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

**CONTROL ID:** 2211026

**CONTACT (NAME ONLY):** [Reginald Rogers](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Materials Chemistry - Oral

**SESSION HOST:** Organizer (Kristina Hugar)

**AUTHORS (LAST NAME, FIRST NAME):** Dichiaro, Anthony B.<sup>1</sup>; Litts, Benjamin S.<sup>1</sup>; [Rogers, Reginald E.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2211365

**CONTACT (NAME ONLY):** [Garegin Papoian](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Biochemistry - Oral

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** Papoian, Garegin<sup>1</sup>; Winogradoff, David<sup>1</sup>; Echeverria, Ignacia<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2212021

**CONTACT (NAME ONLY):** [Morton Hoffman](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Oral

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** Hoffman, Morton Z.<sup>1,2</sup>; Lerman, Zafra M.<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2212253

**CONTACT (NAME ONLY):** [Ruth Williams](#)

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Food Chemistry - Oral

**SESSION HOST:** Organizer (Joy Swanson)

**AUTHORS (LAST NAME, FIRST NAME):** [Williams, Ruth E.](#)<sup>1</sup>

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2212366

**CONTACT (NAME ONLY):** [Cristina Dubceac](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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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. 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

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

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

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** [Dubceac, Cristina](#)<sup>1</sup>; Filatov, Alexander S.<sup>1</sup>; Zabula, Alexander V.<sup>1</sup>; Petrukhina, Marina A.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2226113

**CONTACT (NAME ONLY):** [Cristina Dubceac](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 (C<sub>20</sub>H<sub>10</sub>) 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  $\pi$ -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  $\pi$ -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

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

**ABSTRACT SYMPOSIUM NAME:** Inorganic Chemistry - Poster

**SESSION HOST:** Organizer (Andrew Roering)

**AUTHORS (LAST NAME, FIRST NAME):** Spisak, Sarah N.<sup>1</sup>; [Dubceac, Cristina](#)<sup>1</sup>; O'Neil, Natalie J.<sup>1</sup>; Zhou, Zheng<sup>1</sup>; Filatov, Alexander S.<sup>1</sup>; Zabula, Alexander V.<sup>1</sup>; Petrukhina, Marina A.<sup>1</sup>

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**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2215282

**CONTACT (NAME ONLY):** [Ralph Stuart](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**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

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

**ABSTRACT SYMPOSIUM NAME:** Green Labs - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Ralph Stuart)

**AUTHORS (LAST NAME, FIRST NAME):** [Stuart, Ralph](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2212742

**CONTACT (NAME ONLY):** [Mariana Huerta Francos](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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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

**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.

**ABSTRACT SYMPOSIUM NAME:** Materials for Energy - Oral

**SESSION HOST:** Organizer (Nikolay Dimitrov)

**AUTHORS (LAST NAME, FIRST NAME):** [Huerta Francos, Mariana](#)<sup>1</sup>; [Espinosa, Mercedes](#)<sup>2</sup>; [Sanchez, Maria](#)<sup>3</sup>; [Menéndez, Mariluz](#)<sup>4</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2212715

**CONTACT (NAME ONLY):** [Mercedes Espinosa](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

**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.

**ABSTRACT SYMPOSIUM NAME:** Materials for Energy - Oral

**SESSION HOST:** Organizer (Nikolay Dimitrov)

**AUTHORS (LAST NAME, FIRST NAME):** [Espinosa, Mercedes](#)<sup>2</sup>; [Menendez, Mariluz](#)<sup>3</sup>; [Huerta Francos,](#)

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Mariana<sup>1</sup>; Sanchez, Maria<sup>4</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2213145

**CONTACT (NAME ONLY):** [Shashank Jain](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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, 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  $\alpha$ -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

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

2. Chemistry, University Of Vermont, Burlington, VT, United States.

**ABSTRACT SYMPOSIUM NAME:** Environmental Chemistry - Oral

**SESSION HOST:** Organizer (Theodore Dibble)

**AUTHORS (LAST NAME, FIRST NAME):** [Jain, Shashank](#)<sup>2</sup>; Petrucci, Giuseppe<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2213214



APRIL 1, 2015

**CONTACT (NAME ONLY):** [Amanda Aldous](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

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

**ABSTRACT SYMPOSIUM NAME:** Biochemistry - Oral

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** [Aldous, Amanda R.](#)<sup>1</sup>; Kritzer, Joshua<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2213336

**CONTACT (NAME ONLY):** [Geoffrey Coates](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Green Polymers - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Richard Gross)

**AUTHORS (LAST NAME, FIRST NAME):** [Coates, Geoffrey W.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2223197

**CONTACT (NAME ONLY):** [Brian Duffy](#)

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry - Poster

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** [Duffy, Brian](#)<sup>2</sup>; Chisholm, John D.<sup>1</sup>

