

INSTITUTIONS (ALL): 1. Department of Chemistry, Yale University, New Haven, CT, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Transition metal catalyzed cross-coupling has found applications in diverse areas of chemistry and is widely considered to be one of the most powerful and general synthetic methods. The most effective cross-coupling catalysts tend to utilize Pd and feature sterically demanding, electron rich phosphine or N-heterocyclic carbene ancillary ligands. Traditionally, the active species in catalysis, often monoligated Pd(0), has been generated through the addition of excess ligand to a Pd(0) source. However, in recent years the cost of the specialized ligands utilized in most cross-coupling reactions has become comparable to the Pd(0) source and the use of excess ligand is no longer attractive. Instead, a variety of well-defined Pd(I) and Pd(II) precatalysts (Figure 1), which feature a 1:1 Pd:ligand ratio have been developed, and are now commercially available. A key feature in the effectiveness of these Pd(I) and Pd(II) precatalysts is the rate and efficiency of their conversion into the monoligated L-Pd(0) active species under the reaction conditions. Studies have been performed on the mechanism of activation of the Mingos/Hartwig, Buchwald and Organ precatalysts and these activation pathways, which are important for designing improved precatalysts, are now relatively well understood. In contrast, relatively little work has been performed on the mechanism of activation of Nolan type precatalysts. In this presentation we outline the pathway by which Nolan type precatalysts are activated and use this information to design a far more efficient precatalyst.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Inorganic Chemistry - Poster

CONTROL ID: 2280571

TITLE: [The effect of 2-pyridone substitutions on the magnetic exchange of pyrazine in 2-pyridone/pyrazine linear chain complexes of copper \(II\) perchlorate.](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. Monk](#)¹, C. P. Landee⁴, M. M. Turnbull², J. L.

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Wikaira³

INSTITUTIONS (ALL): 1. Biochemistry, Clark University, Columbia, CT, United States.
2. Chemistry, Clark University, Worcester, MA, United States.
3. Chemistry, University of Canterbury, Christchurch, New Zealand.
4. Physics, Clark University, Worcester, MA, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Compounds containing a 1:1:2 ratio of copper to pyrazine to 2-pyridone exhibit a wide range of magnetic exchange through the pyrazine moiety varying from 0-25K. The strength of magnetic exchange depends on the molecular structure and substituents on the complex. In order to better understand the varying exchanges, we have studied the effect of varying the electron density at the copper ion by placing different substituents at the n = 4, 5, and 6 positions of the 2-pyridone ligands. A family of crystallized coordination polymers with the formula [Cu (n-S-2-pyridone)₂(H₂O)₂(pyrazine)](ClO₄)₂ [S = substituent] have been prepared with the Cu(II) ions bridged by the pyrazine molecules. The effect of the identity and position of the 2-pyridone substitutions on the magnetic exchange has been studied and the crystalline structures characterized.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Medicinal Chemistry - Poster

CONTROL ID: 2280684

TITLE: [The Role of Water in the DNA Doxorubicin Intercalation Mechanism](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [J. Finan](#)¹

INSTITUTIONS (ALL): 1. Chemistry, St. Lawrence University, Canton, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: The chemotherapeutic drug doxorubicin intercalates into the DNA double helix preventing DNA replication. The highly effective drug is also toxic; therefore the specifics of the intercalation mechanism are of unique interest to minimize side effects. It is known that there is a hydration layer around the DNA double helix that is involved with the mechanism. The titration of doxorubicin with different DNAs is used to enhance the understanding of the mechanism of intercalation; specifically the importance of water in the binding of doxorubicin to DNA. The binding constant of doxorubicin is found by measuring the fluorescence of the drug molecule in solution with gradually added osmolyte. The binding constants with various DNAs (calf thymus, poly(dA•dT), and poly (dG•dC) are tested with two osmolytes: acetamide and triethyleneglycol (TEG). Our data fitting procedure uses the Gibbs-Duhem equation to evaluate the number of water molecules exchanged in the intercalation of doxorubicin. The water exchange values for the DNAs are different, although the CT and AT values are similar at +37 (acetamide) and +38 (TEG) water, respectively. The GC DNA has a much lower but also positive exchange of +8 waters. Differences in water exchange values for different osmolytes in the GC and AT studies will be investigated by DNA melting experiment that are sensitive to DNA stability in the presence of acetamide and TEG.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Inorganic Chemistry - Oral

CONTROL ID: 2281107

TITLE: [Asymmetric Ligand Approach to Design Heterometallic Molecular Precursors](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [H. Han](#)¹, Z. Wei¹, E. Dikarev¹

INSTITUTIONS (ALL): 1. Chemistry, University at Albany, SUNY, Albany, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Asymmetric ligands, that feature different substituents at the two ends of the ligand, have been utilized for the preparation of three molecular heterometallic precursors $\text{Li}_2\text{Co}_2(\text{dhd})_6$ (dhd = 2,2-dimethyl-hexanedionate), $\text{Li}_2\text{Co}_2(\text{tbaoc})_6$ (tbaoc = *tert*-butyl acetoacetate), and $\text{Li}_2\text{Co}_2(\text{ptac})_6$ (ptac = 1,1,1-trifluoro-5,5-dimethyl-2,4-hexanedionate). The nature of the asymmetric ligands employed results in a different bridging connectivity properties at the two coordinating oxygen sites and allows one to design the heterometallic assembly with discrete molecular structure. The title heterometallic compounds were shown to act as effective single-source precursors for the low-temperature preparation of the LiCoO_2 battery cathode material. Diamagnetic complex $\text{Li}_2\text{Mg}_2(\text{tbaoc})_6$, an analogue of $\text{Li}_2\text{Co}_2\text{L}_6$ molecules, was isolated and utilized to investigate the retention of heterometallic structure in solution by multinuclear NMR spectroscopy.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: resubmitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials Chemistry - Poster

CONTROL ID: 2281335

TITLE: [Engineered pervious layer for pathogen removal during rainwater harvesting](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [S. Hwang](#)¹, H. Smith²

INSTITUTIONS (ALL): 1. University of Puerto Rico at Mayagüez, Mayagüez, Puerto Rico, Puerto Rico.
2. University of the Virgin Islands, St. Thomas, Virgin Islands (U.S.).

