



**The PR-LSAMP Annual
Best Practices Conference
on Teaching and Learning**

ABSTRACT BOOK

November 6, 2009

Ponce Hilton Hotel

ABSTRACTS OF PRESENTATIONS



**Felice Frankel
Harvard University**

More Than Pretty Pictures

Visual representations now appear widely in science and engineering and are having a profound impact on how we communicate science among experts and to lay communities. The visual expression of scientific data and concepts using photographs, graphs, animations, and web interfaces, for example, are designed to convey complex information. Yet, despite the best intentions of research scientists and designers, many attempts to visually communicate science are confusing rather than clarifying. While new technologies and capabilities make visual communication possible, we need to develop a shared understanding and significant collaboration among researchers, computer scientists and graphic artists on how to represent scientific information effectively across disciplines and to the public. This talk will discuss one person's attempts, including her failures, describing how the process of making a representation clarifies understanding as well as creating a more accessible scientific vocabulary.

Science photographer Felice Frankel holds concurrent positions at Harvard University and the Massachusetts Institute of Technology. Working in collaboration with scientists and engineers, Frankel's images have been published in over 300 journal articles and/or covers and various other publications for general audiences. Her most recent book, co-authored with chemist George M. Whitesides, *No Small Matter, Science on the Nanoscale* will be published November 1, 2009 (Harvard University Press).

Frankel was awarded a Guggenheim Fellowship, and has received grants from the National Science Foundation, the National Endowment for the Arts, the Alfred P. Sloan Foundation, the Graham Foundation for the Advanced Studies in the Fine Arts and the Camille and Henry Dreyfus Foundation. She was elected as a Fellow of the American Association for the Advancement of Science and was a Loeb Fellow at Harvard University's Graduate School of Design for her previous work photographing the built landscape and architecture.

Her previous books are *Envisioning Science, The Design and Craft of the Science Image*. (The MIT Press), *On the Surface of Things, Images of the Extraordinary in Science* (Harvard University) co-authored with George Whitesides and *Modern Landscape Architecture, Redefining the Garden*, with Jory Johnson (Abbeville Press). She is founder of the Image and Meaning conferences whose purpose is to develop new approaches to promote the public understanding of science through visual expression (www.imageandmeaning.org). She is also leading a National Science Foundation program, *Picturing to Learn*, an effort to study how making representations by students, aids in teaching and learning, (www.picturingtolearn.org).

Frankel's work has been profiled in the New York Times, LIFE Magazine, the Boston Globe, the Washington Post, the Chronicle of Higher Education, National Public Radio's All Things Considered, Science Friday, and the Christian Science Monitor among others. Her images and graphical representations have appeared on the covers and inside pages of Nature, Science, Angewandte Chemie, Advanced Materials, Materials Today, PNAS, Wired, Newsweek, Scientific American, Discover Magazine, New Scientist and others. She exhibits throughout the United States and in Europe. Her limited edition photographs are included in a number of corporate and private collections.



Silvia Ronco
Program Officer, Research Corporation for Science Advancement

“Effective Undergraduate Research Programs: The Tale of a Traveling Chemist”

As a former academic at a public institution and a current program officer at a private foundation for the advancement of science, I've had the opportunity to work closely with the scientific community and have helped a large number of early career faculty and students to establish and grow productive programs of research. This presentation will cover a number of professional activities and initiatives with a common goal - the support of interdisciplinary undergraduate research as a way of teaching and learning. Effective programs to help shape the future of science, educate the future workforce, and influence institutional change will also be presented and discussed.

Silvia Ronco is currently a program officer at Research Corporation for Science Advancement where she directs both the Cottrell College Science Awards and the Partners in Science programs and actively participates in all Science Advancement programs. Silvia joined Research Corporation in September 2003 after a faculty career at the University of South Dakota (USD) where she moved through the ranks as assistant professor (1992-1997), associate professor (1997-2002) and full professor (2002-2003). Her research interests involve the synthesis and study of the photochemistry and photophysics of transition metal complexes with applications in solar energy conversion, luminescence probes and photocatalysts. At the University of South Dakota, she maintained an active research program and taught inorganic and freshman chemistry courses for undergraduate and graduate students and worked diligently to institutionalize undergraduate research on campus. She also served as the chair of the USD undergraduate research program (1999-2003), and as the program director of an interdisciplinary NSF-REU site, “Retracing the Lewis

and Clark Expedition: Contemporary Aspects of Culture and Environment along the Missouri River.”

Before joining the University of South Dakota faculty in 1992, Silvia received a PhD in inorganic chemistry from the National University of La Plata (Argentina) where she worked under the supervision of Dr. Pedro Aymonino, and conducted postdoctoral work with Guillermo Ferraudi at the Notre Dame Radiation Laboratory (1986-1989) and with John D. Petersen at Clemson University (1991-1992). In addition, she was a visiting professor at the University of California-San Diego (sabbatical leave, 2000-2001) where she worked in collaboration with Cliff Kubiak, and a Program Officer for the Photochemical and Radiation Sciences Program at the U.S. Department of Energy (1995-1996).

Silvia is currently the Chair-elect for the Council on Undergraduate Research (CUR) Chemistry Division and is serving a fourth term as a Chemistry Councilor. At CUR she has been part of many leadership roles including her participation as the co-chair 2008 CUR National Conference. As a CUR Councilor and a Program Officer her main interest has been to help early career faculty at PUIs and R1s to establish and sustain long-term research programs. Silvia also served two terms as a member of the National Conference on Undergraduate Research (NCUR) Board of Governors (2002-2008).



Dr. Ana Rita Mayol
Institute for Functional Nanomaterials, University of Puerto Rico

Bringing Research Into The Classroom, Our Community and General Public: An Interdisciplinary Approach

A.-R. Mayol, M. Gomez, N. Cardona, R. Palai

The Institute for Functional Nanomaterials (IFN) at the University of Puerto Rico is a multicampus research institute composed of 36 scientists. It has a very effective Education and Outreach Program lead by a Nano Interdisciplinary Education Team (NIET). The goal of the program is to bring research into the classroom. Graduate and undergraduate students use cutting edge results as motivators to bring key concepts and applications in Nanoscience to the general public, students and teachers in the K-16 levels. This project has catalyzed the development and implementation of a Nanoscience Exhibits for general public; fourteen workshops for the K-14 level; five new laboratory experiences for advanced undergraduates; and four interdisciplinary graduate course, reaching more the 6000 people during the first two years; the objective of all these activities is to motivate students to pursue careers in nanoscience. The IFN successfully participated in NanoDays developing demonstrations to teach the core concepts and applications in the field in an interactive and approachable fashion to all ages. The Nanoscience Display used trained high school students as presenters. The IFN has created strong collaborations network with NSF-funded education programs such as National Center for Learning and Teaching (NCLT) and Cornell Center for Materials Research (CCMR), and a PR based non-profit organization Operación Exito (OE) and Boys and Girls Clubs of Puerto Rico to ensure breadth and depth in reaching all educational levels. Dissemination of these materials has been done via the IFN website and collaborators' web-based libraries. The program is introducing the Master Teachers Training Program and a Lending Library this fall. These programs will train master teachers in the implementation of educational materials. Once train they will be able to borrow equipment for a short period of time to use the educational materials in the classroom.

Ana-Rita Mayol is an Assistant Professor in the Department of Chemistry at the University of Puerto Rico – Rio Piedras Campus. She received her M.S. and Ph.D. degree in Organometallic Chemistry from Cornell University in 2000.