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2213588

**CONTACT (NAME ONLY):** [Kristin Gublo](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**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

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Oral

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** [Gublo, Kristin I.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2215755

**CONTACT (NAME ONLY):** [Catherine Stephens](#)

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**ABSTRACT STATUS:** resubmitted [Withdraw](#)

**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

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

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

**SESSION HOST:** Organizer (Michael Haaf)

**AUTHORS (LAST NAME, FIRST NAME):** [Stephens, Catherine H.](#)<sup>1</sup>

**ABSTRACT STATUS:** resubmitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2216492

**CONTACT (NAME ONLY):** [Dan Lehnher](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**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

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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

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

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry - Oral

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** [Lehnherr, Dan](#)<sup>1</sup>; Ford, David D.<sup>1</sup>; Rajapaksa, Naomi S.<sup>1</sup>; Jacobsen, Eric N.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2251061

**CONTACT (NAME ONLY):** [Dan Lehnherr](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 structures. For example, *ortho*-arylethynyls 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

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

**ABSTRACT SYMPOSIUM NAME:** Materials Chemistry - Oral

**SESSION HOST:** Organizer (Kristina Hugar)

**AUTHORS (LAST NAME, FIRST NAME):** [Lehnherr, Dan](#)<sup>1</sup>; Alzola, Joaquin M.<sup>1</sup>; Dichtel, William<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

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**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2223728

**CONTACT (NAME ONLY):** [David Hilmey](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** The Legacy of Minority Institution - Oral

**SESSION HOST:** Organizer (Kishore Bagga)

**AUTHORS (LAST NAME, FIRST NAME):** [Hilmey, David G.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2216740

**CONTACT (NAME ONLY):** [Ayten Ay](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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, 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

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

APRIL 1, 2015

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Biochemistry - Poster

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** Muok, Laureana<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2216719

**CONTACT (NAME ONLY):** [Ayten Ay](#)

**ABSTRACT STATUS:** resubmitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Analytical Chemistry - Poster

**SESSION HOST:** Organizer (Jun Wang)

**AUTHORS (LAST NAME, FIRST NAME):** Muok, Christiane<sup>1</sup>; Mahmoud, Fatma<sup>1</sup>

**ABSTRACT STATUS:** resubmitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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**TITLE:** [Bactericidal Effect of Hexamethylenetetramine](#)

**CONTROL ID:** 2268200

**CONTACT (NAME ONLY):** [Ayten Ay](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 organisms<sup>1</sup>. Hexamethylenetetramine (HMTA) is an organic compound with the formula (CH<sub>2</sub>)<sub>6</sub>N<sub>4</sub>. 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

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hydrolyze to formaldehyde and ammonia,<sup>2</sup> 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/](http://www.cdc.gov/ecoli/general/)
2. <http://www.epa.gov/opprd001/inerts/hexamethyl.pdf>

**CONTACT (COUNTRY ONLY):** United States

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

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

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Biochemistry - Poster

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** Rowser-Grohol, Lemire<sup>2</sup>; Dingra, Nin N.<sup>1</sup>; McCue, Kaitlyn<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2217746

**CONTACT (NAME ONLY):** [Ayten Ay](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

#### 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

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

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Food Chemistry - Poster

**SESSION HOST:** Organizer (Joy Swanson)

**AUTHORS (LAST NAME, FIRST NAME):** Garcia Maso, Claudia E.<sup>1</sup>; Alquraishi, Rasha<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2217816

**CONTACT (NAME ONLY):** [Juan Duchimaza Heredia](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

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**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  $\beta$ -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

**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.

**ABSTRACT SYMPOSIUM NAME:** Physical Chemistry - Oral

**SESSION HOST:** Organizer (Sarah Nathan)

**AUTHORS (LAST NAME, FIRST NAME):** Duchimaza Heredia, Juan<sup>1</sup>; Yan, KaKing<sup>1</sup>; Sadow, Aaron D.<sup>3</sup>; Gordon, Mark S.<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2218598

**CONTACT (NAME ONLY):** [Kamruz Zaman](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Oral

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** Zaman, Kamruz<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)



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**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2219752

**CONTACT (NAME ONLY):** [Todd Krauss](#)

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**ABSTRACT BODY:**

**Abstract:** Homogeneous molecular-based systems for light-driven reduction of protons to H<sub>2</sub> 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 (DHLA) as the solar energy harvester and a soluble Ni<sup>2+</sup>-DHDLA 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