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: This study aimed to develop engineered pervious layer (EPL) capable of reducing and/or inactivating pathogens during rooftop rainwater harvesting. Contamination in rainwater is due mostly to urban pollution, bird and reptile waste materials, roof material deterioration, and particulate matter deposition. The presence of pathogens in the harvested rainwater can lead to serious health problems for those exposed to it. Fecal coliforms (FC) were tested in the current study as indicator microorganisms. The EPL was designed to have the structural integrity and hydraulic permeability. For this end, EPLs were made using coarse aggregate with size of 4.75 -9.5 mm, cement from a local supplier, fly ash (FA) from the AES Puerto Rico, and different nanomaterials ($\text{nanoFe}_3\text{O}_4$ and nanoSiO_2). Preliminary results showed, in general, that a higher compressive strength was achieved for the EPLs containing nanomaterials than for the control EPL. However, the permeability was lower for the EPLs containing nanomaterials than for the control EPL, although the values fell into the recommended ones. A lower FC inactivation was accomplished with the EPL specimens containing $\text{nano-Fe}_3\text{O}_4$ than those with the control EPL that developed higher pHs during the experiment. The impact of the additions of other nanomaterials (photocatalytic nanoTiO_2 and/or biocidal nanoZnO) on FC inactivation by EPL is under investigation and will be included in the presentation. This study was financed in part by the U.S. Department Interior, United States Geological Survey, through the

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Virgin Islands Water Resources Research Institute.

CONTACT (COUNTRY ONLY): Puerto Rico

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials for Energy - Oral

CONTROL ID: 2281449

TITLE: [Correlating nanoscale reactivity with photocurrent reveals optimal catalyst sites on photoanodes](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [J. B. Sambur](#)¹

INSTITUTIONS (ALL): 1. Chemistry, Cornell University, Brooktondale, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Photoelectrochemical solar energy conversion to electricity or fuels is often limited by the reactivity of photogenerated holes and electrons on photoelectrode surfaces, requiring modification with catalysts to improve efficiency. It is unclear, however, on what surface sites to optimally deposit catalysts, and to what extent the same surface sites, responsible for fuel-forming reactions, also cause recombination. Here we use super-resolution imaging of hole and electron surface reactivity and sub-nanorod photoelectrochemical measurements to reveal that on TiO₂ nanorod photoanodes, the sites reactive for water oxidation also contribute most to recombination, and the photocurrent efficiency and onset potential are surprisingly uncorrelated at the nanoscale. Guided by hole and electron reactivity maps, site-selective catalyst deposition on individual nanorods reveals that the optimal sites for oxygen evolution catalysts are the low reactivity and high onset potential sites, contrary to what is obtainable under typical deposition conditions, leading to a strategy for rationally engineering photoelectrodes with catalysts.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Medicinal Chemistry - Oral

CONTROL ID: 2282389

TITLE: [Flavonoids & its Complexes in the Treatment of Diabetes](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [P. shukla](#)¹

INSTITUTIONS (ALL): 1. Chemistry, University of Delhi, Delhi, Delhi, India.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: NIDDM (Non-insulin dependent diabetes mellitus), a metabolic disorder leading to chronic morbidity and increasing mortality due to changing life styles particularly in urban Indian population. Different module of drugs targeting insulin modulation are known to treat the disease as insulin sensitizer and/or stimulator of insulin secretion. However due to non-responsiveness of patients after treatment for some time, requires drugs acting with some other mechanisms. Agonists of β_3 -adrenergic and PPAR receptor modulators stimulate the oxidative pathway to dissipate heat without the synthesis of ATP and thereby lower plasma sugar and lipids profiles. Oxidative stress plays a key role in diabetes for macrovascular complications.

Flavonoids are polyphenolic compounds that are ubiquitous in nature and are categorized, according to chemical structure, into flavonols, flavones, flavanones, isoflavones, catechins, anthocyanidins and chalcones. The flavonoids have aroused considerable interest recently because of their potential beneficial effects on human health. An imbalance between antioxidants and ROS results in oxidative stress, leading to cellular damage. Oxidative stress has been linked to different diseases. Flavonoids are known to possess antioxidant property which therefore led us to utilize them for synthesis of hybrid molecules for the treatment of diabetes. The inhibition of PTP-1B is a potential target for treatment of type-2 diabetes. V & Zn complexes have insulin-enhancing activities, and while vanadium compounds inhibit PTP-1B, little is known on the mode of action about Zn compounds.⁴ V is not only an important trace element for organisms but also the necessary element for human body. It has been demonstrated that many V-Compounds possess therapeutic effects as insulin mimetics.^{1,2} Many clinical trials of V-compounds have also been reported^{3,4} in which vanadium salts such as VOSO₄ and NaVO₃ were administered to diabetic patients. There are various V and Zn compounds have reported for anti-diabetic activity.

On the basis of above points, I have synthesized the flavonoids and its metal complexes for antidiabetic activity.

CONTACT (COUNTRY ONLY): India

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Organic Chemistry - Oral

CONTROL ID: 2283034

TITLE: [A General Approach for Catalytic \$\beta\$ -Selective Glycosidation](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): N. Kuhl^{1,2}, K. Harper², Y. Park², R. Y. Liu³, E. N. Jacobsen¹

INSTITUTIONS (ALL): 1. Harvard Univ, Cambridge, MA, United States.

2. Harvard University, Cambridge, MA, United States.

3. Harvard University, Cambridge, MA, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Decorating the cell surfaces of every organism, oligosaccharides are involved in various signaling pathways at a cellular level. Despite their biological prevalence and importance, the efficient synthesis of oligosaccharides, and in particular, selectively linking monosaccharide units through glycosidic bonds, still represents a major challenge for synthetic chemists.

A glycosidic linkage can exist in two different configurations, α or β , depending on its stereochemistry at the anomeric position. The stereochemical outcome of a glycosidation reaction can vary significantly by slightly changing the steric and electronic nature of the substrate or the reaction conditions. This adds additional complexity and renders the development of general and practical methods similar to those of other biopolymers, such as polypeptides and polynucleotides, difficult.

To allow selective formation of glycosidic linkages independent from inherent substrate bias, the use of anion-binding thiourea-catalysts has been invoked as an alternative approach. A new macrocyclic thiourea-catalyst was developed that mimics the stereospecific mechanism of glycosyltransferases and allows for the selective formation β -linked disaccharides from α -configured glycosyl chlorides. The net invertive transformation proved to be generally applicable for different classes of glycosides. 1,2-*trans*- β -linked disaccharides using galactosyl-, glucosyl- and related 2-acetamido-donors, as well as the more challenging classes of β -linked deoxy-sugars, 1,2-*cis*- β -linked mannosides and rhamnosides could be generated in synthetically useful yields and selectivities. Details of this novel, catalytic glycosidation method, including

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preliminary mechanistic studies and first attempts towards a related α -selective approach are presented.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Analytical Chemistry - Oral

CONTROL ID: 2283063

TITLE: [Nutritional Supplement and Diesel Fuel Application Development for Benchtop NMR Systems Operating at 42, 60, and 80 MHz – Equivalency with Supercon NMR](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [J. C. Edwards](#)^{1, 2}, G. Hernandez^{2, 3}, P. J. Giammatteo⁴

INSTITUTIONS (ALL): 1. Process NMR Assoc LLC, Danbury, CT, United States.

