ABSTRACTS FOR POSTER SESSION

Agricultural Sciences

Latoni, Elena, UPR-MAYAGUEZ; Vaz, Melissa, Dept. of Crops and Agroenvironmental Sciences; Rivera, Lydia I., Dept. of Crops and Agroenvironmental Sciences

[Agricultural Sciences 01]

Identification of Oidium Neolycopersici, A Powdery Mildew of Tomato Using Scanning Electron Microscopy and DNA analysis

Tomato production in Puerto Rico is valued at $11 million per year. Powdery mildews are an important limiting factor in tomato production. These Ascomycetes, Order Erysiphales, commonly cover foliage with a profuse white-to-grayish growth, which often results in reduced yield. Recent research has established the existence of two powdery mildews species affecting tomato. One, *Oidium lycopersici*, is restricted to Australia, and the other, *O. neolycopersici*, is a newly described species of worldwide distribution. The objective of this research was to identify the Erysiphales attacking tomato in Puerto Rico. Tomato leaf samples with powdery mildew symptoms were field collected. Species determination was performed using both light and scanning electron microscopy. In addition, PCR was used to amplify rDNA's ITS region, followed by nucleotide sequencing. Criteria for species determination were conidial production and germination, shape of appresoria, presence or absence of fibrosin bodies, and fimbriate patterns of the conidial wall. Using these criteria, we can confirm the presence of the newly described O*. neolycopersici* infecting tomatoes in Puerto Rico.

Chemistry

Arroyo-Ramirez, Lisandra, UPR-RIO PIEDRAS; Raptis, Raphael G., Chemistry, UPR-Rio Piedras; Cabrera, Carlos R., Chemistry, UPR-Rio Piedras

[Chemistry 01]

Palladium and Palladium-Cobalt Catalysts for the Oxygen Reduction Reaction with High Methanol Tolerance

The metallic nanoparticles are important in the development of catalysts for direct methanol fuel cells (DMFC). The cathode electrodes for direct methanol fuel cells (DMFC) have the problem that required high cost catalysts and degradation in this catalyst occurs due to the methanol crossover. Also, the

deposition methods for the catalysts are complex and time consuming. To solve this drawback we used Pd-based catalysts with high methanol tolerance and simple methodology for the catalysts deposition. Our focus is on the nanoparticles synthesis by single source precursor on carbon support (Vulcan XC-72R) to be used for fuel cell applications.

In this work, we describe the study of reductive decomposition of the $Pd_3(\mu\text{-}3\text{-}Phpz)_6$ (Pd), $[NH_4]_2CoPd_2(Me_2Ipz)_4Cl_4$ (Pd_2Co) and $[NH_4]_2Co_2Pd(Me_2Ipz)_4Cl_4$ ($PdCo_2$) complexes on Vulcan XC-72R surfaces. The Pd and Pd-Co catalyst synthesis will be done by thermal and chemical reduction using organometallic complex as precursor. The Pd nanoparticles were characterized by electrochemical and surface analysis techniques, such as: TEM, STEM/EDS, XPS, CV and LSV.

TEM images for Pd and Pd-Co on Vulcan show nanoparticles with average sizes of 3.3 nm and 6.0 nm, respectively. The palladium nanocatalysts will be studied by cyclic and linear sweep voltammetry. The catalytic activity toward oxygen reduction was evaluated with LSV in 0.5 M H_2SO_4 and methanol tolerance in 1 M MeOH solutions saturated with oxygen. These preliminary results suggest that the Pd-Co nanoparticles might be a promising a cathode catalysts for fuel cells.