Mayol completed a postdoctoral appointment in Food Chemistry at Cornell University, under the supervision of Dr. Terry Acree, and a Research and Development appointment at Consorzio di Ricerca Lattiero Caseario (CorFiLaC), in Sicily, Italy. Mayol has been an active researcher in Chemical Education since August 2001 in the Department of Chemistry where she has done work in module development, implementation and assessment in the areas on Organic, NanoScience and Physical Chemistry. Mayol is developing innovative laboratory experiences for advanced undergraduate courses and the final goal is to develop a Nanoscience curriculum. Since June 2007, she is the Education and Outreach Director of the Institute of Functional Nanomaterials (IFN), where she has build a strong Education and Outreach Program reaching more than 1000 persons at all levels. She also directs the Education and Outreach Program of NASA: Center for Advanced Nanoscale Materials and is the Project Director of the NSF funded projects PR-AGEP and a G K-12 Program: "From Hectares to Nanometers: GK-12 Multidisciplinary Explorations of Tropical Ecosystems and Functional Nanoscience". Mayol was the Academic Coordinator for the Department of Chemistry from July 2002 to January 2005 and the Assistant Dean of Student Affairs in the College of Natural Sciences from August 2007 to May 2008.

ABSTRACTS OF POSTERS

Almodóvar, Edgard; UPR-RIO PIEDRAS, Ciencias Naturales
edgardalmodovar@gmail.com

Statistical Analysis of Eclosion Success Rates for Hawksbill Turtle Nests in Mona Island

The hawksbill turtles, when procreating, return to their own nesting grounds, utilizing the same resources, and influenced by similar environmental factors. We want to study how demography is affected in this case, by focusing on eclosion success rate as a response to both nest clutch size and region on Mona Island. Sets of data were collected, provided by CREST-CATEC, which included dates taken, beaches where they were taken from, clutch size, eclosion rate, and observations regarding the nesting grounds. We want to analyze the hypothesis of whether or not eclosion rate is dependent on clutch size and region where the nest is located given a certain reproductive episode. We propose a generalized linear model in order to represent this phenomenon and be able to test the hypothesis.

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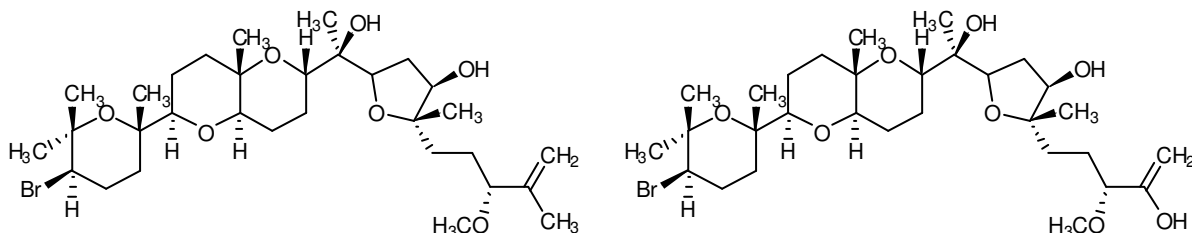
Aviles, Edward; UPR-RIO PIEDRAS, Chemistry Department/Natural S
edward.aviles@prlsamp.org

Aplysqualenols A and B: Squalene-Derived Polyethers with Antitumoral and Antiviral Activity from the Caribbean Sea Slug *Aplysia dactylomela*

Brunilda Vera, Abimael D. Rodríguez, Edward Avilés and Yasuyuki Ishikawa, Department of Chemistry, University of Puerto Rico, Rio Piedras Campus, San Juan, PR

The novel bromotriterpene polyethers aplysqualenol A (1) and aplysqualenol B (2) have been isolated from the Caribbean sea slug *Aplysia dactylomela* collected in Puerto Rico, and their structures established from spectroscopic data. Although both these compound may be conceived as polyoxycyclic derivatives of the C₃₀ squalene skeleton, remarkably 1 and 2 possess an unprecedented C₁₅ to C₂₄ flexible chain of 14S* spatial disposition that contains a unique ether bridge between C₁₆ and C₁₉. Biological activity screening test revealed that although aplysqualenol A (1) does not have significant anti-infective properties, it possesses potent antitumoral and antiviral activity.

RISE



Avilés, Sully Mar; UPR-MAYAGUEZ, Chemical Engineering
sullymar29@gmail.com

Synthesis and Characterization of Sulfonated Poly(Styrene-Isoprene-Styrene): Effects of Linear vs Branched Morphology and Counter-ion Substitution

This investigation studied the resulting nanostructure of ionic membranes composed of sulfonated copolymers with thermoplastic and elastomeric blocks. Linear poly(styrene-isoprene-styrene) (L-SIS) and branched poly(styrene-isoprene) (B-SI), were sulfonated to various levels of ion exchange capacity (IEC). Since the sulfonation occurred in both the poly(styrene) (PS) blocks and the double bonds of the poly(isoprene) (PI) segments, the resulting sulfonated polymer lost the elastomeric component of the membranes; therefore, physical blends of sulfonated and unsulfonated L-SIS and B-SI were casted and analyzed. The resulting membranes were then characterized with several techniques including: elemental analysis (EA), thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FT-IR) and Small angle X-Ray scattering (SAXS). These techniques provided thermal and physical properties of the membranes, which allowed us to compare the resulting morphologies and selectivities. Counter-ion substitution (Mg^{+2} , Ca^{+2} , Ba^{+2}) was used to cross-linked the sulfonated polymers to create more selective membranes. Vapor permeabilities were measured at 308K using dimethyl methylphosphonate (DMMP), a chemically similar stimulant to Sarin Gas (GP), and water as permeates, in order to analyze the selectivity of the resulting membranes for chemical and biological protective clothing (CBPC). Results show a similar IEC to sulfonated poly(styrene-isobutylene-styrene) (SIBS), although the reaction kinetics was significantly faster due to the unsaturated bonds of the isoprene block. However, lower sulfonation levels and blends of sulfonated/unsulfonated linear/branched resulted in unique morphologies capable of selective separations and significant differences were observed between linear and branched morphologies. Some applications for these membranes include: chemical and biological protective clothing for the US military forces, fuel cells and gas sensors among others.

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Avilés-Barreto, Sonia L.; UPR-MAYAGUEZ, Chemical Engineering
lizmar_s@hotmail.com

Sulfonated Poly(styrene-isobutylene-styrene) Metal Nanocomposites for Gas Sensor Applications

Many potential applications have been proposed for nanocomposite polymer membranes including conductive and high-strength composites; energy storage and energy conversion devices; and high sensitivity sensors. These

amperometric sensors are increasingly important for industrial safety. They consist of a proton exchange membrane (PEM) that work as an electrode to detect the presence of different gases as H₂, SO₂, CO, CH₄, Cl₂, and NH₃ among others. In this study, sulfonated poly(styrene-isobutylene-styrene) (SIBS), a triblock copolymer, has been proposed as a PEM to detect the presence of H₂ in air. SIBS was functionalized with sulfonic groups in order to obtain more selective membranes for gas sensor applications. Sulfonated SIBS was characterized with elemental analysis (EA) to determine accurate sulfonation levels. Subsequently, the sulfonated polymer was neutralized with three +2 cations, Mg⁺², Ca⁺² and Ba⁺², to create highly selective polymer-metal nanocomposite membranes. Since the potential interconnectivity of the membrane pores is very important for the performance of these dielectric materials, the proton conductivity of the samples was measured using AC impedance spectroscopy in a range of frequency from 10mHz up to 100kHz. Although proton conductivity increases with sulfonation, the effect of metal type and concentration will be further discussed based on the changes in nanochannel size and electronic configuration.