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

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

**SESSION HOST:** Organizer (Luis Velarde)

**AUTHORS (LAST NAME, FIRST NAME):** [Krauss, Todd](#)<sup>1</sup>; [Qiu, Fen](#)<sup>1</sup>; [Eisenberg, Richard](#)<sup>1</sup>; [Han, Zhiji](#)<sup>1</sup>; [Holland, Patrick L.](#)<sup>2</sup>; [Liu, Cunming](#)<sup>1</sup>; [Peterson, Jeffrey](#)<sup>1</sup>

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2277927

**CONTACT (NAME ONLY):** [Nidia Trejo](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**Abstract:** In this study carboxylic acid coated iron oxide nanoparticles (CA-Fe<sub>3</sub>O<sub>4</sub> 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

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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 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

**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.

**ABSTRACT SYMPOSIUM NAME:** Materials Chemistry - Poster

**SESSION HOST:** Organizer (Kristina Hugar)

**AUTHORS (LAST NAME, FIRST NAME):** Trejo, Nidia K.<sup>1</sup>; Frey, Margaret<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2222118

**CONTACT (NAME ONLY):** [Catherine Lavin](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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- $\pi$  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

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

**ABSTRACT SYMPOSIUM NAME:** Inorganic Chemistry - Oral

**SESSION HOST:** Organizer (Andrew Roering)

**AUTHORS (LAST NAME, FIRST NAME):** Lavin, Catherine M.<sup>1</sup>; Goos, Alan G.<sup>1</sup>; Allis, Damian G.<sup>1</sup>; Ruhlandt-Senge, Karin<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2223687

**CONTACT (NAME ONLY):** [William Dichtel](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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-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

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

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

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** [Dichtel, William](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2224847

**CONTACT (NAME ONLY):** [Kent Marshall](#)

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**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 methods reported for their construction. This project was based on the procedure of Davidson and Shovronek<sup>1</sup> 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 hydrophobic 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.

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

**CONTACT (COUNTRY ONLY):** United States

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

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Organic Chemistry - Poster

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** [Marshall, Kent S.](#)<sup>1</sup>

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**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2225924

**CONTACT (NAME ONLY):** [Melissa Charlton-Smith](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

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

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

**ABSTRACT SYMPOSIUM NAME:** Green Labs - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Ralph Stuart)

**AUTHORS (LAST NAME, FIRST NAME):** [Charlton-Smith, Melissa](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2225973

**CONTACT (NAME ONLY):** [Ellen Sweet](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

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**ABSTRACT SYMPOSIUM NAME:** Green Labs - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Ralph Stuart)

**AUTHORS (LAST NAME, FIRST NAME):** [Sweet, Ellen](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2227508

**CONTACT (NAME ONLY):** [Evgeny Dikarev](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 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

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

**ABSTRACT SYMPOSIUM NAME:** Materials for Energy - Oral

**SESSION HOST:** Organizer (Nikolay Dimitrov)

**AUTHORS (LAST NAME, FIRST NAME):** [Dikarev, Evgeny](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2228067

**CONTACT (NAME ONLY):** [Wei Zhang](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**Abstract:** Organocatalysis has advantages such as free of toxic heavy metals, mild reaction conditions, novel mode 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 fluorinated organocatalysis provides an efficient way to address the issue. In addition to phase tag separation, the stereoelectronic effect of the fluorinated 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

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addition, Robinson annulation, and one-pot addition/cyclization for asymmetric synthesis of biologically interested molecules.

**CONTACT (COUNTRY ONLY):** United States

**INSTITUTIONS (ALL):** 1. University of MA Boston, Dorchester, MA, United States.  
2. Nanjing university of Science and Technology, Nanjing, Jiangsu, China.

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry - Oral - INVITED ONLY

**SESSION HOST:** Organizer (George Ruger)

**AUTHORS (LAST NAME, FIRST NAME):** Zhang, Wei<sup>1</sup>; Hung, Xin<sup>1</sup>; Yi, Wenbin<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2229645

**CONTACT (NAME ONLY):** [Michael Cann](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**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

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

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry - Oral - INVITED ONLY

**SESSION HOST:** Organizer (George Ruger)

**AUTHORS (LAST NAME, FIRST NAME):** Cann, Michael C.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2228298

**CONTACT (NAME ONLY):** [Adiel Coca](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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.

