

March 9, 2015 NERM Abstract Submissions

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

CONTROL ID: 2211026

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

ABSTRACT STATUS:

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)

TITLE: [A Study of Hydrophobic vs. Hydrophilic Components 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

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 Shovronek¹ which involved a one pot reaction between 1 eq. of amide, 1.1 eq. of acid anhydride and 1 eq. of acid chloride to prevent nitrile formation. The current project was to study the relationship between the hydrophobic side chain and the hydrophilic carbonyl moiety during imide formation. At what carbon size does the 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.

¹D. 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)

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

CONTROL ID: 2223197

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

ABSTRACT STATUS: decisioned_accepted

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)

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

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.

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ABSTRACT SYMPOSIUM NAME: Food Chemistry - Oral

SESSION HOST: Organizer (Joy Swanson)

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

CONTROL ID: 2216719

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

ABSTRACT STATUS: re

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)

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

CONTROL ID: 2215755

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

ABSTRACT STATUS: re

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)

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

CONTROL ID: 2234330

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

ABSTRACT STATUS:

ABSTRACT BODY:

Abstract: Choline is an essential nutrient often grouped with the B vitamins. Choline biomolecules participate in various biological processes including growth and development, cellular membrane formation, neurotransmission and one-carbon metabolism. The demand for choline increases substantially during pregnancy. Dietary recommendation for choline has been established at 450 mg/d in the form of Adequate Intake for pregnant women, yet the actual requirement of this nutrient is unknown. Supplementing third trimester pregnant women with extra choline (930mg/d versus 480 mg/d) beneficially influences maternal vasculature and fetal markers of stress.

Choline supplementation improves maternal glucose tolerance and prevents fetal overgrowth in part by activating placental fat catabolism in mice with high-fat diet-induced gestational diabetes. Maternal choline supplementation may be an effective prophylaxis for the improvement of perinatal health.

(Advances in Food Chemistry and Nutritional Biochemistry Symposium)

CONTACT (COUNTRY ONLY):

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)

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

CONTROL ID: 2233424

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

ABSTRACT STATUS:

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.

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

SESSION HOST: Organizer (Catherine DeBlase)

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

CONTROL ID: 2231173

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

ABSTRACT STATUS:

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)

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:

ABSTRACT BODY:

Abstract: An automated surface-sampling technique called liquid extraction surface analysis (LESA), coupled with infusion nano-electrospray high-resolution mass spectrometry and tandem mass spectrometry (MS/MS), will be described and applied to the qualitative determination of surface chemical residues resulting from the artificial spraying of selected fresh fruits and vegetables with representative pesticides. When the surface of a spinach leaf was analyzed by LESA, trace levels of diazinon were readily detected on the spinach purchased directly from a supermarket before they were sprayed with the five-pesticide mixture. A 30 s rinse under hot running tap water appeared to quantitatively remove all remaining residues of this pesticide. This report showed that representative

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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)

TITLE: [Titanium minerals and biochemistry](#)

CONTROL ID: 2229772

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

ABSTRACT STATUS:

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)

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:

ABSTRACT BODY:

Abstract: In 2009 planetary boundaries were proposed that define a "safe operating space for humanity." The nine

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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)

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:

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)

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

CONTROL ID: 2228819

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

ABSTRACT STATUS:

ABSTRACT BODY:

Abstract: N-Nitrosoacetamides undergo thermal rearrangements into acetates, and the relative ease and efficiency

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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)

TITLE: [From Strained Carbocycles to Heterocycles](#)

CONTROL ID: 2228356

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

ABSTRACT STATUS:

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 ONLY

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

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

CONTROL ID: 2228308

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

ABSTRACT STATUS:

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)

TITLE: [Antibiotic Activity of 5-Substituted 1H-Tetrazoles](#)

CONTROL ID: 2228298

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

ABSTRACT STATUS:

ABSTRACT BODY:

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

CONTACT (COUNTRY ONLY): United States

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)

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

CONTROL ID: 2228067

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

ABSTRACT STATUS:

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 fluororous organocatalysis provides an efficient way to address the issue. In addition to phase tag separation, the stereoelectronic effect of the fluororous chain can be used to modify the reactivity and selectivity of the catalysts. This presentation highlights our recent effort on the development of recyclable organocatalyst-promoted fluorination, Michael addition, Robinson annulation, and one-pot addition/cyclization for asymmetric synthesis of biologically interested molecules.

CONTACT (COUNTRY ONLY): United States

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)

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

CONTROL ID: 2227508

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

ABSTRACT STATUS:

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)

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

CONTROL ID: 2226113

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

ABSTRACT STATUS:

ABSTRACT BODY:

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

CONTACT (COUNTRY ONLY): United States

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

ABSTRACT SYMPOSIUM NAME: Inorganic Chemistry - Poster

SESSION HOST: Organizer (Andrew Roering)

TITLE: [A Strategy with Lab Ventilation Management to Enhance Sustainability](#)

CONTROL ID: 2225973

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

ABSTRACT STATUS:

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.

ABSTRACT SYMPOSIUM NAME: Green Labs - Oral - INVITED ONLY

SESSION HOST: Organizer (Ralph Stuart)

TITLE: [Green Chemistry & Chemical Hygiene, a marriage made in an undergraduate program?](#)

CONTROL ID: 2225924

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

ABSTRACT STATUS:

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)

TITLE: [A Community-Based Learning Archetype for Science : Native American Health and Medicine](#)

CONTROL ID: 2223728

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

ABSTRACT STATUS:

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

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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)

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

CONTROL ID: 2223687

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

ABSTRACT STATUS:

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)

TITLE: [Semiconductor Nanocrystals for Robust and Efficient Solar Hydrogen Production](#)

CONTROL ID: 2219752

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

ABSTRACT STATUS:

ABSTRACT BODY:

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

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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)

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

CONTROL ID: 2218598

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

ABSTRACT STATUS:

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)

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

CONTROL ID: 2217746

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

ABSTRACT STATUS:

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

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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)

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

CONTROL ID: 2216740

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

ABSTRACT STATUS:

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.

ABSTRACT SYMPOSIUM NAME: Undergraduate Biochemistry - Poster

SESSION HOST: Organizer (Katherine Hicks)

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

CONTROL ID: 2215282

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

ABSTRACT STATUS:

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.

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ABSTRACT SYMPOSIUM NAME: Green Labs - Oral - INVITED ONLY

SESSION HOST: Organizer (Ralph Stuart)

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

CONTROL ID: 2213588

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

ABSTRACT STATUS:

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)

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

CONTROL ID: 2213336

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

ABSTRACT STATUS:

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)

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

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CONTROL ID: 2213214

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

ABSTRACT STATUS:

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)

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:

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 α -pinene-derived SOA. This method allows for the real-time determination of SOA phase state for polydisperse aerosols, permitting studies of the relationship between SOA phase, oxidative formation and chemical aging. The proposed method allowed us to evaluate the impact that various parameters, such as SOA precursor, relative humidity, oxidation type and mixing ratio, can have on the phase of atmospheric organic particulate.

CONTACT (COUNTRY ONLY): United States

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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)

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:

ABSTRACT BODY:

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

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

CONTACT (COUNTRY ONLY): Mexico

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)

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

CONTROL ID: 2212715

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

ABSTRACT STATUS:

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)

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

CONTROL ID: 2212366

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

ABSTRACT STATUS:

ABSTRACT BODY:

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

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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)

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:

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)

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

CONTROL ID: 2211365

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

ABSTRACT STATUS:

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

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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 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)