PR-LSAMP Grant: HRD-0832961

Bobea, Milena; UPR-RIO PIEDRAS, Natural Sciences
becky_543@yahoo.com

Application of the Magnetoelectric Effect to Exchange Bias in Fe/Cr₂O₃ and Ni/Cr₂O₃ Heterostructures

Since the discovery of exchange bias effect in ferromagnetic(FM)/antiferromagnetic(AFM) heterostructures, it has been used in numerous applications, such as magnetic recording media, data storage and magnetoresistive sensors. Several FM/AFM systems have been explored to understand the mechanics of exchange bias effect. Systems with room temperature FM/AFM property are widely investigated for device applications. Antiferromagnetic films with magnetoelectric properties can facilitate the fabrication of new types of memory devices where both electric and magnetic fields can serve as control parameters.

By using Cr₂O₃ as the antiferromagnetic layer, it is possible to investigate the response of the magnetoelectric effect at electric fields on fabricated multilayers of Fe/Cr₂O₃ and Ni/Cr₂O₃ thin films.

Caceres, Rita; UPR-RIO PIEDRAS, Institute of Tropical Ecosystems
ritirene@hotmail.com

Effects of salinity in the development and survival of tadpoles of *Peltophryne lemur*

Tadpole growth rates, duration of larval period, size at metamorphosis and survival to metamorphosis can be influenced by the physical environment. Salinity is an abiotic factor that has raised concern for herpetologists due to an increase in anthropogenic salinisation of aquatic habitats. Freshwater organisms present different salinity tolerance ranges but most of what is known is the effect of salinity in adults and not on embryonic or larval stages. Some of the negative effects of increased salinity for tadpoles include reduced growth rate, delayed metamorphosis, physical abnormalities and increased mortality. The Puerto Rican Crested Toad (*Peltophryne lemur*) is the only endemic toad in Puerto Rico. *P. lemur* breeds in the only natural breeding pond found in Tamarindo, Guánica. This pond has been known to have salt intrusion in the past and it is believed that this may affect negatively the development of the tadpoles. In order to address this issue a laboratory experiment was developed to see the effect of different salt concentrations on the growth and survival of *P. lemur* tadpoles. There were 6 salinity treatments (0, 2, 4, 6, 8, 10 ppt) with 10 replicates of each. Our preliminary results show that tadpoles die after 24 - 48 hours exposure to 10ppt. With increasing salinity, weight and size of the tadpole decrease. Tadpoles raised at 4 ppt seemed to do better than the rest. Tadpoles raised at 8 ppt took three months to metamorphose, two months longer than the rest. These preliminary results show the importance to monitor salt concentrations in the natural pond in order to promote the success of breeding events in the only naturally occurring breeding pond.

PR-LSAMP and CATEC

Cardona, Gloriell; UPR-RIO PIEDRAS, Natural Sciences/ Applied Math
gloriell_m@yahoo.com

PVA

Gloriell M. Cardona-Meléndez, María E. Pérez, Ph.D

The Mona Island iguana, *Cyclura cornuta stejnegeri*, is an endangered species since 1973. Its population is decreasing by the predation of introduced mammals, such as cats and pigs. In addition, the incorporation of *Casuarina equisetifolia* (Australian pine) has affected the nesting site. Currently, a research effort for developing a Population Viability Analysis for Mona Island Iguana has been undertaken in order to predict the future size of the population of this species and to evaluate current conservation efforts. As part of this effort, data relating the size of a female (snout-vent length –SVL-, tail length and body mass) and the

number of eggs laid in each clutch are analyzed using Generalized Linear Models based on the Poisson distribution. All calculations were done with the statistical software R. The method used consists in analyzing the data using the software package R. From the fitted models, it can be seen that bigger sizes are related to bigger clutch sizes.

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Carpenna, Jennifer; UPR-RIO PIEDRAS, Physics
jennifercarpenna@gmail.com

Development of Expertise in In-Situ Experiments of Nanostructures

Four *Nanofactory* In-Situ holders (2 STM, 1 AFM, 1 Nanoindenter) were recently acquired for the University's Transmission Electron Microscopy (TEM) Facility and a new High Resolution Transmission Electron Microscope (HRTEM) that is currently being installed. My current research consists on developing expertise on In-Situ experiments of nanostructures with these new tools acquired. These holders are able to measure important properties, such as a material's resistance, mechanical properties and responses to applied voltage, radiofrequency and mechanical stress, among many others. Initial tests are being conducted on CrSi□ nanowires and Pd. These tests are to measure the current as a function of an applied voltage (the so called IV curves) when a tungsten tip in the STM holder is in physical and electrical contact with the sample. Others tests involve silica rods and the use of this STM holder and a radiofrequency source to make the rod vibrate. Future experiments with the HRTEM will be conducted for the carbon nanotrees, where the STM holder will apply a current to the nanotrees and some heating will occur. This heating is predicted to cause some reorganization of the atomic structure of the nanotrees, thus reorganizing the amorphous carbon of the nanotree into graphite. Many other experiments on these In-Situ holders in these microscopes will be of great scientific value and benefit to further analyses.

PR-LSAMP

Colon, Jennifer; Ortiz, Noelia; Santiago, Jennifer; UIA-METROPOLITANO,
Science
jennifer.colon06@gmail.com

Plasmid DNA Content of Bacteria from the Environment

Tania D. Gracia Pagán, Jennifer Santiago Freytes, Jennifer M. Colón Mercado, Noelia Ortiz Aponte, and Livier I. González- Cordero. Interamerican University of Puerto Rico, Metropolitan Campus, Faculty of Science and Technology, Department of Natural Sciences

Plasmid presence in bacteria may provide advantage against environmental factors. One of these factors could be the presence of antimicrobial agents in water. Bacteria from the families of total and fecal coliforms, and enterococci were obtained from water samples of three stations: Laguna Tortuguero, Bahía de San Juan and Rio Piedras river. Water samples were filtrated; bacteria were subcultured and subjected to plasmid DNA isolation with a commercial kit. Agarose gel electrophoresis was used to separate plasmid DNA according to molecular weight. Plasmid DNA weight was found to be between 16kb and 2.0kb. Plasmid DNA weight was not related to a specific bacterial family. This suggests that the plasmids identified may have been transferred by conjugation between the different bacterial groups. Isolated strains of bacteria with plasmid DNA will be subject to antibiotic susceptibility tests. Plasmid DNA content and antibiotic susceptibility are expected to correlate.

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Davila, Melissa; UIA-METROPOLITANO, Ciencias Naturales
melidavila@yahoo.com

Chemical Metrology of Trace Explosives Detection

The NIST surface and Microanalysis Science Division is working to build a chemical metrology program to support the widespread operational deployment and effective utilization of explosive trace detectors (ETD's) currently deployed throughout the United States in support of security screening for homeland security. One objective of our research is to optimize the detection of trace explosives by manipulating the analysis conditions in the ETD's, to increase the overall sensitivity of detection. In this work, we have conducted a series of experiments to optimize the desorber temperature for several common explosives. By modifying the desorber temperature, order of magnitude increases in sensitivity have been obtained for several high explosives. Optimal temperatures (the ones giving the highest sensitivity) were 60°C for TNT, 100°C for PETN, 140°C for RDX and 200°C for HMX. This data will be discussed in the context of developing optimized conditions for screening applications. Additional experiments were also designed and performed to provide insights into the possible mechanisms of the observed sensitivity enhancements. Ongoing research is focused on more complex explosives such as plastic bonded explosives and ammonium nitrate fuel oil.