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**CONTACT (COUNTRY ONLY):** United States

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

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Medicinal Chemistry - Poster

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** [Coca, Adiel](#)<sup>1</sup>; Roberts, Elizabeth<sup>2</sup>; Dudley, Joshua<sup>1</sup>; Feinn, Liana A.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2228308

**CONTACT (NAME ONLY):** [Adiel Coca](#)

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry - Oral

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** Dudley, Joshua<sup>1</sup>; Feinn, Liana A.<sup>1</sup>; [Coca, Adiel](#)<sup>1</sup>

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2228356

**CONTACT (NAME ONLY):** [Peter Wipf](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

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



APRIL 1, 2015

ONLY

**SESSION HOST:** Organizer (Catherine Malele)|Organizer (Maurice Odago)

**AUTHORS (LAST NAME, FIRST NAME):** Wipf, Peter<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2228819

**CONTACT (NAME ONLY):** [Charles Jakobsche](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry - Poster

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** Jakobsche, Charles E.<sup>1</sup>; Wang, Linshu<sup>1</sup>; McCarthy, Blaine G.<sup>1</sup>; MacArthur, Nicholas S.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Preferred

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

**CONTROL ID:** 2229078

**CONTACT (NAME ONLY):** [Jarod Grossman](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 H<sub>2</sub>O<sub>2</sub> 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

APRIL 1, 2015

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

**ABSTRACT SYMPOSIUM NAME:** Environmental Chemistry - Oral

**SESSION HOST:** Organizer (Theodore Dibble)

**AUTHORS (LAST NAME, FIRST NAME):** [Grossman, Jarod](#)<sup>1</sup>; Kahan, Tara F.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2229177

**CONTACT (NAME ONLY):** [J Brenna](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

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

**SESSION HOST:** Organizer (Joy Swanson)

**AUTHORS (LAST NAME, FIRST NAME):** [Brenna, J](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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**TITLE:** [Design of the first volatile precursors for low-temperature synthesis of up-conversion NaREF<sub>4</sub> materials.](#)

**CONTROL ID:** 2247191

**CONTACT (NAME ONLY):** [Matthew Barry](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**Abstract:** A new approach to design single-source precursors for the most efficient up- and down-conversion

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materials is reported. Heterobimetallic fluorinated  $\beta$ -diketonates  $\text{NaRE}(\beta\text{-dik})_4$  (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 diketonate precursors affords target fluoride materials in the form of  $\alpha$ -cubic or  $\beta$ -hexagonal  $\text{NaREF}_4$  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

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

**ABSTRACT SYMPOSIUM NAME:** Inorganic Chemistry - Oral

**SESSION HOST:** Organizer (Andrew Roering)

**AUTHORS (LAST NAME, FIRST NAME):** Barry, Matthew C.<sup>1</sup>; Dikarev, Evgeny<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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**TITLE:** [Titanium minerals and biochemistry](#)

**CONTROL ID:** 2229772

**CONTACT (NAME ONLY):** [Ann Valentine](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

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

**SESSION HOST:** Organizer (Emily Garcia Segal)|Organizer (Kathryn Cole)

**AUTHORS (LAST NAME, FIRST NAME):** Valentine, Ann<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2230612

**CONTACT (NAME ONLY):** [John Henion](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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(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.

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

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

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

**SESSION HOST:** Organizer (Joy Swanson)

**AUTHORS (LAST NAME, FIRST NAME):** Henion, John D.<sup>1</sup>; Eikel, Daniel<sup>1</sup>; Sousou, Nigel<sup>1</sup>; Hao, Changtong<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2251530

**CONTACT (NAME ONLY):** [Robert Stewart](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

2. Chemistry, Pennsylvania State University, State College, PA, United States.

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**ABSTRACT SYMPOSIUM NAME:** Physical Chemistry - Oral

**SESSION HOST:** Organizer (Sarah Nathan)

**AUTHORS (LAST NAME, FIRST NAME):** [Stewart, Robert J.](#)<sup>1</sup>; Asbury, John B.<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2231173

**CONTACT (NAME ONLY):** [Nicholas Kotov](#)

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**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 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

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

2. Chemical Engineering, University of Michigan, Ann Arbor, MI, United States.

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

**SESSION HOST:** Organizer (Luis Velarde)

**AUTHORS (LAST NAME, FIRST NAME):** [Kotov, Nicholas](#)<sup>1</sup>; Kim, Yoonseob<sup>2</sup>; Tung, Siu O.<sup>1</sup>; Yeom, Bongjun<sup>1</sup>; Shyu, Terry<sup>1</sup>

**ABSTRACT STATUS:** decisioned\_accepted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2232061

**CONTACT (NAME ONLY):** [Alexander Bayden](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

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**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

**INSTITUTIONS (ALL):** 1. CMD Bioscience, 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.

**ABSTRACT SYMPOSIUM NAME:** Biochemistry - Oral

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** Bayden, Alexander S.<sup>1</sup>; Yakovlev, Vasily A.<sup>2</sup>; Mikkelsen, Ross B.<sup>3</sup>; Kellogg, Glen E.<sup>4</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2233424

**CONTACT (NAME ONLY):** [Adam Whalley](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

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

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** [Whalley, Adam](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

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**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2233563