2. SpinMetrix SRL, Montevideo, Uruguay.

3. Vis Magnetica, Montevideo, Uruguay.

4. Process NMR Associates, LLC, Danbury, CT, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Benchtop high-resolution NMR systems are available at a number of field strengths and probe configurations. However beyond the obvious academic instruction market for these instruments very few applications have been demonstrated across all available platforms and thus proving the general applicability of benchtop NMR technology to industrial quality control. We will present two chemometric-based applications that have been developed at 4 different field strengths utilizing Varian Mercury 300 MHz, Magritek Spinsolve 42 MHz, Aspect AI 60 MHz, and Thermo Picospin 80 MHz NMR systems. Partial-least-squares (PLS) regression correlations were obtained on all 4 platforms relating to:

- 1) Omega-3 fatty acid composition of samples taken from various points in a nutritional supplement manufacturing process. Excellent correlations were obtained on all 4 NMR instruments proving that NMR technology is applicable to in-lab, at-line, or on-line analysis of fish oil derived omega-3 fatty acid supplements. The 40 second NMR analysis effectively replaces a 60+ minute GC analysis.
- 2) Physical and chemical property determination of diesel fuels where excellent correlations were obtained between ¹H NMR variability and parameters such as density, aromatic content by GC, hydrogen content by ¹H TD-NMR (ASTM D7171 method), and sulfur content.

Finally, we will present the concept and initial results from an independent server-based NMR application software that can be utilized in conjunction with the NMR software of the current benchtop NMR systems, or alternatively as a stand-alone application platform. This software would effectively make chemometric and direct measurement NMR application ubiquitous across all NMR platforms.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Food Chemistry - Poster

CONTROL ID: 2283171

TITLE: [¹H qNMR of Alcoholic Cider - Analysis of Small Molecule and Residual Sugar Chemistry](#)

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AUTHORS (FIRST NAME INITIAL, LAST NAME): J. C. Edwards¹

INSTITUTIONS (ALL): 1. Process NMR Assoc LLC, Danbury, CT, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: ¹H qNMR has been utilized to assess the the small molecule and carbohydrate chemistry of a number of home-brewed and commercial alcoholic ciders. A quantitative chemistry distribution of the products of the various fermentations that occur in cider making. Malolactic fermentation as well as fermentation by saccharomyces and wild yeasts occur in the cider making process which traditionally occurred without the intentional addition of yeast by the manufacturer. The distribution of small molecules produced by the yeast and bacterial metabolomes at work in the process can yield information of the sensory perception of ciders produced in different ways. An investigation of the residual sugar chemistry of commercial ciders gives some indication of the process of sweetening commercial cider products with sugar additions after fermentation is complete. These typical commercial ciders are very different in chemistry distribution compared to very dry cider styles such as those found in the Basque region of Spain where fermentation is taken to the extreme resulting in complete conversion of sugars to alcohol but also glycerols to 1,3 propanediol. Finally it was decided to determine how much quantitative chemistry information could be obtained from benchtop NMR systems operating in the 60 MHz range. These benchtop NMR systems have a price and cost-of-ownership that would allow small laboratories of manufacturers to think about their use in QA and QC roles.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Food Chemistry - Oral

CONTROL ID: 2283153

TITLE: [From Mash to Bottle: Chemistry of the Beer Brewing Process and NMR-based Quality Control](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): A. DiCaprio¹, J. C. Edwards¹

INSTITUTIONS (ALL): 1. Process NMR Assoc LLC, Danbury, CT, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: Due to the complexity of the complete brewing process, there are multiple opportunities for the application of quantitative NMR (qNMR) in brewery quality control. NMR and multivariate analysis have been applied as quality control measures previously, but never throughout the entire brewing process. In conjunction with a number of commercial brewing companies, this project seeks to utilize NMR and chemometrics to describe the full chemical changes that occur during the brewing process, as well as variations occurring between separate production lots. qNMR is utilized to provide bulk chemistry information on small organic acids, residual dextrans, esters, and fusel alcohols. Equipped with the knowledge of brewing process variables and their consequential chemical effects, brewers would be able to use NMR as a quality control measure to not only identify when production issues occur, but also where and why they occur.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

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ABSTRACT SYMPOSIUM NAME: Medicinal Chemistry - Oral

CONTROL ID: 2283105

TITLE: [Survey of Low Field NMR Spectrometer Platforms for Successful Screening of Sexual Enhancement and Weight Loss Supplements for Adulteration with Drugs and Drug Analogs](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): J. C. Edwards¹, A. Bzhelyansky², K. M. Adams³

INSTITUTIONS (ALL): 1. Process NMR Assoc LLC, Danbury, CT, United States.

2. Dietary Supplements, United States Pharmacopeial Convention, Rockville, MD, United States.

3. United States Pharmacopeial Convention, Rockville, MD, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: The adulteration of dietary supplements (or natural health products) with synthetic pharmaceuticals is an area of increasing concern, which presents substantial risk to public health. Widely available in retail and via the Internet, these products are often marketed as sexual enhancement, weight loss and/or bodybuilding supplements.

Development of analytical tools for screening and identification of adulterated products in the marketplace represents a significant step forward in the fight against adulterated dietary supplements. Several organizations, including AOAC and USP, have undertaken initiatives to evaluate and recommend analytical methodologies for screening supplements for adulteration. HPLC and mass spectrometry have so far dominated the screening and quantitation studies published in the literature, with NMR spectroscopy often relegated to the status of structure elucidation tool. In this work, we investigate the ability of several-low field NMR spectrometric platforms to successfully identify and quantify the presence of adulterating drug substances in sexual enhancement and weight loss supplements purchased online and in US retail. ¹H qNMR of both types of samples was performed with 300 MHz NMR to confirm the presence of adulterants such as sildenafil, tadalafil, and their structural analogues (sexual enhancement supplements) and various synthetic stimulants (weight loss supplements). We have concluded that a simple sample preparation protocol combined with straightforward ¹H NMR spectroscopic analysis yields a rapid, robust and reliable screening test for adulterated supplements, presenting an attractive alternative to more labor-intensive, expensive and expertise-demanding techniques *du jour*.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Inorganic Chemistry - Oral

CONTROL ID: 2283120

TITLE: [Unusual Redox Reactions in the Synthesis of Copper Coordination Compounds: The Synthesis of bis\(5-NAP\)CuCl₂ and Multiple Polymorphs of bis\(5-NAPH\)CuCl₂](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): A. G. Bellesis¹, M. M. Turnbull¹, C. P. Landee², J. L. Wikaira³, M. Polson³

INSTITUTIONS (ALL): 1. Chemistry, Clark University, Worcester, MA, United States.