NIST

del Hoyo, Natalie; UPR-RIO PIEDRAS, Chemistry
guachunat@yahoo.com

Modulation of the Nicotinic Acetylcholine Receptor Function by Cholesterol

The nicotinic acetylcholine receptor (nAChR), located in the cell membranes of neurons and muscle cells, mediates the transmission of nerve impulses across cholinergic synapses. The nAChR is also found in the electric organs of electric rays (e.g. *Torpedo californica*). Cholesterol is a key lipid for maintaining the correct functionality of membrane proteins and has been found to alter the nAChR function. We were thus interested to probe the changes in the functionality of different nAChRs when expressed in cell membranes with modified cholesterol to phospholipid ratios (C/P). In this study, we examined. The effect of increasing the C/P of *Xenopus laevis* oocytes expressing the muscle-type, *Torpedo californica*, neuronal α -7 or α 4 β 2 nAChRs in the function of the nAChR was studied. Using the two-electrode voltage clamp technique it was found that the neuronal α -7 and *Torpedo* nAChRs are significantly more sensitive to small increases in C/P than the muscle-type nAChR. This study clearly illustrates that a physiologically relevant increase in membrane cholesterol concentration alters the neuronal α -7 and *Torpedo* nAChRs functionality whereas the muscle-type nAChR tends to resist this inhibition in function.

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Delgado, Diana; UPR-RIO PIEDRAS, Natural sciences
dianadelourdes@hotmail.com

Fluctuating asymmetry in Puerto Rican populations of Papilionidae butterflies

The intricate vein patterns in butterfly's wings are maintained by a variety of mechanisms that prevent changes during development. Among these, developmental stability stands out for its role in the maintenance of symmetry in bilateral traits. Under ideal conditions, symmetry is expected with small random deviations, otherwise known as fluctuating asymmetry (FA), which may occur when developmental stability fails due to environmental stresses. The goal of this project was to evaluate variation in FA among four Puerto Rican species of butterflies within the Papilionidae and associate this variation with the characteristics of their collection sites. The specimens were photographed with a digital camera, and the images were used to collect data of homologous landmarks along the wing-cell of both the fore- and hindwings using the TPS software package. Differences between the centroid size of the set of landmarks in the right and left wing were used to estimate FA. This information was entered in a GIS to the specimens with known locations. We established that variation between right and left wings corresponded to FA in the four species. FA ranged

between -37.77 to 50.89 pixel units in the forewing and 18.54 to 40.05 pixel units in the hindwing. We observed one case of extreme asymmetry in an individual with an extra vein in the left but not right forewing. In consequence there was reorganization in the vein pattern manifesting an increase in FA. These extreme cases of FA may be associated with reduced male mating success hence the fitness of the individuals.

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Espinosa, Javier; UIA-BAYAMON, Electrical Engineering
J.23.espinosa.13@gmail.com

Design of a Grid Portal

Grid Portals is a web based gateway to resources in a grid that provides High Performance Computational capacity from a secure entry point. Portals will allow students, researchers and scientist to accomplish tasks in much less time than with average computation, by reducing task completion time by more than half. In this paper we proposed a new Grid Portal which is more user friendly and simple than others Grid Portals. The purpose of this research is to design and implement a grid portal that meets our computational research needs at the Inter American University Bayamon-campus.

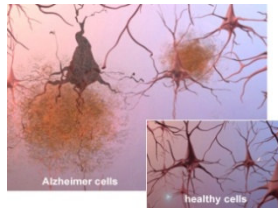
Figuroa, Cindy; UPR-RIO PIEDRAS, Natural Science
cindyfm@gmail.com

Interaction between DAHK and HSA with A β -Cull: Understanding Alzheimer's disease

Figuroa, C.1, Faller, P.2 University of Puerto Rico, Rio Piedras Campus, Chemistry Department1, Laboratoire de Chimie de Coordination, Centre National de la Recherche Scientifique, Université Paul Sabatier, Toulouse, France2

The amyloid hypothesis was proposed, to study the Alzheimer's disease, and is focused on the aggregation of fragments of the protein APP known as beta-amyloid, A β . This is believed to be responsible for neuronal death which leads to memory loss and irrational behavior. The oxidative stress coupled with the reductive environment in our brain is thought to be the metabolic key to kill neurons. When the O₂ reacts with a reduced metal ion, it produces reactive oxygen species, or ROS, such as HO \cdot , H₂O₂, O₂ \cdot^- that destroy proteins, cellular membranes, and DNA. This process starts when A β aggregates and interrupt neurons communication. With metals ions like Cu^I and O₂ these aggregates produce ROS that concludes in neuronal death.





In this project we study the interaction between the peptide DAHK and $A\beta_{40}\text{-Cu}^{\text{II}}$. We selected the peptide DAHK because it is believed to be a stronger chelator than $A\beta$, it might remove Cu^{II} from the $A\beta_{40}\text{-Cu}^{\text{II}}$ complex. DAHK has a specific Cu^{II} binding site and it is the terminal Cu-binding domain of HSA, human serum albumin, a protein present in the human brain and blood. We expect that the DAHK- Cu^{II} complex inhibits the ROS production and produces a negligible aggregation rate when compared to $A\beta_{40}\text{-Cu}^{\text{II}}$. Using several methods and techniques we should be able to obtain enough information about their interactions. Throughout the realization of this project, we were able to provide evidence that DAHK and HSA have a stronger affinity to Cu^{II} than $A\beta_{40}$. They can remove Cu^{II} from the original compound, $A\beta_{40}\text{-Cu}^{\text{II}}$. DAHK and HSA can decrease HO^{\cdot} production and aggregation coming from $A\beta_{40}\text{-Cu}^{\text{II}}$.

AMP Bridge to Doctorate

Figuerola, Cielo; UPR-RIO PIEDRAS, Biology/Natural Sciences
cfiguerola@gmail.com

Evaluation of Potential Demographic Differences in the Subpopulations of the Mona Island Iguana (*Cyclura Cornuta Stejnegeri*) Located in Different Microclimates in Mona Island, Puerto Rico

Cielo E. Figuerola-Hernández and Elvia Meléndez-Ackerman
Institute for Tropical Ecosystem Studies, University of Puerto Rico, Río Piedras Campus

Rock iguanas have a high degree of endemism. Timely research has been directed to endangered species which typically exhibit limited dispersal capabilities, low population numbers and dependency for special habitats for breeding or foraging purposes, this is the case of the Mona rock iguana. The increase of these iguanas in Mona Island has been possible in part to the presence of smaller depression sites. Given the distribution of depression forests across the landscape, different-sized depression sites may have distinctive roles in the Mona rock iguana life cycle. Mona Island is located in the middle of the Mona Channel, between the coasts of Dominican Republic and Puerto Rico. It is an oceanic island with a subtropical dry forest climate. The largest (93%) habitat type of the island is the limestone rocky "plateau". Another unique habitat type (1%) are the forest depressions located in the plateau. With this study, we want to address the importance of these two sites in regard to habitat suitability and population dynamics of Mona rock iguanas. Our objectives for this study include

1) assessing the reproductive biology of the Mona island iguana, 2) assessing differences in the movement patterns for the different demographic stages of the Mona island iguana between microclimates and 3) assessing the differences in the utilization of the habitat by the Mona iguana between microclimates. The methodology will include visual censuses to determine the distribution of the iguanas in the depression forests and platform, spatial analysis to develop distribution maps by season, microclimate and by habitat use. Finally, head start iguanas will be used to determine movement patterns of the three life stages in both microclimates with GPS radio collars.

PR-LSAMP Bridge to the Doctorate and CATEC (Center for Applied Tropical Ecology and Conservation)

Garcia, Karla & Mejia, Daniel; UIA-METROPOLITANO, Ciencias y Tecnologia
kaki_bff@hotmail.com

Study of the Microbial and Physical-Chemical Water Quality at Tortuguero Lagoon, Vega Baja P.R.