Aviles, Edward, UPR-RIO PIEDRAS; Aviles, Edward, Chemistry, University of Puerto Rico; Rodriguez, Abimael, Chemistry, University of Puerto Rico; Mayer, Alejandro, Pharmacology, Midwester University, Chaudhri, S., Pharmacology, Midwester University; Hall, M.L., Pharmacology, Midwester University

[Chemistry 02]

Marine Sponge Hymeniacidon SP. Amphilectane Metabolites Potently Inhibit Rat Brain Microglia Thromboxane B2 Generation

Neuroinflammation appears to involve release of thromboxane B_2 (TXB_2) and superoxide anion (O_2^-) by brain microglia (BMG). The purpose of this investigation was to determine the effect of five *Hymeniacidon* sp. amphilectane) (1-5) and two semi-synthetic analogs (6 and 7) on TXB_2 and O_2^- generation frmetabolites (1-5om *E. coli* LPS-activated rat BMG. Short and long term cell viability was assessed by lactate dehydrogenase (LDH) release (1.5 h) and mitochondrial dehydrogenase (MTH) activity (2.5-18 h), respectively. O_2^- levels were determined via superoxide dismutase-inhibitable reduction of ferricytochrome C and TXB_2 by EIA. Results were the following (n=3-4): all *Hymeniacidon* sp. metabolites and analogs potently inhibited TXB_2 (IC50=0.20-5.69 μM) with low LDH release and minimal MTH inhibition. Comparison of IC_{50} of closely related amphilectane diterpenes 1 (IC50~0.20 μM) and 2 (IC50~0.23 μM) supports the observation that bioactivity is associated with presence of two isonitrile groups. However, the amphilectane diterpenoid skeleton plays a

significant role, as suggested by comparison between IC_{50} of these two compounds and 6 (IC50~3.14 μM), where original isonitriles have been replaced by formamide groups. Lack of O_2^- inhibition would appear to suggest that all *Hymeniacidon* sp. metabolites and derivatives inhibit TXB_2 synthesis by a cyclooxygenase-dependent mechanism. Supported by Midwestern University and the RISE and SCORE Programs, University of Puerto Rico at the Río Piedras Campus.

Bailon, Sonia, UPR-MAYAGUEZ; Perales-Perez, Oscar, Engineering Science & Materials, UPRM; Singh, Surinder, Engineering Science & Materials, UPR-Mayaguez

[Chemistry 03]

Effect of Doping on the Structural and Optical Properties of Microwave-Assisted Synthesis of ZnSe@ZnS Core-Shell Quantum Dots

Semiconductors Quantum Dots (QD's) have attracted much attention because of their optical properties can be tuned just by controlling their crystal-size, composition and shape at the nanoscale. The incorporation of Cu species into II-VI semiconductors structures to allow tunability of the resulting luminescence properties and the enhancement of the quantum yield. We report here the microwave-assisted synthesis of water-soluble non doped ZnSe@ZnS core-shell quantum at pH 6.0, 7.0 and 8.0 and the effect of the concentration of the dopant (Cu ions) on the optical properties of these QD's. Quantum dots were synthesized from zinc chloride and selenide aqueous solutions in presence of 3-mercaptopropionic acid (MPA). The concentrations of Copper ions ranged from 0.001 to 0.125mM. The average crystallite sizes were estimated from the X-Ray Diffraction pattern. They were 4.1 ± 0.4 nm for non doped QD's and 3.6 ± 0.3 nm for Cu-doped (0.001mM of Cu) QD's. The HRTEM image of non doped QD's evidenced the crystallinity of the QD's. The ICP-MS analysis confirmed the presence of zinc, selenium and copper in the QD's. Non doped QD's and Cu-doped QD's synthesized at pH 7.0 showed excitonic peaks at 320 nm. The position of the emission band in Cu-doped QD's changed from 412nm (non doped ZnSe@ZnS) to 515 nm in Cu-doped (0.001mM) QD's. The observed strong green emission in the doped nanocrystals was attributed to the internal incorporation of copper in the lattice of the host chalcogenide.