**CONTACT (NAME ONLY):** [Patrick Cost](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

**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.

**ABSTRACT SYMPOSIUM NAME:** Physical Chemistry - Poster

**SESSION HOST:** Organizer (Sarah Nathan)

**AUTHORS (LAST NAME, FIRST NAME):** [Cost, Patrick](#)<sup>2</sup>; Collison, Christopher<sup>1</sup>; Cody, Jeremy A.<sup>1</sup>; Zheng, Chenyu<sup>1</sup>; Jalan, Ishita<sup>1</sup>; Cona, Brandon<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Preferred

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

**CONTROL ID:** 2234330

**CONTACT (NAME ONLY):** [Xinyin Jiang](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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



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of perinatal health.  
(Advances in Food Chemistry and Nutritional Biochemistry Symposium)

**CONTACT (COUNTRY ONLY):**

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

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

**SESSION HOST:** Organizer (Joy Swanson)

**AUTHORS (LAST NAME, FIRST NAME):** [Jiang, Xinyin](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2265029

**CONTACT (NAME ONLY):** [Dominic Ventura](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Poster

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** [Ventura, Dominic](#)<sup>1</sup>; Poblocki, Angela<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2245913

**CONTACT (NAME ONLY):** [Christopher Nomura](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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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

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

**ABSTRACT SYMPOSIUM NAME:** Green Polymers - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Richard Gross)

**AUTHORS (LAST NAME, FIRST NAME):** Nomura, Christopher T.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2247382

**CONTACT (NAME ONLY):** [Gang Wu](#)

**ABSTRACT STATUS:** resubmitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Materials for Energy - Oral

**SESSION HOST:** Organizer (Nikolay Dimitrov)

**AUTHORS (LAST NAME, FIRST NAME):** [Wu, Gang](#)<sup>1</sup>

**ABSTRACT STATUS:** resubmitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2248457

**CONTACT (NAME ONLY):** [Gerald Takacs](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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.

**CONTACT (COUNTRY ONLY):** United States

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Poster

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** [Bailey, Alla](#)<sup>1</sup>; Li, Xinyun<sup>1</sup>; Toro, Marc<sup>1</sup>; Mastrangelo, Brenda<sup>1</sup>; Takacs, Gerald A.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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**TITLE:** [Water adsorption and oxidation on anatase TiO<sub>2</sub>](#)

**CONTROL ID:** 2248371

**CONTACT (NAME ONLY):** [Annabella Selloni](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**Abstract:** Semiconductor-based photocatalysis for the degradation of pollutants and the decomposition of water into H<sub>2</sub> and O<sub>2</sub> has been an important area of research for decades. Due to its abundance, non-toxicity,

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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 (TiO<sub>2</sub>). I shall discuss recent applications of first principles electronic structure calculations and molecular dynamics simulations to understand materials properties and reaction mechanisms relevant to TiO<sub>2</sub>-based photocatalysis, with focus on water adsorption and the mechanism of water oxidation at the surface of anatase TiO<sub>2</sub>.

**CONTACT (COUNTRY ONLY):** United States

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

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

**SESSION HOST:** Organizer (Luis Velarde)

**AUTHORS (LAST NAME, FIRST NAME):** Selloni, Annabella<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2250543

**CONTACT (NAME ONLY):** [Edward Brush](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Oral

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** Brush, Edward J.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2252753

**CONTACT (NAME ONLY):** [Michael Campbell](#)

APRIL 1, 2015

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 reported for sensors based on carbon nanotubes (CNTs), conductive organic polymers, and metal chalcogenides (*e.g.*  $\text{MoS}_2$ ). 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

**INSTITUTIONS (ALL):** 1. MIT, Cambridge, MA, United States.  
2. Building 2-321, MIT, Cambridge, MA, United States.  
3. Chemistry, MIT, Cambridge, MA, United States.

**ABSTRACT SYMPOSIUM NAME:** Inorganic Chemistry - Oral

**SESSION HOST:** Organizer (Andrew Roering)

**AUTHORS (LAST NAME, FIRST NAME):** [Campbell, Michael G.](#)<sup>3</sup>; Sheberla, Dennis<sup>3</sup>; Liu, Sophie<sup>3</sup>; Swager, Timothy M.<sup>1</sup>; Dinca, Mircea<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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**TITLE:**

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

**CONTROL ID:** 2254913

**CONTACT (NAME ONLY):** [John Evans](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

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

**SESSION HOST:** Organizer (Emily Garcia Segal)|Organizer (Kathryn Cole)

**AUTHORS (LAST NAME, FIRST NAME):** [Evans, John S.](#)<sup>1</sup>

APRIL 1, 2015

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2254937

**CONTACT (NAME ONLY):** [Lars Gundlach](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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.

In the first part excited state dynamics of a phlorin macrocycle attached to TiO<sub>2</sub> nanoparticles will be discussed. The dynamics was measured after excitation to the S<sub>1</sub> and the S<sub>2</sub> 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 S<sub>2</sub> state, while the S<sub>1</sub> does not show ultrafast HET.