The Tortuguero Lagoon Natural Reserve is a highly valuable ecological and hydrological resource located on the north coast of Puerto Rico. This natural reserve is the only and largest coastal freshwater body in the Island. Over the years this natural resource has been impacted by urban development and contaminants as result of human activities. This study allowed to characterize the water quality near the fishery and recreational area of the lagoon. Five sampling stations were selected to measure temperature, pH, Dissolved Oxygen, Total Dissolved Solid, and salinity along a hole year. Also qualitative microbial test (Colilert™) was conducted to identify the presence of total coliforms and Escherichia coli. The bacterial densities for total coliforms and fecal coliforms were determined using the Membrane Filtration technique. A total of 70 water samples were taken over a period six months and submitted to microbial tests. According to the results for the physical-chemical parameters the obtained averages were: temperature=28.34 °C, pH=7.98, DO= 6.14mg/l, TDS= 398.4mg/L and salinity=1.32mg/L. The results for the bacterial densities demonstrated a minimum average of 2 CFU/100ml and a maximum of 37 CFU/100ml for total coliforms. On the other hand, the minimum average of 18 CFU's/100ml and a maximum of 64 CFU's/100ml were obtained for fecal coliforms. The results of the physical-chemical and microbiological tests suggest that the quality of the water does comply with the standards that have been established for this type of natural resources. This research will be useful for amplifying the database that is needed for the development of management and protection plans for the lagoon, and for future investigations. The study was sponsored with funds provided by PRLS-AMP and CECIA-IAUPR.

PRLS-AMP & UIPR-CECIA

Guzman, Haydee; UPR-RIO PIEDRAS, Matematicas/Ciencias Naturales
garnethgl83@gmail.com

Some Results on Edwards Elliptic Curves and Their Applications to Cryptography

The main focus of this research is to study binary Edwards Curves, their form and find their zeta function. We give examples of best elliptic curves. This study is directed towards an understanding of the Edwards curves the field with two elements. As a part of this poster, we present a basic foundation of Edwards elliptic curves and their applications to Elliptic Curve Cryptography, in the process demonstrating the importance of the zeta function, the number of rational points of an elliptic curve and the point at infinity. We use concepts from Abstract Algebra at the Graduate Level including Galois Theory. In this work we give special emphasis to Edwards curve over F_8 . We give implementation of some of the best Edwards Elliptic curve we have discussed in applications to cryptosystems using MAPLE.

NSF Fellowship-Bridge to the Doctorate

Laguna Torres, Jessenia Yaris; UPR-RIO PIEDRAS, Biology/Neuroscience
jessenialaguna@gmail.com

DNA Recombination, Remote Memory and Hippocampal Synaptic Plasticity.

Jessenia Yaris Laguna Torres¹, Melissa Colón Cesario², Edgardo Castro¹, Iván Santos Soto¹, Yarelis Soto¹ & Sandra Peña de Ortiz¹
¹Department of Biology, University of Puerto Rico, San Juan, Puerto Rico 00931-3360
²Department of Biology, University of Puerto Rico, Humacao, Puerto Rico 00791-4300

DNA recombination mechanisms, involving DNA endonucleases and ligases, may contribute to long-term memory formation in the brain. We previously showed that 1- β -D-arabinofuranosylcytosine triphosphate (ara-CTP), a known inhibitor of DNA ligases, blocks consolidation of context fear conditioning (Colón-Cesario et al., 2006). Now, we hypothesized that inhibition of brain DNA ligases also interferes with remote memory and hippocampal synaptic plasticity. Adult male C57BL/6 mice received systemic injections of ara-CTP or vehicle, 1 h prior to context fear conditioning. Animals were then used to test for remote memory 40 days after training. On the next day after the remote memory test, the mice from both groups were subjected to brain perfusion and Timm's staining analyses in order to assess the effects of ara-CTP on hippocampal synaptogenesis. ara-CTP blocked both remote memory of context fear conditioning and hippocampal synaptogenesis. This research has helped establish DNA recombination as a

molecular mechanism involved in structural synaptic plasticity necessary for consolidation of important and long-lasting memories.

PR-LSAMP/BDP

Malavé, Josué; UPR-MAYAGUEZ, Biology
luxarian@gmail.com

Study of Microbial Community Structure using Phospholipid Fatty Acid Analysis (PLFA) in Chromium Contaminated Site before Lactate Biostimulation

Josué Malavé-Orengo¹, Sharon Borglin², Carlos Ríos-Velázquez¹, and Terry Hazen²

¹ University of Puerto Rico at Mayagüez. ² Center for Environmental Biotechnology, Lawrence Berkeley National Laboratory, Berkeley, CA

Microbial communities have always performed a crucial role in almost any type of environment. Through research strong evidence supports microbes being able to modify toxic metals into a more stable form. A common example is hexavalent chromium (Cr VI), which can be reduced to non-hazardous trivalent state (Cr III). The main focus of this study is to examine the community composition in a chromium contaminated environment in Hanford, Washington before biostimulation. Phospholipid Fatty Acid Analysis (PLFA) was used as a biochemical approach to analyze the microbial community structure based on their different signature lipids biomarkers (SLB). Due to the extreme low biomass of the Hanford soil samples, various enrichment approaches were applied to increase the biomass by promoting microbial growth. The PLFA shows that the biomass of the samples belong mainly to bacteria, that all major groups of microbial communities are present. *Geobacter* sp., sulfate reducers, and gram-positive bacterial species increased after the enrichments. A modified cell extraction method for PLFA analysis of low biomass samples are also shown.

Montalvo, Stephanie; UPR-RIO PIEDRAS, Ciencias Naturales
einaphetsm@hotmail.com

Silicide Nanorods for Spintronics Applications

Spintronics is a technology that uses the spin, the electron, its magnetic moment, and the electronic charge. Transition metal silicide nanorods are new materials with great potential for spintronics applications. This is due to their simplicity integration into conventional silicon base electronics and the high thermal oxidation stability. These properties have been shown by chromium silicide, iron silicide and cobalt silicide. We use the Chemical Vapor Transport (CVT) technique for the synthesis of metal silicide nano scaled and micro scaled rods and tubes. When the material is in a scale of nano, the electrical and magnetic properties might show significant differences from their bulk counterparts. At this moment, we have synthesized nanorods of CrSi_2 and we are planning to synthesize nano and microrods of Fe-silicide, and $\text{Cr}_x\text{Fe}_y\text{Si}_z$. We plan to modify

the rod's composition using ion implantation and investigate the average and the local magnetic responses of the materials.

Nocua, Jose; UPR-RIO PIEDRAS, Ciencias Naturales
joenob30@gmail.com

Bacterial Behavior of E.Coli and C.Xerosis on Micro and Nano Diamond Surfaces, and Carbon Nanotubes

Olga Medina¹, José E. Nocua,¹ J. Avalos^{2,3}, Ramón Gomez³, Diana Guzman³
B.R. Weiner^{1,4}, and G. Morell^{1,2}

¹*Department of Physics, University of Puerto Rico, San Juan, PR, USA*

²*Institute for Functional Nanomaterials, University of Puerto Rico, USA*

³*Department of Physics, University of Puerto Rico at Bayamón, PR, USA*

⁴*Department of Chemistry, University of Puerto Rico, San Juan, PR, USA*

The possible risk of infection due to microbial presence on the surfaces of implants in the human body and in the surgery tools, require materials with improved features (in addition to biocompatibility and thromboresistivity). Serious problems associated with the colonization of these surfaces appear due to microbial adhesion and the consequent biofilms formation. The medical industry can greatly benefit from coatings designed to reduce the bacterial viability on implants and medical tools. In the present work, we have analyzed a mechanism of estimation of susceptibility for E. coli and C. xerosis bacteria colonization of surfaces made of microcrystalline diamond (MCD) and nanocomposite carbon (NCS) films and compared to stainless steel and quartz surfaces. The results indicate that they exhibit resistance to C. xerosis and E. coli bacterial colonization with respect to Stainless Steel and other materials. Furthermore, measurements of the growth curves of these bacteria in presence of commercial carbon-nanotubes(1-2nm dia.), bamboo-carbon-nanotubes(100-200nm dia.) and single-wall carbon-nanotubes(8-10nm dia.), shown different behavior respect to the standard curve. The carbon-nanotubes curve show a adaptation period of several hours more than the standard curve, for both bamboo and single walls nanotubes the logarithm period shows all along over his standard curve , indicating probably an accelerating ratio of population growing. The convenient use of these nanotubes will can to minimize or active the presence of these bacterias on surfaces.