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[Chemistry 04]

Low Temperature Aqueous Synthesis of ZnO Nanorods for Enhanced Raman Spectroscopy

Semiconductor oxide nanorods exhibit chemical properties and thermodynamic stability associated to their size, which improves the present problem of steric stabilization that silver and gold colloids present. Shape-controlled synthesis of zinc oxide films is very important since almost all properties of thin films are dependent of shape and size. Magnetron sputtering is a convenient technique to make particle size in a uniform manner by sowing seed. In contrast to other methods which result in high polydispersity and a variety of shapes, this method offers narrow size distribution and near spherical particles. ZnO seed film were prepared by Radio frequency (RF) magnetron sputtering. After was conducted to thermal decomposition Zn^{2+} amino complex (wet chemistry). A second but important goal was to test the substrates as suitable for SERS detection of 4-nitrobenzenethiol. Two samples of Au-coated on rod and nanorods on growth were prepared to investigate the size dependence of the surface enhanced Raman scattering (SERS). The diameter of the nanorods was controllable during the synthesis by wet chemistry different average diameters of 250 and 50-131 nm were prepared to investigate the size dependence of the surface enhanced Raman scattering (SERS). High SERS enhancement was observed from Au-coated ZnO nanorod arrays. Raman spectra of 4-nitrobenzenethiol were measured as low as 1.0 picograms. The average diameter of the ZnO was approached between 50-131 nm and at an excitation wavelength of 532 nm was used for Raman excitation. The SERS was explained by the field enhancement effect induced by surface plasmon polaritons of Au-coated nanorods.

Betancourt, José, UPR-RIO PIEDRAS; Jose M. Rivera, Department of Chemistry, University of Puerto Rico, Río Piedras Campus

[Chemistry 05]

Host-Guest Recognition inside Nanoglobules from Thermoresponsive Supramolecules

Here we show 8-(meta-carbonylphenyl)-2'-deoxyguanosine derivatives that self-assemble in aqueous media into discrete supramolecular hexadecamers and

exhibit the lower critical solution temperature (LCST) phenomenon. Spectroscopic, calorimetric and optical microscopy studies support the fact that above transition temperature (Tt) the supramolecules further assemble into nanoscopic spherical globules of low polydispersity. Also we will show the use of these globules for the inclusion of a flavin-functionalized polystyrene copolymer as model guest molecules. This nanoglobules provide a versatile scaffold for "host-guest" recognition in aqueous media. This approach exhibits great interests in preparing monodisperse thermosensitive microcapsules for encapsulating bioactive materials or drugs.

Casañas, Barbara, UPR-RIO PIEDRAS; Barbosa, Cindy, Department of Chemistry, UPR-RP; Colón, Jorge L., Department of Chemistry, UPR-Rio Piedras

[Chemistry 06]

Zirconium Phosphates for use in Bionanotechnology

Zirconium bis(monohydrogen orthophosphate) monohydrate (Zr(HPO4)2•H2O, α-ZrP) is the best characterized zirconium phosphate (ZrP). The highly hydrated phase of the layered ZrP, known as the 10.3 Å phase, is an acidic ion exchanger that has been used for the immobilization of several photo-, bio- and redox-active compounds. Among these compounds is a metallocene derivative known as titanocene dichloride which has been proposed and investigated as a potential anticancer drug. We use the 10.3 Å phase of ZrP as a host to intercalate by direct ion exchange this metallocene derivative and chemically and electrochemically characterize it for possible applications in biotechnology. ZrP is suitable to produce robust titanocene dichloride-intercalated nanomaterials that will have better stability as biosensors and drug carriers compared to non-layered materials. The direct intercalation reaction of the titanocene dichloride into 10.3 Å ZrP was performed. The intercalated materials were characterized using IR spectroscopy, X-ray powder diffraction (XRPD) and X-ray photoelectron spectroscopy (XPS). The XRPD data indicates that new intercalated phases with expanded interlayer distances of 9.9 Å and 10.0 Å were obtained. We will present the characterization of the unintercalated metallocene derivative as well as those of the intercalated materials.