2. Physics, Clark University, Worcester, MA, United States.

3. Chemistry, University of Canterbury, Christchurch, New Zealand.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: We are involved in a project to synthesize and magnetically characterize copper coordination compounds of the type L₂CuX₂, where L is a substituted pyridine ligand and X is a halide ion. These compounds are low-dimensional Heisenberg Antiferromagnets; the magnetic behavior is known to depend on

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superexchange pathways that are dependent on structure. The synthesis of this family of compounds is important in expanding knowledge in both synthetic inorganic chemistry and applications of theoretical physics.

Here, we present the synthesis, crystal structure, and magnetic properties of bis(2-amino-5-nitropyridine)CuCl₂. The synthesis is of particular interest due to unusual oxidation-reduction reactions. When dissolved in various organic solvents at high temperatures, bis(2-amino-5-nitropyridine)CuCl₂ reacts with atmospheric oxygen and is reduced to produce multiple polymorphs of bis(2-amino-5-nitropyridinium)CuCl₄. The reduced and oxidized compounds exist in a temperature-dependent equilibrium in solution and are stable in air as the dry solids. Synthesis, crystallographic information, magnetic data and proposed reaction mechanisms will be presented.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Analytical Chemistry - Poster

CONTROL ID: 2283283

TITLE: [Determination of bisphenol A analogues and their photochemical degradation in fresh and marine coastal waters](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): Y. Zuo¹, M. Alshantiti¹, A. L. Francis¹, J. Michael¹

INSTITUTIONS (ALL): 1. Univ Massachusetts Dartmouth, North Dartmouth, MA, United States.

PRESENTATION TYPE: Poster Preferred

ABSTRACT BODY:

Abstract: Bisphenol A is widely used in plastic and other industrial consumer products. Release of bisphenol A and its analogues into the aquatic environment during manufacture, use and disposal has been a great scientific and public concern due to their toxicity and endocrine disrupting effect on aquatic wildlife and even human beings. More recent studies have shown that these alkylphenols may be bioaccumulated in crustacean tissues and other aquatic organisms from polluted water and affect the molting processes and survival of American lobster, crab, shrimp and other wild lives in natural water [Y. Zuo and Z. Zhu (2014) Simultaneous identification and quantification of 4-cumylphenol, 2,4-bis-(dimethylbenzyl)phenol and bisphenol A in prawn *Macrobrachium rosenbergii*. Chemosphere 107, 447-453]. Thus, it is important to examine BPA analogues and their photodegradation in natural waters. In this study, we have developed GC-FID and GC-MS methods for the determination of bisphenol A and its analogues in fresh and coastal marine waters. Bisphenol A, 2,4-bis-(dimethylbenzyl)phenol and 4-cumylphenol were found in the concentration ranges of 2.07–2.55, 2.07–2.43, and 0.217-0.223 ng/L, respectively, in a fresh lake water. In New Bedford Harbor water samples, bisphenol A and 2,4-bis-(dimethylbenzyl)phenol were detected in the concentration ranges of 2.16-2.82 and 2.70-4.62 ng/L, respectively; and no 4-cumylphenol was observed. The detailed kinetic study on the photodegradation of BPA and its analogues will be reported at the presentation.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Analytical Chemistry - Poster

CONTROL ID: 2283446

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TITLE: [Occurrence and identification of bisphenol A and other alkylphenols in sea crabs](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): Y. Zuo¹, J. Michael², M. Alshantiti², F. Albalawi²

INSTITUTIONS (ALL): 1. Univ Massachusetts Dartmouth, North Dartmouth, MA, United States.

2. University of Massachusetts Dartmouth, North Dartmouth, MA, United States.

PRESENTATION TYPE: Poster Preferred

ABSTRACT BODY:

Abstract: The global industrialization in recent decades has led to an increase in environmental pollutants from the development of commercial products, especially those from plastic components. Plastics are organic materials that are used in everyday households for a variety of functions. With the increase in volume of plastics in common everyday items like baby bottles, food cans and drinking bottles, there is a concern over the health effects that come with the exposure of plasticizers to humans and wild lives because plasticizers, such as alkylphenols and bisphenol A, are endocrine-disrupting chemicals (EDCs). Determining the levels of these EDCs in the environment and animals is important so that certain thresholds can be set to limit the health effects to the wildlife and humans. Both GC and HPLC techniques have been developed for determining BPA in the environment [Zuo, Y. Ed., *High-Performance Liquid Chromatography (HPLC): Principles, Procedures and Practices*. Nova Science Publishers, Inc., New York (2014)]. The purpose of this experiment is to identify and quantify alkylphenols and bisphenol A in a local Asian Shore Crab species using GC-FID and GC-MS techniques. BPA and two of its analogues, 2,4-bis-(dimethylbenzyl)phenol and 4-cumylphenol, have been found in Asian crab samples. Further details will be discussed at the presentation.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials for Energy - Oral

CONTROL ID: 2283792

TITLE: [The Ultimate Limits of Li-Ion Batteries, and What's Next - A Reality Check on Beyond Li-Ion](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. S. Whittingham](#)¹

INSTITUTIONS (ALL): 1. NECCES, Binghamton University, Binghamton, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Li-Ion batteries, based on intercalation reactions, are around 40 years old. They have steadily increased in performance and now dominate portable energy storage from electronic devices to cars and buses. They are also finding use in the grid for load leveling, smoothing and to support renewable resources such as wind and solar. They have still much room for improvement, and their ultimate limits of around 1 kWh/L and 355 Wh/kg at the cell level is still in the future. Some approaches to attain these values will be discussed including 2 Li systems and "Closing the Gap" on the layered oxides, MO₂. A number of Beyond Li-ion systems have been proposed; a number of these including Li/O₂ do not pass a reality check. This research is supported by the DOE-EFRC-NECCES at Binghamton.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

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ABSTRACT SYMPOSIUM NAME: Materials Chemistry - Oral

CONTROL ID: 2284573

TITLE: [Metal-organic frameworks as platform to arrange and protect single-molecule magnets in multidimensional arrays](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): M. Wriedt¹, J. Pyser¹, D. Aulakh¹, A. Yakovenko³, X. Zhang⁴, K. R. Dunbar²

INSTITUTIONS (ALL): 1. Chemistry Biomolecular Science, Clarkson University, Potsdam, NY, United States.