**CONTACT (COUNTRY ONLY):** United States

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

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

**SESSION HOST:** Organizer (Luis Velarde)

**AUTHORS (LAST NAME, FIRST NAME):** [Gundlach, Lars](#)<sup>1</sup>; [Nieto-Pescador, Jesus](#)<sup>1</sup>; [Abraham, Baxter](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2255304

**CONTACT (NAME ONLY):** [Valerie Lopez](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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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

**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.

**ABSTRACT SYMPOSIUM NAME:** Inorganic Chemistry - Oral

**SESSION HOST:** Organizer (Andrew Roering)

**AUTHORS (LAST NAME, FIRST NAME):** Lopez, Valerie<sup>1</sup>; Lijewski, Matthew D.<sup>1</sup>; Bampoh, Victoria N.<sup>3</sup>; Ruhlandt-Senge, Karin<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2255429

**CONTACT (NAME ONLY):** [Trevor Douglas](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

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

**SESSION HOST:** Organizer (Emily Garcia Segal)|Organizer (Kathryn Cole)

**AUTHORS (LAST NAME, FIRST NAME):** Douglas, Trevor<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only



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**TITLE:** [\[Lewis Acid\]<sup>+</sup>\[Co\(CO\)<sub>4</sub>\]<sup>-</sup> Catalysts for Enantio- and Regioselective Transformations of Epoxides](#)

**CONTROL ID:** 2257682

**CONTACT (NAME ONLY):** [Jessica Lamb](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**Abstract:** This talk addresses recent advances in epoxide transformations using catalysts of the form [Lewis acid]<sup>+</sup>[Co(CO)<sub>4</sub>]<sup>-</sup>. 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

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

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry - Oral

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** [Lamb, Jessica R.](#)<sup>2</sup>; Coates, Geoffrey W.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2257841

**CONTACT (NAME ONLY):** [Suzanne O'Handley](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Biochemistry - Poster

**SESSION HOST:** Organizer (Katherine Hicks)

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**AUTHORS (LAST NAME, FIRST NAME):** [Dass, Lucinda<sup>1</sup>](#); [Moreno, Isreal<sup>1</sup>](#); [O'Handley, Suzanne F.<sup>1</sup>](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2258527

**CONTACT (NAME ONLY):** [Suzanne O'Handley](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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).

**CONTACT (COUNTRY ONLY):** United States

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

**ABSTRACT SYMPOSIUM NAME:** Biochemistry - Poster

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** [Moreno, Isreal<sup>1</sup>](#); [Dass, Lucinda<sup>1</sup>](#); [Ramirez, Sebastian A.<sup>1</sup>](#); [Hill, Jacqueline<sup>1</sup>](#); [Blake, Kimbria<sup>1</sup>](#); [Thomson, Joshua<sup>1</sup>](#); [O'Handley, Suzanne F.<sup>1</sup>](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2258020

**CONTACT (NAME ONLY):** [Kimberly O'Brien](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 (<sup>58</sup>Fe). 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

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the labeled  $^{58}\text{Fe}$ -pork fed as chili, and the other test dose was administered as ferrous sulfate ( $^{57}\text{FeSO}_4$ ). 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 ( $^{58}\text{Fe}$ ) compared to  $^{57}\text{Fe}$  (non-heme Fe) ( $47.7 \pm 14.4$  vs.  $40.0 \pm 13.2\%$ ,  $p=0.04$ ,  $n=18$ ). Of interest, neonates at birth had a significantly greater percentage of maternally absorbed  $^{58}\text{Fe}$  compared to  $^{57}\text{Fe}$  ( $5.4 \pm 2.4$  vs.  $4.0 \pm 1.6\%$ ;  $p<0.0001$ ) suggesting a preferential fetal use of maternally ingested Fe derived from a dietary, animal-based heme source. The net amount of  $^{57}\text{Fe}$  ( $p=0.002$ ) and  $^{58}\text{Fe}$  ( $p=0.004$ ) 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 ( $p=0.003$ ,  $r^2=0.43$ ). 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

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

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

**SESSION HOST:** Organizer (Joy Swanson)

**AUTHORS (LAST NAME, FIRST NAME):** O'Brien, Kimberly O.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2258581

**CONTACT (NAME ONLY):** [Ian Rhile](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 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

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Poster

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** Rhile, Ian<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Preferred

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

**CONTROL ID:** 2258933

**CONTACT (NAME ONLY):** [Markus Hoffmann](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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<sub>2</sub>mim][MeSO<sub>3</sub>]) 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.<sup>1</sup> 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.<sup>2</sup> While the concentration dependence of a number of measured physical properties is very similar to [C<sub>2</sub>mim][MeSO<sub>3</sub>] the temperature dependence shows marked differences with respect to activation energies for a number of physical properties as well as T<sub>1</sub>-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