Cedeño-Mattei, Yarilyn, UPR-MAYAGUEZ; Perales-Perez, Oscar, Engineering Science & Materials, UPR-Mayaguez; Uwakweh, Oswald N.C., Engineering Science & Materials, UPR-Mayaguez; Xin, Yan, Magnet Science & Technology Division, National High Magnetic Field Laboratory

[Chemistry 07]

Colossal Room-Temperature Coercivity in Size-Selected Cobalt Ferrite Nanocrystals

It has been well-established that a fine tuning in cobalt ferrite nanocrystal size within the single domain region would lead to the achievement of extremely high coercivity values at room-temperature. If so, the high coercivity and chemical stability expected for this ferrite will increase its attractiveness for magneto-optical recording applications. The present work addresses the development of a size-sensitive phase separation method for cobalt ferrite nanocrystals that is based on selective dissolution of the superparamagnetic fraction and subsequent size-sensitive magnetic separation of single-domain nanoparticles. Ferrite nanocrystals synthesized under size-controlled conditions were first contacted with acidic solutions under precise conditions of acid concentration and contact time, followed by a magnetically-assisted phase separation in water. Produced nanocrystals were characterized by X-Ray Diffraction (XRD), Transmission Electron Microscopy (TEM), Energy Dispersive X-Ray Spectroscopy (EDS), Vibrating Sample Magnetometry (VSM), and Mössbauer Spectroscopy techniques. The attained coercivity value of 9.4 kOe was mainly attributed to the enlargement of the average crystal size within the single domain region coupled with the removal of the superparamagnetic fraction in the ferrite powders.

Contés, Enid, UPR-RIO PIEDRAS; Li, Jing, NASA Ames, Moffet Field, CA; Cabrera, Carlos, Chemistry Dept, UPR Rio Piedras

[Chemistry 08]

Methane Detection Using Functionalized Carbon Nanotubes Based Sensors

Gas sensors have been widely investigated because of their applications in the aerospace industry, space missions, defense and homeland security, to monitor environmental pollution, and for medical diagnosis as well. Pristine carbon nanotubes (CNTs) have been used for the detection of polar, non-polar and organics molecules. It has been stated that pristine CNTs are not suitable for the detection of non-polar gases but the inclusion metallic nanoparticles might help in their detection. In our work, we used electrochemical deposition and chemical synthesis to decorate single wall carbon nanotubes with platinum nanoparticles. Pt/CNTs samples were characterized using energy dispersive spectroscopy (EDS) and X-Ray Diffraction (XRD). The samples were tested for the detection of methane at different concentrations in the parts per million (ppm) range.

Cunci, Lisandro, UPR-RIO PIEDRAS; Scibioh, Aulice, Department of Chemistry, University of Puerto Rico; Cabrera, Carlos, Department of Chemistry, University of Puerto Rico

[Chemistry 09]

Diamond Doping and Preparation of Supported Catalysts for the Oxygen Evolution Reaction

The need for a new energy carrier is well established and there is no doubt that the world's current use for hydrocarbons as a primary energy source is not sustainable. Regenerative fuel cell is considered one of the most attractive options for future on-board energy generation in space applications due to its possibility of on-site hydrogen and oxygen regeneration. However, even though platinum is proved to work as catalyst for the hydrogen evolution reaction (HER), improvement needs to be made in catalysts for the oxygen evolution reaction (OER).

Since OER catalysts found in literature are either not stable at the potentials needed or have low performances providing low current densities, a diamond supported stable and high performance catalyst is the best alternative. Boron doped diamond nanoparticles provide the most suitable stable support for the catalyst to help increase the surface area, and together with ruthenium and iridium oxides make the best option for the OER catalyst. In this work, diamond nanoparticles are doped with boron and used as a support for the electrodeposition of platinum nanoparticles. XPS was used to analyze the composition and electrochemical voltammetry was used to test the catalysts on a glassy carbon substrate. Rotating disk electrode slurry technique was used to electrodeposit platinum on boron doped diamond. Boron doped diamond high conductivity indicated the success of the doping procedure and the electrochemical voltammetry showed the successful platinum electrodeposition.

del Hoyo, Natalie, UPR-RIO PIEDRAS; Báez Pagán, Carlos, Chemistry Department, UPR-RP; Quesada, Orestes, Physics Sciences Department, UPR-RP, Lasalde, José A., Biology Department, UPR-Rio Piedras

[Chemistry 10]

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 α4β2 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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[Chemistry 11]

In Vitro and in Silico Enantioselective Transesterification Catalysis by Nanosized Serine Protease Subtilisin Carlsberg in Tetrahydrofuran (THF)