Nasa

Nogueras, Carlos J.; UPR-RIO PIEDRAS, Natural Sciences
c.noguerasortiz@gmail.com

Purification and Characterization of the High -Temperature Requirement A (HtrA1) – an Essential Protease of Mycobacterium Tuberculosis

Carlos J. Nogueras Ortiz,¹ Nilofar N. MohamedMohaideen,² Satheesh K. Palaninathan,² and James C. Sacchettini²

¹ Department of Natural Sciences, University of Puerto Rico, Río Piedras Campus; ² Department of Biochemistry and Biophysics, Texas A&M University

Tuberculosis (TB) is a disease caused by bacteria called *Mycobacterium tuberculosis* (Mtb), responsible for more than 2 million deaths per year. The emergence of new drug-resistant Mtb strains has made this disease a serious threat throughout the years; there is an urgent need for new drugs and drug targets. The high-temperature requirement A (HtrA) family of serine proteases has been demonstrated to play an important role in the environmental and cellular stress damage control system in *Escherichia coli*, Mtb having three membrane bound HtrA protease homologs -HtrA1, HtrA2, and HtrA3-. Gene knock out studies have reveal that Mtb HtrA1 is essential for bacterial survival in the host, making the gene product a promising drug target against TB. We over expressed and purified HtrA1 without its trans-membrane and cytoplasmic region (residues 221-528). The crystal structure of the purified truncated HtrA1 (Δ HtrA1) have revealed that residues 221-490 form the protease domain and 491-528 form the PDZ domain; the protein either forms a trimer or a hexamer in the crystal lattice. Δ HtrA1 consistently produced a ~10 kDa autolytic fragment in different pH and temperature conditions. N-terminal amino acid sequencing analysis of the ~10 kDa fragment confirmed that this product is the intact PDZ domain of HtrA1. Interestingly, the Native-PAGE characterization of Δ HtrA1 showed a ~100 kDa, ~200 kDa and ~242 kDa protein bands. The subsequent SDS- PAGE and N-terminal amino acid sequencing analyses suggested that the ~100 kDa and ~200 kDa bands are the trimeric and hexameric forms of HtrA1 respectively. Surprisingly, the majority of the PDZ ~10 kDa products form the ~242 kDa assembly shown in the Native-PAGE. Autolysis of Δ HtrA1 is not restricted to the production of PDZ complexes as six other time-regulated autolytic products were identified and characterized. Light-scattering analysis for the inhibition of aggregate formations of citrate synthase showed that both, Δ HtrA1 and PDZ domains have temperature regulated chaperone-like activity. The biological role of the autolysis and the significance of the oligomeric assemblies are not clear at this point. Perhaps more importantly, the selective autolysis, the oligomeric assembly of HtrA1, and the chaperone and protease activity suggests that the HtrA1 may play a central role in the periplasmic stress response system of Mtb.

PRLSAMP-BDP

Ocasio Torres, María; UPR-RIO PIEDRAS, Biology
mariapr_24@hotmail.com

Long Rostrum as a Defense Mechanism for *Xiphocaris Elongata*

María Ocasio Torres¹, Alberto Sabat¹ & Tugrul Giray¹
University of Puerto Rico, Department of Biology

Amphidromous shrimp *Xiphocaris elongata* possess a short rostrum (3.9 mm \pm 2.1 mm SD) in headwater streams where predatory fishes are absent, but have a long rostrum (10.6 \pm 2.9 mm SD) below waterfalls where predators are present. Natural barriers such as steep waterfalls limit the upstream migration of catadromous predatory fishes such as mountain mullets (*Agonostomus monticola*) and eels (*Anguilla rostrata*) to headwater streams (Fievet et al. 2001). Shrimps may avoid fish predation by migrating above waterfalls or altering their morphology where predatory fishes are present (Hein, 2009). The objective of our investigation was to examine if the long rostrum exhibited by some *X. elongata* reduces their susceptibility to predatory attacks by *A. monticola* by measuring handling time and attack success in short vs. long rostrum shrimps. If *X. elongata* used their long rostrum as a defense mechanism against predatory fish, we expected *A. monticola* to undergo more failed attacks, more rejections and a longer handling time for the shrimp with long rostrum than for the shrimp with short rostrum. Since *A. monticola* is known for being a visual predator, we also hypothesized the fish to initially attack the shrimp with short rostrum. We videotaped attacks by six *A. monticola* individuals on long and short rostrum shrimps in a 20 gl. liter aquaria. The shrimp had similar post-orbital length (t-test, $p=0.994$) but different rostrum length (t-test, $p<0.001$). Tests consisted of two 15 minutes trials every other day for a total of 5 test days in which we fed the fish one shrimp with long rostrum and one shrimp with short rostrum simultaneously. Long rostrum shrimps were attacked significantly more than short rostrum individuals ($X^2=11.7$, $N=534$, $p=0.001$) for the same amount of consumptions ($N_1=N_2=45$). Long rostrum shrimps were also rejected significantly more than short rostrum individuals ($X^2=10.5$, $N=475$, $p=0.001$). *A. monticola* attacked first shrimp with short rostrum ($X^2=28.0$, $N=112$, $p<0.0001$). Handling time was significantly higher in long rostrum shrimps than short rostrum shrimps (t-test, $p=0.005$). This study suggests that *X. elongata* may avoid or delay predation by increasing their rostrum length. Long rostrum may be an adaptation to avoid predation from catadromous fish.

PRLSAMP

Ríos Franceschi, Alejandro; UPR-MAYAGUEZ, Biology
guasabara@gmail.com

Cambios en la distribución geográfica del coquí *Eleutherodactylus portoricensis*

El coquí *Eleutherodactylus portoricensis* o como se conoce comúnmente “coquí de la montaña” habita en las regiones de altas elevaciones en Puerto Rico. Comúnmente se encontraba en toda la Cordillera Central, en los bosques de Puerto Rico, como por ejemplo los bosques de El Yunque, Carite, Toro Negro, Maricao y Guilarte.

Para junio de 2008 se realizó un estudio en conjunto con la Universidad de Nuevo México (UNM), con la estudiante doctoral Brittany Barker en el cual se visitaron puntos previamente censados (Villanueva, 2005), como también se visitaron muchos de los lugares de colecta de la Colección de Herpetología de la Universidad de Puerto Rico Recinto de Mayagüez. Durante las visitas se obtuvo datos de presencia y ausencia. Para el 2008 la mitad de estos bosques ya mencionados carecía de la especie. Estos datos fueron analizados y plasmados en mapas geográficos utilizando programas tales como ArcGIS e Idrisi Kilimanjaro.

Para esta especie se generó un mapa de adecuación utilizando dos parámetros: Elevación y Cobertura Vegetal. Cada mapa se generó por separado y luego mediante una composición se unieron generando así un mapa donde solo se muestran las áreas en que la elevación y la cobertura vegetal se solapan.

Según la información obtenida la parte oeste ha sido más afectada. Para entender cuales fueron las razones para la disminución o desaparición de esta especie en estas áreas es necesario realizar estudios a mayor profundidad. Algunas razones que pudieron afectar esta especie lo son el calentamiento global, destrucción de hábitat y un hongo llamado *Batrachochytrium dendrobatidis* que afecta la piel de los anfibios.