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

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry - Oral - INVITED ONLY

**SESSION HOST:** Organizer (George Ruger)

**AUTHORS (LAST NAME, FIRST NAME):** [Hoffmann, Markus M.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2259218

**CONTACT (NAME ONLY):** [Geoffrey Peterson](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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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

**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.

**ABSTRACT SYMPOSIUM NAME:** Environmental Chemistry - Oral

**SESSION HOST:** Organizer (Theodore Dibble)

**AUTHORS (LAST NAME, FIRST NAME):** Peterson, Geoffrey<sup>1</sup>; Jones, Timothy <sup>2</sup>; Rispoli, Diana<sup>2</sup>; Niri, Vadoud<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2259385

**CONTACT (NAME ONLY):** [Edurne Gonzalez](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Materials Chemistry - Poster

**SESSION HOST:** Organizer (Kristina Hugar)

**AUTHORS (LAST NAME, FIRST NAME):** Gonzalez, Edurne<sup>1</sup>; Buttaro, Larissa<sup>1</sup>; Frey, Margaret<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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APRIL 1, 2015

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

**CONTROL ID:** 2260926

**CONTACT (NAME ONLY):** [Andrei Yudin](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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, 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

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

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

**SESSION HOST:** Organizer (Catherine Malele)|Organizer (Maurice Odago)

**AUTHORS (LAST NAME, FIRST NAME):** [Yudin, Andrei K.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2261861

**CONTACT (NAME ONLY):** [Jinglin Fu](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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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

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

**ABSTRACT SYMPOSIUM NAME:** Biochemistry - Oral

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** [Fu, Jinglin](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2262624

**CONTACT (NAME ONLY):** [Joseph Kraai](#)

**ABSTRACT STATUS:** resubmitted [Withdraw](#)

**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  $7.5 \pm 0.1$   $\mu$ M, similar to the natural substrate which has a  $K_d$  of  $11.2 \pm 1.5$   $\mu$ 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

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



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

**ABSTRACT SYMPOSIUM NAME:** Biochemistry - Poster

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** [Kraai, Joseph](#)<sup>1</sup>; Christie, Crissana<sup>1</sup>; Hicks, Katherine<sup>2</sup>

**ABSTRACT STATUS:** resubmitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2263116

**CONTACT (NAME ONLY):** [Narayan Das](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 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

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

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

**ABSTRACT SYMPOSIUM NAME:** Materials for Energy - Oral

**SESSION HOST:** Organizer (Nikolay Dimitrov)

**AUTHORS (LAST NAME, FIRST NAME):** [Das, Narayan C.](#)<sup>1</sup>; Ganguly, Sayan<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2265130

APRIL 1, 2015

**CONTACT (NAME ONLY):** [Courtney Kellogg](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**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

**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.

**ABSTRACT SYMPOSIUM NAME:** Biochemistry - Poster

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** [Kellogg, Courtney](#)<sup>1</sup>; Blake, Kimbria<sup>1</sup>; O'Handley, Suzanne F.<sup>1</sup>; Gehret, Austin<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2266445

**CONTACT (NAME ONLY):** [Elena Margine](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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  $\pi$ -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

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

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

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** [Margine, Elena](#)<sup>1</sup>

APRIL 1, 2015

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2266651

**CONTACT (NAME ONLY):** [Timothy Vaden](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Physical Chemistry - Oral

**SESSION HOST:** Organizer (Sarah Nathan)

**AUTHORS (LAST NAME, FIRST NAME):** Yu, Lei<sup>2</sup>; [Vaden, Timothy D.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2266660

**CONTACT (NAME ONLY):** [Han Jia](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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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):**

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

**ABSTRACT SYMPOSIUM NAME:** Biochemistry - Oral

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** [Jia, Han](#)<sup>1</sup>; Farinas, Edgardo T.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2267076

**CONTACT (NAME ONLY):** [Peter Csernica](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

**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.

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Materials Chemistry - Poster

**SESSION HOST:** Organizer (Kristina Hugar)

**AUTHORS (LAST NAME, FIRST NAME):** [Csernica, Peter](#)<sup>3</sup>; McKone, James R.<sup>3</sup>; Abruna, Hector D.<sup>1</sup>; DiSalvo, Francis J.<sup>2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Preferred

APRIL 1, 2015

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

**CONTROL ID:** 2268535

**CONTACT (NAME ONLY):** [Samuel Lothridge](#)

**ABSTRACT STATUS:** resubmitted [Withdraw](#)

**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-dihydroxypyridine 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.