Enzyme catalysis in organic solvents is a powerful tool for stereo- and regio-selective synthesis of chiral intermediates. However, enantioselectivity of an enzyme is still hard to predict. To overcome this obstacle, we employed subtilisin Carlsberg (SC) co-lyophilized with methyl-beta-cyclodextrin (MβCD) and designed a series of 14 structurally related racemic alcohols. They were employed in the model transesterification reaction with vinyl butyrate and the enantioselectivities were determined. The aim of this study was explored the efficiency of the additive MβCD to enhance the enantioselectivity of the subtilisin C. in THF comparing the experimental with the theoretical results. In general, short alcohol side chains led to low enantioselectivties, while larger and bulky side chains caused better discrimination of the enantiomers by the enzyme. With several bulky substrates high enantioselectivities with E >100 were obtained. Computational modeling highlighted that key to high enantioselectivity is the discrimination of the *R* and *S* substrates by the sole hydrophobic binding pocket based on their size and bulkiness. While bulky *S* enantiomer side chains could be accommodated within the binding pocket, bulky *R* enantiomer side chains could not. However, when also the *S* enantiomer side chain becomes too large and does not fit into the binding pocket anymore, enantioselectivity accordingly drops.

Enríquez, Yanira, UPR-RIO PIEDRAS; Ana R. Guadalupe, Department of Chemistry, University of Puerto Rico, Río Piedras Campus; Yashira Negrón, Department of Chemistry, University of Puerto Rico, Río Piedras Campus

[Chemistry 12]

Development of an Electrochemical Biosensor for the detection of Pseudomona aeruginosa

Pseudomonas aeruginosa (PA) is an opportunistic pathogen and is considered one of the most common bacterium found in nosocomial infections. We are interested in designing an electrochemical biosensor for the detection of PA. A free radical copolymerization of Styrene and NAS has been prepared to generate a film on carbon surfaces in order to anchor a β-NAD^+ electroactive analog. A Ferrocene-labeled NAAD cofactor (Fc-NAAD) was prepared by attaching Ferrocene Succinimide (Fc-NHS) to the primary amine in the adenine moiety of NAAD. The synthesis was done at room temperature for 8-15 days. The Square Wave Voltammetry (SWV) analysis of the unpurified product showed the signal for Fc-NHS at 600 mV decreasing with time of reaction while, a new band was forming between 500-520 mV that is tentatively assigned to the oxidation of Ferrocene in the Fc-NAAD cofactor. The product was purified using a column of Sephadex G-25 and the electrochemical analysis of the final product showed only one signal at 340 mV in SWV which is assigned to the oxidation of Ferrocene in the Fc-NAAD. The FT-IR analysis confirms the disappearance of the carbonyl signal from the amide in the succinimide group of Fc-NHS, the presence of the carbonyl group of the carboxylic acid from NAAD and the carbonyl group from the new amide link formed in Fc-NAAD which is an indication that the modification was in the primary amine of the adenine moiety. Our work is now focused on the full characterization of the Fc-NAAD cofactor and electrode surface modification.

Feliciano, Ileana, UPR-RIO PIEDRAS; Nicolau, Eduardo, Chemistry, UPR Rio Piedras; Zavala, Zarixia, Biochemistry, UPR Rio Piedras; Zulic, Zana, Chemistry, St. Louis University, Minteer, Shelley, Chemistry, St. Louis University; Cabrera, Carlos, Chemsitry, UPR Rio Piedras

[Chemistry 13]

Expression, Purification and Characterization of PQQ-dependent Alcohol Dehydrogenase from Gluconobacter and use in L-cysteine monolayer on Palladium Surface

In the last decade, the ability for an enzyme to undergo direct transfer electron has been of increasing interest for the development enzymatic biosensor. The pyrroloquinolinequinone dependent alcohol dehydrogenase

(PQQ-ADH) enzyme catalyzes the direct electron transfer between the active center of the enzyme and the electrode which is use for biosensor application.