2. Texas AM Univ, College Station, TX, United States.

3. Advanced Photon Source, Argonne National Laboratory, Argonne, IL, United States.

4. Department of Chemistry, Texas A&M University, College Station, TX, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Next-generation computer technologies will require ultrahigh-density data storage devices and quantum computing based on isolated spin-carriers, so-called molecular spintronics. [1] Single-molecule magnets (SMMs) have shown great potential for such applications. [2] Their unique magnetic properties enable SMMs to be used in spintronics for switching from total spin up to total spin down on a molecular level, and therefore each molecule can be used as a magnetic bit of information. Although a broad community works on the design of new SMMs with improved properties, [3] coupling of the nanoscale units to the macroscopic world remains as a key challenge. [4] Any practical application of SMMs requires in the first step their organization in 2D or 3D networks to allow read-and-write processes. Moreover, they are very delicate molecules that break down easily and thus, they need to be protected to retain their unique magnetic properties. Owing to their crystalline nature and tunability, metal-organic frameworks (MOFs) provide an excellent means to overcome this challenge. We investigated the unprecedented incorporation of SMMs into multidimensional MOF matrixes, yielding new nanostructured composite materials that combines key SMM properties with the functional properties of MOFs (Fig. 1). We believe that these findings might be crucial for the development of spintronics in real world applications. In this presentation we will focus on the fundamental understanding in the exciting structure-property relationships of these SMM@MOF composite materials.

Figure 1. Schematic representation of a MOF hosting SMM molecules.

References

(1)Sanvito, S. *Chem. Soc. Rev.* **2011**, *40*, 3336.

Bogani, L.; Wernsdorfer, W. *Nat Mater* **2008**, *7*, 179.

(3)Woodruff, D. N.; Winpenny, R. E. P.; Layfield, R. A. *Chem. Rev.* **2013**, *113*, 5110.

(4)Domingo, N.; Bellido, E.; Ruiz-Molina, D. *Chem. Soc. Rev.* **2012**, *41*, 258.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Inorganic Chemistry - Poster

CONTROL ID: 2284628

TITLE: [The mechanochemical synthesis of 2-amino-5-substitutedpyridine copper \(II\) halide complexes and their magnetic properties](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): P. C. Farris¹, J. E. Chellali¹, C. P. Landee², M. M.

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Turnbull¹

INSTITUTIONS (ALL): 1. Chemistry, Clark University, New York, NY, United States.
2. Physics, Clark University, Worcester, MA, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Research has been completed surrounding the salts with the general formula (2- amino-5-S-pyridine)₂CuX₄, in which S is a substituent and X is a halide ion (Cl or Br). There is less known about the crystal structures and magnetic properties of neutral compounds made with 2-amino-5-S-pyridines and cupric halides. We have begun working to synthesize compounds with the general formula (5CAP)_nCuX₂, [5CAP = 2-amino-5-chloropyridine; n = 1, 2] where X is either chloride or bromide. These structures either tend to form dimers or chains in the solid state, but it has yet to be discovered why certain processes or starting materials will yield one structure over another. By working to produce this compound under different conditions by using different various methods, we are hoping a reason for either trend will become clear. We have been utilizing mechanochemistry, which can be used to synthesize products without solvents. The reactions are facilitated between solid materials by applying a grinding force to increase the thermal energy of the molecules to break and form the bonds. This process is carried out by using a mortar and pestle, as it is the most convenient and affordable technique. By using this method the new compound can be produced quickly, although the technique may produce a less pure product. The products are characterized using methods such as infrared spectrometry and X-ray diffraction to determine their purity and composition. Once pure substances have been acquired the next task is to form crystals from them and determine their crystalline structures.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Organic Chemistry - Oral

CONTROL ID: 2284759

TITLE: [A new boron intermediate in carbonyl reduction by borohydride](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [P. S. Murthy](#)¹, R. Winkler¹

INSTITUTIONS (ALL): 1. Chemistry and Biochemistry, Georgian Court University, Lakewood, NJ, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: The stereoselectivity induced in the borohydride reduction of carbonyl compounds with a α -chiral carbon has been studied for five decades. Mechanistic models that take into account the nature of the substituents on the α -carbon have been used to account for the induced stereoselectivity. These existing models fail to explain the high stereoselectivity observed in the borohydride reduction of the multifunctional substrate benzil (**A**) proceeding *via* the intermediate **B** (a carbonyl compound with an α -chiral carbon), to mainly (~89%) the *meso*-hydrobenzoin (**F**) – a common undergraduate laboratory experiment. To address this lack of mechanistic insight, we studied this reaction using stoichiometric and hydrogen-deuterium isotope exchange studies and ¹¹B spectroscopy. We have obtained evidence for the intermediate spiroborate with *syn*, *syn* configuration (**E**), formed from the dimeric dialkoxy dihydridoborate dimer (**D**) – a new, hitherto unknown borate species with bridged hydrogens and penta-coordinated boron atoms. Stereospecific intramolecular hydride transfer within this rigid dimer could be the cause of the selective formation of the *syn*, *syn*-spiroborate (**E**) and hence the *meso*-diol (**F**) observed in this reaction. The newly discovered dimerization equilibria is likely to be present in all reduction reactions with borohydride and could be a significant factor in influencing selectivity in the borohydride reduction of carbonyl compounds with a α -

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chiral carbon.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Environmental Chemistry - Oral - INVITED ONLY

CONTROL ID: 2284771

TITLE: [Biomonitoring of Human Exposure to Phthalates and Environmental Phenols](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [K. Kannan](#)¹

INSTITUTIONS (ALL): 1. New York State Department of Health, Wadsworth Center , Albany, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Phthalates, parabens and bisphenol A (BPA) are used in a wide variety of consumer products. Although human exposure to these endocrine disrupting chemicals is inevitable, the exposure doses for these chemicals are still not well known. A biomonitoring approach, that involves measurement of concentrations of target chemicals in human urine and by use of a simple pharmacokinetic model, we estimated total daily exposure doses of these chemicals. We also measured these contaminants in various exposure sources including foodstuffs for the calculation of daily exposure doses. A comparison was made between exposure doses calculated using biomonitoring approach and direct measurement of contaminants in food, indoor air and dust.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Biochemistry - Poster