**CONTACT (COUNTRY ONLY):** United States

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

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Biochemistry - Poster

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** [Lothridge, Samuel](#)<sup>1</sup>; Simone, Gregory<sup>1</sup>; Hicks, Katherine<sup>1</sup>

**ABSTRACT STATUS:** resubmitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2268709

**CONTACT (NAME ONLY):** [Brandon Tiegs](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Materials Chemistry - Poster

**SESSION HOST:** Organizer (Kristina Hugar)

**AUTHORS (LAST NAME, FIRST NAME):** [Tiegs, Brandon J.](#)<sup>1</sup>; Coates, Geoffrey W.<sup>1</sup>

APRIL 1, 2015

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2268900

**CONTACT (NAME ONLY):** [Wei Feng Zhen](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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):**

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

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Biochemistry - Poster

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** [Zhen, Wei Feng](#)<sup>1</sup>; Hicks, Katherine<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Only

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

**CONTROL ID:** 2269651

**CONTACT (NAME ONLY):** [Arunkumar Sharma](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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existing experiments into discovery oriented experiments, there is no significant burden to the laboratory budget.

**CONTACT (COUNTRY ONLY):** United States

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Oral

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** Sharma, Arunkumar K.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2270019

**CONTACT (NAME ONLY):** [Alexander Nazarenko](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 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

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Oral

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** Nazarenko, Alexander Y.<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)



APRIL 1, 2015

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2270628

**CONTACT (NAME ONLY):** [Daniel Rabinovich](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

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

**SESSION HOST:** Organizer (Peter Baran)

**AUTHORS (LAST NAME, FIRST NAME):** [Rabinovich, Daniel](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2270645

**CONTACT (NAME ONLY):** [Daniel Rabinovich](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

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

APRIL 1, 2015

**SESSION HOST:** Organizer (Michael Haaf)

**AUTHORS (LAST NAME, FIRST NAME):** [Rabinovich, Daniel](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2270686

**CONTACT (NAME ONLY):** [Ting Chen](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Environmental Chemistry - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Theodore Dibble)

**AUTHORS (LAST NAME, FIRST NAME):** [Chen, Ting](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2271609

**CONTACT (NAME ONLY):** [Gita Perkins](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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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 it's 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

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

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Poster

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** Perkins, Gita<sup>1,2</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Preferred

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

**CONTROL ID:** 2274207

**CONTACT (NAME ONLY):** [Jeffrey Whitford](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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**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

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

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry - Oral - INVITED ONLY

**SESSION HOST:** Organizer (George Ruger)

**AUTHORS (LAST NAME, FIRST NAME):** [Whitford, Jeffrey](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2274559

**CONTACT (NAME ONLY):** [Timothy Owen](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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 IC<sub>50</sub> of 5X10<sup>-6</sup> 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<sub>N</sub>Ar 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

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

**ABSTRACT SYMPOSIUM NAME:** Biochemistry - Poster

**SESSION HOST:** Organizer (Katherine Hicks)

**AUTHORS (LAST NAME, FIRST NAME):** [Owen, Timothy](#)<sup>1</sup>; [Ngoje, George](#)<sup>1</sup>; [Callahan, Brian P.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Poster Preferred

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

**CONTROL ID:** 2274747

**CONTACT (NAME ONLY):** [Keith Baessler](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

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**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

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Oral

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** [Baessler, Keith A.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Preferred

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

**CONTROL ID:** 2277692

**CONTACT (NAME ONLY):** [Swarna Basu](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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

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

**ABSTRACT SYMPOSIUM NAME:** Chemical Education - Oral

**SESSION HOST:** Organizer (Jenny Novotny)

**AUTHORS (LAST NAME, FIRST NAME):** [Basu, Swarna M.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2278402

**CONTACT (NAME ONLY):** [Andrey Rogachev](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**ABSTRACT BODY:**

**Abstract:** Recent experimental achievements in chemistry of reduced corannulene (C<sub>20</sub>H<sub>10</sub>, the smallest buckybowl) 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 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<sup>+</sup> to Na<sup>+</sup>, K<sup>+</sup>, Rb<sup>+</sup>, and Cs<sup>+</sup>) 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

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

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

**SESSION HOST:** Organizer (Catherine DeBlase)

**AUTHORS (LAST NAME, FIRST NAME):** [Rogachev, Andrey Y.](#)<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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

**CONTROL ID:** 2278510

**CONTACT (NAME ONLY):** [Nilay Hazari](#)

**ABSTRACT STATUS:** submitted [Withdraw](#)

**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.

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**CONTACT (COUNTRY ONLY):** United States

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

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

**SESSION HOST:** Organizer (Peter Baran)

**AUTHORS (LAST NAME, FIRST NAME):** Hazari, Nilay<sup>1</sup>

**ABSTRACT STATUS:** submitted [Withdraw](#)

**PRESENTATION TYPE:** Oral Only

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