Programa Graduado de Biología

Rivera, Adriana; UPR-RIO PIEDRAS, Natural Sciences, Dept. of Che
adriannarivera@gmail.com

Optical and Electronic Properties of Rare-Earth Nitride Semiconductors

A. Rivera, J. Wu, and R. Palai*

Department of Physics, University of Puerto Rico, Río Piedras Campus, SJ, PR.
adriana.rivera@prlsamp.org, *r.palai@gmail.com

Rare-earth nitrides are emerging materials for novel microelectronics applications because of their interesting optical and electronic properties, from metallic or semimetallic to semiconductor. The optical and electronic properties of rare-earth nitrides have not been widely investigated. In the present work, thin films of YbN, ErN, and Rare-earth doped GaN will be grown by Molecular Beam Epitaxy using different substrate with different buffer layers to understand the growth mechanism and to minimize lattice mismatch. X-Ray diffraction, atomic force microscopy, Hall effect, photoluminescence, cathodeluminescence, and magnetoelectric properties will be investigated for better understanding of optical and electronic properties.

Rivera-Vélez, Nelson E.; UPR-RIO PIEDRAS, Natural Sciences
nelsonerivera@gmail.com

Substrate Effect on Electrochemically Prepared High Surface Area Catalysts for Oxygen Evolution Reaction

Nelson E. Rivera-Vélez, Richard T. Kinch, Lisandro Cunci, Aulice M. Scibioh, Carlos R. Cabrera*

We present a comparative study of different substrates modified electrochemically with high surface area Ir and Ru particles focusing on the oxygen evolution reaction (OER) for water electrolysis applications. Modified platinum, glassy carbon, and boron-doped diamond (BDD) substrates were prepared by electrodepositing the aforementioned metals. Ir and Ru have been widely studied and are among the best working catalysts in the literature for the OER process. The metals were electrochemically deposited using cyclic voltammetry (CV) and linear sweep voltammetry (LSV) was used to characterize these electrodes by measuring the onset potential and the current density for the OER. On glassy carbon and BDD it was necessary to electrodeposit platinum particles before any further modification. Comparison of the OER by LSV for the Ir, Ru, and Ir/Ru modified electrodes suggests that the Ir-Ru combination shows the highest current density and lowest onset potential. This trend is consistent for all the studied substrates. The onset potential appears to be much less when the metallic particles are electrodeposited on the BDD, compared to GC and Pt solid substrate.

AMP

Rivero, Kennett; UPR-RIO PIEDRAS, Chemistry
rivero_kenny@yahoo.com

Redox Active Iron-Oxo Pyrazolate Clusters

Kennett I. Rivero, Richard Rivera Ocasio, Indranil Chakraborty and Raphael G. Raptis*
Chemistry Department, University of Puerto Rico-Río Piedras, San Juan PR
00931-3346

Iron-sulfur cubane-type clusters have drawn much attention in bioinorganic chemistry due to their role in biological electron-transfer pathways, and model complexes containing Fe₄S₄ have been studied for a long time. Their ability to cycle between two or more oxidation states with minimal change in structure, allows for the rapid transfer of electrons in metalloproteins. Polynuclear oxo-ferric complexes self-assemble with bridging ligands in diverse structures. An iron-oxygen cluster [Fe₈(μ₄-O)₄(μ-pz)₁₂Cl₄] (pz= pyrazolato anion, C₃H₃N₂-) containing an all-ferric Fe^{III}₄O₄ cubane core, which can reversibly accept four electrons across a potential window of ~1.1 V, has been synthesized in our lab. Impressively, Fe₈ complexes can be regarded as electron storage machines that can have tantalizing implications in electronic devices, catalysis, photodyads, etc. Preliminary data are consistent with a first one-electron step of the reduction process that is localized largely on the cubane core rather than on the peripheral iron centers for the parent cluster. Tunability of the redox processes is achieved by substitution of the terminal ligands. A simple Indium adduct, mer-InCl₃(4-H-pzH)₃, has been synthesized for the preparation of a In₄Fe₄O₄ cluster. A one-pot synthetic approach that was used to synthesize a mixed-metal cluster containing Ga and Fe atoms, yielded Fe₇Ga(μ₄-O)₄(μ-H-pz)₁₂Cl₄. Lower nuclearity clusters have been studied with the purpose of understanding electronic communication within the iron centers. Also, analogous compounds of trinuclear iron carboxylates are being used as precursors for the synthesis of higher nuclearity iron pyrazolate clusters.

PRLSAMP

Robles, Emily; UPR-RIO PIEDRAS, Ciencias Naturales
emily.robles@gmail.com

Synthesis of Fe₄O₄-core dendrimers

In Nature, redox centers that are required to reach potentials far from those of their environment are protected within protein pockets. Using Nature as an inspiration, scientists have encapsulated redox active complexes for biomimetic studies¹ in order to understand Nature's extraordinary behaviors and simulate

them. Encapsulated complexes are also useful as memory and electronic storage devices.^{2,3}

Fe₄O₄-core complexes of the type Fe₈(μ₄-O)₄(μ-4-Rpz)₁₂X₄ (where pz is pyrazolate and X is Cl, NCS) show four consecutive, closely-spaced, reversible redox processes in cyclic voltammetry.⁴ These electrochemical properties make them very attractive.

The main objective of this project is to encapsulate the Fe₈ complex into a covalent cage since electrochemical properties can be changed by encapsulating redox active complexes by covalently attaching dendrons to their core. The first part of the project consists in the Fe₈ cluster modification. An Fe₄O₄-core complex, namely Fe₈(μ₄-O)₄(μ-4-Clpz)₁₂(NCS)₄, was synthesized starting from FeCl₃, 4-chloropyrazole, base, and ammonium thiocyanate. The first generation dendron, [Ga-1], was synthesized separately following literature procedures.^{5,6} Once the first generation dendron was prepared it was reacted with the cluster previously made. The expected Fe₄O₄-core dendrimer, Fe₈(μ₄-O)₄(μ-4-Clpz)₁₂([Ga-1])₄, was identified as monoreduced (Bu₄N)[Fe₈(μ₄-O)₄(μ-4-Clpz)₁₂(NCS)₄].

Ruiz, Francheska; UPR-RIO PIEDRAS, Ciencias Naturales
falula18@hotmail.com

A New Way to Tag Small Frogs

Marking animals in general is an important tool to be able to study and understand their populations. Small animals present a challenge as most techniques are either designed for large animals or are way too expensive to make a study cost efficient. For frogs the challenge is even greater as no technique that involves the surface of the skin can be applied as frogs breathe and absorb water from the environment through their skin. One way to overcome this obstacle is our new technique that involves inserting fluorescent tattoo dye in the hind limbs of the frogs on the ventral and dorsal side with a small insulin needle for a total of 10 combinations per color and 12 combinations when applying two colors. During a thirteen month study the marking technique does not seem to affect growth rates or weight gain of individuals from all age classes and sexes. Individuals have been found with the marks up to 12 months after its application. This new application will allow for the application of mark-recapture studies of small animals which allows for better and more complete populations studies.

