

CONTROL ID: 2211026

TITLE: Adsorption of organic-based pesticides from aqueous solutions using lightweight carbon aerogels

CONTACT (NAME ONLY): Reginald Rogers

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.

SYMPOSIUM NAME: Materials Chemistry - Oral

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2212253

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

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.

SYMPOSIUM NAME: Food Chemistry - Oral

CONTACT (COUNTRY ONLY): Jamaica

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

CONTROL ID: 2216719

TITLE: GC-MS volatile organic compound analysis in drinking water samples

CONTACT (NAME ONLY): Ayten Ay

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.

SYMPOSIUM NAME: Undergraduate Analytical Chemistry - Poster

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2226113

TITLE: Charging fragments of fullerenes and nanotubes with multiple electrons: X-ray structural highlights

CONTACT (NAME ONLY): Cristina Dubceac

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.

SYMPOSIUM NAME: Inorganic Chemistry - Poster

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2225973

TITLE: A Strategy with Lab Ventilation Management to Enhance Sustainability

CONTACT (NAME ONLY): Ellen Sweet

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.

SYMPOSIUM NAME: Green Labs - Oral - INVITED ONLY

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2225924

TITLE: Green Chemistry & Chemical Hygiene, a marriage made in an undergraduate program?

CONTACT (NAME ONLY): Melissa Charlton-Smith

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.

SYMPOSIUM NAME: Green Labs - Oral - INVITED ONLY

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2224847

TITLE: A Study of Hydrophobic vs. Hydrophilic Components of Molecules in C3 to C10 Acyclic Imide Synthesis: An Undergraduate Research Project

CONTACT (NAME ONLY): Kent Marshall

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).

SYMPOSIUM NAME: Undergraduate Organic Chemistry - Poster

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2223728

TITLE: A Community-Based Learning Archetype for Science : Native American Health and Medicine

CONTACT (NAME ONLY): David Hilmey

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.

SYMPOSIUM NAME: The Legacy of Minority Institution - Oral

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2223687

TITLE: Novel Aromatic Architectures Derived from the Benzannulation of Alkynes

CONTACT (NAME ONLY): William Dichtel

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.

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

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2223197

TITLE: Synthetic Studies on Small-Molecule SHIP1 Agonists

CONTACT (NAME ONLY): Brian Duffy

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.

SYMPOSIUM NAME: Organic Chemistry - Poster

CONTACT (COUNTRY ONLY): United States

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

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

CONTROL ID: 2218598

TITLE: Chemical Jokes facilitate learning of important chemistry concepts

CONTACT (NAME ONLY): Kamruz Zaman

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.

SYMPOSIUM NAME: Chemical Education - Oral

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2217746

TITLE: Non-chemical treatment to extend fruit shelf life

CONTACT (NAME ONLY): Ayten Ay

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.

SYMPOSIUM NAME: Undergraduate Food Chemistry - Poster

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2216740

TITLE: The prevalence of batrachochytrium dendrobatidis in Oswego County, NY

CONTACT (NAME ONLY): Ayten Ay

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.

SYMPOSIUM NAME: Undergraduate Biochemistry - Poster

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2215755

TITLE: Degradation of polymers used to make art: origins, measurement, and prevention

CONTACT (NAME ONLY): Catherine Stephens

ABSTRACT BODY:

Abstract: The long term degradation behavior of cotton, linen, wood, and kozo papers all artificially-aged at 90°C and 50% relative humidity to promote hydrolytic breakdown was examined in order better preserve paper-based artifacts 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.

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

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2215282

TITLE: Supporting safe, sustainable laboratories in the 21st century

CONTACT (NAME ONLY): Ralph Stuart

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.

SYMPOSIUM NAME: Green Labs - Oral - INVITED ONLY

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2213588

TITLE: Implementation of a one credit chemical safety course

CONTACT (NAME ONLY): Kristin Gublo

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.

SYMPOSIUM NAME: Chemical Education - Oral

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2213336

TITLE: Development of new routes to benign polymeric materials

CONTACT (NAME ONLY): Geoffrey Coates

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.

SYMPOSIUM NAME: Green Polymers - Oral - INVITED ONLY

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2213214

TITLE: Constrained peptides for metal binding and catalysis

CONTACT (NAME ONLY): Amanda Aldous

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.

SYMPOSIUM NAME: Biochemistry - Oral

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.

CONTROL ID: 2213145

TITLE: A new method to measure aerosol particle bounce and estimating the phase state of atmospheric aerosols

CONTACT (NAME ONLY): Shashank Jain

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.

SYMPOSIUM NAME: Environmental Chemistry - Oral

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.

CONTROL ID: 2212742

TITLE: Determination of optoelectronic and transport properties of sandwich type structures based on organic semiconductors

CONTACT (NAME ONLY): Mariana Huerta Francos

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.

SYMPOSIUM NAME: Materials for Energy - Oral

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.

CONTROL ID: 2212715

TITLE: Preparation of composite films of metal phthalocyanines for optoelectronic applications

CONTACT (NAME ONLY): Mercedes Espinosa

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.

SYMPOSIUM NAME: Materials for Energy - Oral

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.

CONTROL ID: 2212366

TITLE: Site-specific functionalization of Buckybowls: Tailoring properties and structures

CONTACT (NAME ONLY): Cristina Dubceac

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.

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

CONTACT (COUNTRY ONLY): United States

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

CONTROL ID: 2211365

TITLE: The acetylation landscape of the H4 Histone Tail

CONTACT (NAME ONLY): Garegin Papoian

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

SYMPOSIUM NAME: Biochemistry - Oral

CONTACT (COUNTRY ONLY): United States

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