CONTROL ID: 2284852

TITLE: [Probing the interactions between Fmoc Protected Backbone and DNA via Spectroscopy](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. T. Farrier](#)¹, P. E. Sheridan¹, L. A. Levine¹

INSTITUTIONS (ALL): 1. Physical Science Department, Kutztown University, Kutztown, PA, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: The interactions between a 24 base pair duplex DNA strand and a fluorenylmethyloxycarbonyl (Fmoc) and tert-butoxide (OtBu) protected aminoethylglycine (aeg) backbone was observed through the use of fluorescence and absorbance spectrophotometry as well as gel electrophoresis. Fmoc-aeg-OtBu has the potential to interact with DNA through intercalation (Fmoc) and/or groove binding (aeg-backbone) which may disrupt the conformation and functionality of the DNA helix. Methods of analysis included titrating a backbone solution with DNA which was spectroscopically monitored at varying points of saturation. Quenching of the Fmoc tag upon interaction with the DNA was observed through fluorescence spectroscopy. An agarose and polyacrylamide gels were constructed to probe the interactions between a DNA strand and the backbone using gel red indicator as an imaging agent. Future studies include addition of a

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pyridine moiety and subsequently tethered platinum terpyridine pyridine residues to the backbone to further observe intercalation effects with more complex assemblies.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Environmental Chemistry - Oral

CONTROL ID: 2284947

TITLE: [Green Vinyl Ester Resin from Renewable Biowaste Glycerin](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): P. Shah², A. Kokil³, R. F. Kovar¹, Y. Lee³

INSTITUTIONS (ALL): 1. R.F. Kovar Associates, Wrentham, MA, United States.

2. Chemistry, University of Massachusetts Lowell, Lowell, MA, United States.

3. Chemistry, University of Massachusetts at Lowell, Lowell, MA, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: We present here for the first time a novel environmentally benign protocol for synthesis of vinyl ester resin (VER). Our synthetic strategy utilizes a commercial waste material, glycerin, from biodiesel manufacturing, and converts it into a widely utilized resin. The VER was synthesized using bisphenol A (BPA) and glycidyl methacrylate (GMA) as precursors. GMA was synthesized using glycerine obtained from a biodiesel manufacturing waste stream. Glycerine was converted to GMA using a novel multistep synthetic protocol. The structure of intermediate was confirmed by ¹H NMR, HPLC and FT-IR spectroscopy.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Undergraduate Inorganic Chemistry - Poster

CONTROL ID: 2285157

TITLE: [Synthesis, Structure, and Magnetic Behavior of a family of Copper\(II\) halide/isoquinoline salts and complexes.](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): A. D. Richardson¹, T. J. Zirkman¹, C. P. Landee³, M. M. Turnbull¹, M. Rademeyer²

INSTITUTIONS (ALL): 1. Chemistry, Clark University, Worcester, MA, United States.

2. Chemistry, University of Pretoria, Pretoria, South Africa.

3. Physics, Clark University, Worcester, MA, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: There has been extensive research into metal halide complexes and salts of quinoline and the relationship between the structure of those compounds and their magnetic behavior. Isoquinoline, however, has received very limited study. Our objective was to learn more about how isoquinoline affects structure and magnetic characteristics. We have prepared a family of complexes and salts with both copper (II) chloride and copper (II) bromide and isoquinoline. The complexes have the general formula Cu(isoquinoline)₂X₂, or Cu[(isoquinoline)₂X₄](H₂O)_n(n=0,1,2). Discussion on the synthesis and structures, as well as magnetic

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properties of these compounds will be presented. An analysis on the distinctions and similarities of the chloride versus the bromide compounds will be provided. This will also include the difficulty in producing analyzable crystals of the neutral complexes, as well as the synthesis of anhydrous and hydrated crystals.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: resubmitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials for Energy - Oral

CONTROL ID: 2285174

TITLE: [Multilayer Light Harvesting Arrays for Molecular Based Solar Cells](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [P. H. Dinolfo](#)¹

INSTITUTIONS (ALL): 1. Dept of Chemistry Chemical Biology, Rensselaer Polytechnic Inst, Troy, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: We have developed a new layer-by-layer (LbL) fabrication technique for the controlled growth of molecular multilayer assemblies on oxide and electrode surfaces. The nanoscale thin-film structures were fabricated using copper(I) catalyzed azide alkyne cycloaddition (CuAAC) as both a means of anchoring the films to the substrate surface and coupling of the individual molecular layers together. The flexibility and versatility of this process permits us to incorporate a wide variety of individual molecular building blocks into the multilayer thin-films. This in turn allows us to target specific electrochemical and photophysical properties for a variety of electro-optical applications including light harvesting arrays for molecular based solar cells. Herein, we describe the optical properties and growth patterns of the multilayer films using a variety of molecular components. Characterization of the thin films by XRR, AFM, XPS, FTIR, optical spectroscopy, and ellipsometry provide a detailed picture of the multilayer structure. The molecular multilayers show consistent growth over tens of layers and moderate ordering in their molecular structure. When assembled on electrode surfaces, the multilayer films display reversible electrochemical charging, but also insulating properties towards solution redox probes. Additionally, multilayer films composed of donor-acceptor building blocks show evidence of efficient Förster resonance energy transfer between chromophores. Finally, preliminary photocurrent data is presented for the multilayer sensitization of ITO electrodes in a Dye-Sensitized Solar Cell configuration.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Food Chemistry - Oral

CONTROL ID: 2285409

TITLE: [Super berry *Aronia mitchurinii* – cultural management, food and non-food related applications supported by phytochemical and material research](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): B. Aroh¹, H. Goldsborough¹, S. Park¹, T. Ndam², D. Nwaeze¹, M. Fadipe¹, A. Ristvey², [V. Volkis](#)¹

INSTITUTIONS (ALL): 1. Natural Sciences, University of Maryland Eastern Shore, Princess Anne, MD,

United States.

2. University of Maryland Extension, Wye Research and Education Center, Queenstown, MD, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: *Aronia mitschurinii*, commonly known as the Black Chokeberry, is a fruiting bush native to the East Coast of the US and cultivated as a specialty food crop in Eastern Europe. Aronia berries contain a cocktail of antioxidants in significantly higher concentrations than currently future as a super-berry Acai berries. The most notable of these compounds is anthocyanin. It is a valuable nutrient and the compound with some technical applications in addition to nutrition ones.