AGEP

Santos, Sylmar; UPR-RIO PIEDRAS, Ciencias Naturales
sylmarsantos@gmail.com

Life History, Population Structure, and Movement of Gobid Fishes in Tropical Urban and Non-Urban Watersheds

Sylmar Santos-Corujo and Alonso Ramirez
Institute for Tropical Ecosystem Studies, Biology Graduate Program, University of Puerto Rico; Rio Piedras, Puerto Rico

Most fish and shrimp species in tropical island streams have marine ancestors and maintain some degree of association with those environments. Diadromy is a common life history strategy in tropical islands. In Puerto Rico, all seven native fish species are considered as diadromous. However, the ecology and basic life history of these species is not well understood. Improving our understanding of diadromous fish and shrimp species in Puerto Rico is important as the island is urbanizing at a rapid rate. Pollution, canalization and damming are some of the threats to stream ecosystems related with urbanization in Puerto Rico. While previous studies have assessed urbanization impacts on native fish species, we know virtually nothing about impacts on population structure and the migratory behavior of diadromous species. The main objectives of the proposed study are to (1) determine the effect of urbanization on the age structure of gobid fishes (Gobiidae) and (2) assess juvenile dispersal in urban and non-urban streams in Puerto Rico. The study will be conducted in an urban stream (Rio Piedras) and a non-urban stream (Rio Mameyes). Gobid age structure will be determined by collecting fishes at different distances from the estuary and analyzing body size distribution and measuring otolith increments using scanning electron microscopy. In addition, analysis of chloride cells in gills will be used to determine whether fishes were exposed to high salinity environments. Juvenile dispersal will be assessed by marking embryos using food mixed with tetracycline, releasing them into the environment, and recapturing to determine movement along the watershed. From day 50-150, samples will be collected daily in estuary, after then recruits will be collected at different distances upstream using migration traps. Overall, the proposed research will provide critically needed information to further understand and manage fish communities in tropical island streams.

Biology Graduate Program

Santos-Figueroa, Gilmarie; UPR-RIO PIEDRAS, Chemistry
gilmarie17@hotmail.com

The Size-Resolved Carbonaceous Fraction of African Dust Particles over the Caribbean

Gilmarie Santos-Figueroa^{1,2}, Adriana Gioda¹, Olga L. Mayol-Bracero^{1*}, (1) Institute for Tropical Ecosystem Studies, University of Puerto Rico, San Juan, PR. (2) Department of Chemistry, University of Puerto Rico, San Juan, PR.

*omayol@ites.upr.edu

North Africa is the principal source of mineral dust at a global scale. High concentrations of this dust are transported across the Atlantic Ocean during much of the year. Most of these African Dust clouds arrive in the Caribbean between May and August. To understand the effects of dust particles to climate and health we need a better understanding of their specific sources, chemical composition, physical properties, and concentrations. We focused our study on the size-resolved distribution of the carbonaceous fraction (organic and elemental carbon, OC and EC) for aerosol particles in air masses with the influence of African dust. Aerosol samples were collected at Cape San Juan, a marine station located at the most northeastern tip of Puerto Rico, using a 13-stage Dekati low-pressure impactor with quartz filters. Analyses were performed using the EC/OC thermal-optical analyzer. The presence of African dust was supported with satellite images of aerosol optical thickness, with the results from the air masses backward trajectories calculated with the NOAA HYSPLIT model, and with the color of the filters after sampling. Results also showed that OC size distributions during the absence and presence of African seem to be trimodal, with one mode in the fine fraction ($D_p \approx 0.33 \mu\text{m}$) and two modes in the coarse fraction. In the absence of dust, OC concentrations were higher than in the presence of dust. Also, for both cases OC is mainly fine with concentrations around 398 and 225 ng/m^3 in the absence and presence of dust, respectively.

Bridge to Doctorate Program

Sierra, Sergio; UPR-MAYAGUEZ, Chemical Engineering
sergio1200@gmail.com

Sonolysis of Pharmaceutical and Personal Care Products (PPCP's) as an Advanced Oxidation Process for the Remediation Treatment of Wastewater Effluents

PPCP's are a diverse group of chemicals, also known as xenobiotics, treated like potential environmental pollutants. Recently, PPCPs have been detected in trace amounts in surface and ground water resources especially those receiving wastewater effluents. Sonolytic irradiation, an Advanced Oxidation Process (AOP), had received increased attention lately as a possible remediation treatment for these pollutants. However, optimization studies are required in order to minimize operational energy costs. The objective of this research is to study the sonolytic degradation of selected

PPCPs model compounds, at an ultrasonic frequency of 20 kHz. In addition, the rate of formation of H₂O₂ that occurs as a result of the OH· produced during the reaction will be studied. To develop this degradation process, Fenton's reaction reagent and direct addition of H₂O₂ will be used at different reaction temperatures. The pH will also be monitored .

Preliminary sonolytic results utilizing UV-Vis Spectrophotometer and High Performance Liquid Chromatography (HPLC) analytical instruments showed linear calibration curves of some PPCPs in concentrations as low as ppb (µg/L). In addition, partial degradation of caffeine was observed in the first 20 minutes at a temperature of 35°C and 50% transducer voltage amplitude. For Acetaminophen, a possible degradation byproduct at 40°C and 50 % amplitude was detected with HPLC.

PR-LSAMP; University of Puerto Rico

Silva, Diana; UPR-RIO PIEDRAS, Natural Sciences
dianavsilva@gmail.com

Synthesis and Supramolecular Properties of Fluorescent 8-Chalcone-2'-deoxyguanosine Derivatives

Diana Silva Brenes & José M. Rivera
University of Puerto Rico at Río Piedras, College of Natural Sciences,
Department of Chemistry, San Juan, Puerto Rico 00931
dianavsilva@gmail.com, jmrivortz@mac.com

Recently we have reported the construction of discrete and well-defined supramolecular hexadecamers in aqueous environments using a 8-(meta-acetylphenyl)-2'-deoxyguanosine (mAG) derivative. This opens the door to the use of these compounds for biomedical applications such as the development of supramolecular imaging probes and therapeutics. A key element towards achieving these goals is the development of 8ArGs with inherent fluorescence at biologically useful frequencies. Furthermore, ideally such compounds will show a large enhancement in their fluorescence emission upon assembly. This will provide a great tool to probe the dynamics of the assembly in complex biological milieus and facilitate the tracking of such supramolecules in vivo. Our initial design relies on the modification of the mAG scaffold via aldol condensations to give a series of 8-chalcone-2'-deoxyguanosine (chaGx) derivatives. Based on computer aided molecular modeling studies, we hypothesized that, similar to the mAG derivatives, the chaGx derivatives would assemble into hexadameric supramolecules. In the assembly the chalcone moiety is more rigid and relatively isolated from the solvent, which in principle should lead to enhanced fluorescence. We will present the synthetic strategy to make the chaGx derivatives as well as the spectroscopic (1D/2D NMR, fluorescence) characterization in their monomeric and assembled states.

AMP-BDP

Torres, Zally; UPR-RIO PIEDRAS, Natural Science
zallytorres@hotmail.com

Thermal Denaturation of Dabtilisin C. in Scetonitrile/H₂O Mixtures

Zally Torres, Stephanie Velazquez and Gabriel Barletta. University of Puerto Rico-Humacao, Puerto Rico

Background and Objectives: It has been suggested that in organic solvents, the unfolded state of an enzyme is thermodynamically favorable. However, due to the high-energy barrier needed for them to unfold most enzymes are thought to be kinetically stable. The melting temperature (T_m) of subtilisin C. was studied in acetonitrile/H₂O mixtures by Differential Scanning Calorimetry (DSC) to determine its melting temperature in pure organic solvents directly, and to determine if the enzyme is kinetically or thermodynamically stable in organic solvents.

Methods: DSC was used to measure the enzyme's T_m in organic/water solutions of different concentrations of acetonitrile. Enzyme activity and structure were determined for each solution by UV/VIS and FTIR.

Results: Initially T_m decreases linearly as the percentage of acetonitrile increases up to 50%. However, a linear increase in T_m is observed as the concentration of acetonitrile increases further (up to 90%), suggesting a change in the enzyme stability thermodynamics. Extrapolating to 100% acetonitrile yields a T_m of about 90°C.

Conclusion: These results, which represent a direct measure of an enzyme's T_m in a pure organic solvent, show that enzymes are thermally stable in organic solvents, and suggest that they are thermodynamically rather than kinetically stable as first thought.

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PR-LSAMP