The first goal of this project is to develop and optimize the horticultural management program for growing aronia in Maryland small farms in order to produce the crop with as high as possible antioxidant capacity. This helps in improving sustainability of local farm business. Our preliminary study of antioxidant capacity of aronia as a function of bush age, sun-shadow ratio, fertilization and pest management influence significantly the antioxidant capacity. Here we present data of the measurements of total polyphenols, anthocyanin content, total flavonoids, pH, juice/pulp ratio, some antioxidant profiles and the ORAC factor of Aronia for 2011, 2013 and 2014 aronia harvests.

We will also present the influence of temperature and exposure time on antioxidant content of Aronia. The aim of this study is to determine the thermal process that would avoid significant decomposition of antioxidants during pasteurization and food processing.

Finally two examples of non-food related applications of Aronia will be presented. The first project aims to testing current resin techniques on the extraction of anthocyanin from both Aronia juice and pulp. Extracted antioxidants can be used in health supplements, food products, and possibly in the future as medication ingredients. Antioxidant profile before and after the resin treatment, comparison of different resins as well as purity analysis of isolated products will be presented. As another example we will present the study in which aronia extracts were incorporated into polymer films for antifouling protection. Available protective coating contain such a danger chemicals as tributyl tin (TBT) and are toxic to marine environments. With the aim to find an alternative to available toxic protecting coatings, extracts of *Aronia mitchurinii* was incorporated into polymers commonly utilized in the paint industry and antifouling tests of these samples have shown significant protecting effect.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Analytical Chemistry - Poster

CONTROL ID: 2285430

TITLE: [Screening for pesticides using enzyme-modified graphene/gold nanoparticle composite film biosensors](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [K. Morrissey](#)¹, O. Kubesa¹, M. R. Hepel¹

INSTITUTIONS (ALL): 1. Department of Chemistry, SUNY Potsdam, Potsdam, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: The extensive use of pesticides in agriculture has significantly contributed to environmental pollution problems. The control of this pollution is of paramount importance to human health due to the high bioactivity of pesticides. Many pesticides have been found to show mutagenicity and their genotoxic properties may include carcinogenicity. Due to the widespread pesticide pollution, there is a need for field testing of water and soil for pesticide contamination. To tackle this challenge, sensitive, robust, and inexpensive sensors are required. One of the solutions is to develop enzymatic biosensors. Biosensors based

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on the principle of enzyme inhibition can be applied for detection of a variety of analytes such as organophosphate, carbamate and benzamide pesticides. We have investigated two types of enzymatic sensors: acetylcholinesterase- and butyrylcholinesterase-based biosensors. Acetylcholinesterase (ACE) and butyrylcholinesterase (BCE) are both used to hydrolyze choline esterase and are the primary targets of inhibition by many different pesticides. The inhibitors bind strongly to the enzyme molecule and block the substrates from entering the active serine site, hindering enzymes from catalyzing their reactions. In the presence of pesticides, the activity of ACE or BCE is inhibited and leads to a decrease in the current signal of an amperometric biosensor. The biosensor performance relies on quantitative measurements of the enzyme activity before and after the exposure to target pesticides. We have successfully developed amperometric biosensors with incorporated graphene into the biosensor surface for highly selective and sensitive determination of the following pesticides: aldicarb, trichlorofuran, carbofuran and diflubenzofuran. The modification with reduced graphene oxide (rGO), gold nanoparticles, and functional molecules has enabled us to increase the enzyme loading and thus the biosensor sensitivity.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Medicinal Chemistry - Poster

CONTROL ID: 2285418

TITLE: [Controlled release of anticancer drug 5-fluorouracil](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): J. Simpkins¹, T. Hughes¹, H. Ilkhani¹, M. R. Hepel¹

INSTITUTIONS (ALL): 1. Department of Chemistry, SUNY Potsdam, Potsdam, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: The administration of chemotherapeutic drugs, which are highly cytotoxic not only to the cancer cells but also to the healthy cells, has been a challenge that only recently has been resolved by the development of novel drug delivery systems based on specialized nanocarriers targeting cancer tissue. One of the carrier systems utilizes functional gold nanoparticles. In this work, we have employed gold-coated magnetic nanoparticles (MNPs) which provide several advantages over gold nanoparticles, such as easy manipulation, separation, and medium exchange during surface modification and drug loading. Also, during the administration, they allow for magnetic focusing on cancer tissue, followed by easy removal and collection. For these reasons, the use of MNPs in cancer research is growing. We have investigated the delivery of an anticancer drug, fluorouracil (5-FU). Effective delivery of 5-FU to malignant tumors is of particular interest because of its high toxicity to the healthy tissues. We have employed surface-enhanced resonance Raman scattering (SERRS) spectroscopy and UV-Vis spectroscopy to monitor the binding and release of 5-FU. SERRS is particularly useful due to its ultra-high sensitivity. The drug release was carried out in the presence of buffer solutions with varying pH (4.5 to 6.5). We have also investigated the effects of surface modification of Au-coated MNPs by immobilizing poly(ethyleneglycol) (PEG) and folic acid (FA) in nanoparticle shells via covalent bonding to a self-assembled monolayer of functional thiol molecules.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: resubmitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Materials for Energy - Oral

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CONTROL ID: 2285468

TITLE: [Engineering and Assembling Nanoscale Building Blocks for Energy Applications](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [R. D. Robinson](#)¹

INSTITUTIONS (ALL): 1. MSE Department, Cornell University, Ithaca, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Our research group works to gain a fundamental understanding of how to program and process nanoscale building blocks into functional structures, and the structure-property relationships of the resulting nanostructured materials. We seek to develop new nano-materials and methods for batteries, supercapacitors, fuel cells, and printable electronics. In this talk I will discuss our recent results overcoming critical challenges to create functional nanostructured assemblies.

I'll discuss our chemical and structural engineering of cobalt nanoparticles to create additive-free battery electrodes, made without polymeric binders or carbon black. We have found that electrophoretic deposition (EPD) of nanoparticles creates a strong electrical and mechanical bond for the batteries to perform at maximum capacity. This innovation increases the power density by reducing the overall volume.

We have applied these techniques to make printable electronics: Using our surface treatment methods to link the nanoparticles, and the EPD method for deposition, we make copper sulfide films with high conductivity and high mobilities. We show that our nanoparticle films have conductivities that are on par with many bulk copper sulfide films (~75 S•cm⁻¹), without the need for heat-treatments.

Finally, I present a comparative study of electrophoretically deposited and dropcast nanoparticulate cobalt oxide thin films for the oxygen reduction/oxygen evolution reactions (ORR and OER). In our work, we compare a conventional dropcast method versus EPD. In examining the film's catalytic properties we find that the electrophoretically deposited nanoparticles outperform the dropcast films by as much as 2.5× for the oxygen reduction reaction and 2.6× and the oxygen evolution reaction when accounting for both surface area and mass. The critical solution-processing technique that we use to obtain high catalytic performance is EPD. EPD binds the metal nanoparticles to the surface of the electrode and to each other in an assembly, creating strong electrical contacts between the particles and electrodes. This process results in this significant catalytic improvement in oxygen reduction/evolution performance which cannot be duplicated by dropcast films with the same loading.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Organic Chemistry - Poster

CONTROL ID: 2285745

TITLE: [Novel heterocyclic methodology for natural products synthesis](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [S. P. Fearnley](#)^{1,2}, [C. Thongsornkleeb](#)¹, [M. E. Domaradzki](#)^{1,2}, [R. C. Lapo](#)^{1,2}, [P. M. Lory](#)¹

INSTITUTIONS (ALL): 1. Dept of Chemistry, CUNY-York College, Jamaica, NY, United States.
2. Ph.D. Program in Chemistry, The Graduate Center of the City University of New York, New York, NY, United States.

PRESENTATION TYPE: Poster Only

ABSTRACT BODY:

Abstract: Our group's research focuses on the development of new heterocyclic methodology for the synthesis of bioactive natural products. Specific efforts include:

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- Investigation and use of oxazolone as a useful heterocyclic scaffold for alkaloid synthesis – chiefly, intramolecular Diels-Alder reactions with oxazolone as the dienophilic species. Application in the synthesis of several alkaloid targets is currently underway.
- Novel organosilane chemistry for approaches to bioactive ether targets – a rapid synthesis of cis-fused bicyclic ether arrays in which oxocarbeniums undergo nucleophilic attack by vinylsilanes via a novel intramolecular annulation process. A wide variety of ether natural product motifs are thus accessible.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Organic Chemistry - Oral

CONTROL ID: 2285789

TITLE: [Oxazolone cycloadducts as versatile frameworks for alkaloid synthesis](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [R. C. Lapo](#)^{1,2}, S. P. Fearnley^{1,2}

INSTITUTIONS (ALL): 1. Dept of Chemistry, CUNY-York College, Jamaica, NY, United States.
2. Ph.D. Program in Chemistry, The Graduate Center of the City University of New York, New York, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: The intramolecular Diels-Alder reaction of N-substituted oxazolones provides a variety of heterocyclic frameworks with obvious potential for alkaloid synthesis. Two main strategies are currently under investigation – either Direct Incorporation of the immediate cycloadduct scaffold itself, or Rearrangement to complementary patterns with further applications. Divergent synthesis of several distinct alkaloid classes from individual cycloadducts is currently underway.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Environmental Chemistry - Oral

CONTROL ID: 2285549

TITLE: [Proteins as Surfactant Synergists for Environmental and Industrial Applications](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [M. G. Goldfeld](#)¹

INSTITUTIONS (ALL): 1. Advanced BioCatalytics Corp., Irvine, CA, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: Data presented on the effect of small proteins on the surface activity of synthetic surfactants and their blends as assessed by standard surface science techniques. Surface tension of aqueous surfactant solutions, interfacial tension between those solutions and water insoluble substrates, and contact angle between these solutions and solid and soft surfaces were determined. It is shown that both small individual proteins, such as lysozyme and b-lactoglobulin, as well as proteins in a yeast extract, significantly and predictively reduce critical micelle concentration of multiple widely used surfactants: ionic, non-ionic and amphoteric. Typically, lower minimal interfacial tension could be achieved with a protein synergist, than with

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the same surfactant in the absence of protein. Examples of industrially important applications of a protein synergist are described. In one of them, the protein accelerates wetting and spreading of surfactant solutions on the hydrophobic surface of green leaves, as well as human skin, with concomitant enhancement of the solution uptake. In another example, the activity of bacterial lipase, an important industrial enzyme, towards a segregated oil substrate is enhanced by a surfactant–protein synergist blend, as compared to the same surfactant(s) in the absence of a protein synergist. Applications in industrial cleaning and remediation of products developed on the above principles will also be presented.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Environmental Chemistry - Oral

CONTROL ID: 2285618

TITLE: [Shale Gas: Unsolvable Local and Global Problems](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [A. Ingraffea](#)¹

INSTITUTIONS (ALL): 1. CEE, Cornell University, Ithaca, NY, United States.

PRESENTATION TYPE: Oral Only

ABSTRACT BODY:

Abstract: We will explore some myths and realities concerning large-scale development of the unconventional natural gas resource in Marcellus and other shale deposits in the Northeast. On a local scale, these concern geological aspects of the plays, and the resulting development and use of directional drilling, high-volume, slickwater, hydraulic fracturing, multi-well pad arrangements, and the impacts of these technologies and their required ancillary infrastructure on waste production and disposal, and on contamination of water supplies. On a global scale, we will also explore the cumulative impact of unconventional gas development on greenhouse gas loading of the atmosphere.

CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)

ABSTRACT SYMPOSIUM NAME: Medicinal Chemistry - Oral

CONTROL ID: 2286136

TITLE: [Investigation of a Vitamin B₁₂ Conjugate as a PET Imaging Probe](#)

AUTHORS (FIRST NAME INITIAL, LAST NAME): [J. L. workinger](#)¹, R. P. Doyle¹

INSTITUTIONS (ALL): 1. Chemistry, Syracuse University, Syracuse, NY, United States.

PRESENTATION TYPE: Oral Preferred

ABSTRACT BODY:

Abstract: <!--StartFragment-->

High nutrient demand is a major characteristic of rapidly proliferating cells. Vitamin B12 (B12) is an essential nutrient for all mammals and is vital for cell proliferation. In this study, we exploited a B₁₂ derivative in detection of preclinical tumor models. Herein, we describe the synthesis and biological evaluation of B₁₂-ethylenediamine-benzyl-1,4,7-triazocyclononane-N,N',N''-triacetic acid, the first example

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of a B₁₂ derivative for positron emission tomography imaging (PET). Small animal imaging shows high tumor uptake at 6 h post-administration. Competition with excess native B₁₂ resulted in a 95% decrease in tumor accumulation, thus indicating the specificity of this radiopharmaceutical for B₁₂ endocytosis transport. These results show that a B₁₂ PET radiopharmaceutical has potential utility for non-invasive imaging.
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CONTACT (COUNTRY ONLY): United States

DECISION STATUS:

ABSTRACT STATUS: submitted [Withdraw](#)