In this work we detail the isolation of PQQ-ADH enzyme from *Gluconobacter* sp. 33 followed by the enzyme purification using ion exchange chromatography technique. Once we have the enzyme was immobilized in L-cysteine monolayer previously formed on palladium surface. The carboxylic acid of the L-cysteine monolayer will serve as the base for the attachment of PQQ–dependent ADH over palladium surface. PQQ-ADH was covalently attached after a coupling reaction of 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (EDC) and N-hydroxysulfosuccinimide (NHS) activation of the carboxyl group of L-cysteine monolayer. This immobilization of PQQ-ADH in L-cysteine monolayer was characterized by Infrared spectroscopy.

Finally, the catalytic activity will be evaluated for the PQQ-dependent alcohol dehydrogenase covalently attached in L-cysteine monolayer in presence of ethanol solution by cyclic voltammetry.

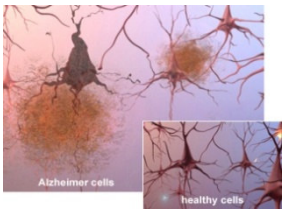
Figueroa, Cindy, UPR-RIO PIEDRAS; Dr. Peter Faller, Biochemistry, CNRS/ Laboratoire de Chimie, Toulouse, France

[Chemistry 14]

Interaction Between DAHK and HSA with Aâ-CuII: Understanding Alzheimer's Disease

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, Aβ. 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 O_2 reacts with a reduced metal ion, it produces reactive oxygen species, or ROS, such as $HO^{\cdot}$, H_2O_2, $O_2^{-\cdot}$ that destroy proteins, cellular membranes, and DNA. This process starts when Aβ aggregates and interrupt neurons communication. With metals ions like Cu^{II} and O_2 these aggregates produce ROS that concludes in neuronal death.

$Ab+Cu^{II} \rightarrow Ab\text{-}Cu^{II} \rightarrow$ Aggregation $\rightarrow$ ROS $\rightarrow$ Neuronal death



In this project we study the interaction between the peptide DAHK and Aβ40-Cu^{II}. We selected the peptide DAHK because it is believed to be a stronger quelator than Aβ, it might remove Cu^{II} from the Aβ40-Cu^{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 ad blood. We expect that the DAHK-Cu^{II} complex inhibit the ROS production and produce a negligible aggregation rate when compared to Aβ40-Cu^{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 stronger affinity to Cu^{II} than Aβ40. They can remove Cu^{II} from the original compound, Aβ40-Cu^{II}. DAHK and HSA can decrease $HO^{\cdot}$ production and aggregation coming from Aβ40-Cu^{II}.

García, Marilyn, UPR-RIO PIEDRAS; Rivera-Sanchez, Maria del C., Chemistry, UPR-Rio Piedras; Hobley, Gerard, Chemistry, UPR-Rio Piedras; Rivera, José M., Chemistry, UPR-Rio Piedras

[Chemistry 15]

Stucture Elucidation and Mechanism of Self-Assembled Guanosine Analogues

The development of self-assembled discrete structures of intermediate molecularity remains a challenge that must be overcome if self-assembly is to become a viable tool for the construction of bio and nanomaterials. To achieve control over the outcome of the self-assembly process, full understanding of the interactions among the individual subunits most be obtain. For the construction of a well-defined discrete structure of intermediate molecularity the scaffold most have the information encoded for the self-termination of the system. Guanosine and its analogues are known to self-assemble into a variety of structures as a result of attractive non-covalent interactions. Guanosine tetramers (G-tetrads) aggregate in the presence of cations to form higher ordered structures known as G-quadruplexes (GQs). We have reported the self-assembly of lipophilic 8-phenyl-2'-deoxyguanosine derivatives into GQs. These compounds were modified by replacing the H8 in the guanine base with a functionalized phenyl group. The position of the functional group in the phenyl ring modulates the molecularity and stability (thermal and kinetic) of the resulting supramolecules. In particular, the **mAG** (*meta*-acetylphenyl), **mECG** (*meta*-ethoxycarbonyl), **3PyG** (3-pyridil) and **pAG** (*para*-acetylphenyl) scaffolds promote the formation of hexadecamers, dodecamers and octamers, respectively, in organic media, figure 1. Herein we report the three-dimensional structure of **mAGi**, **mAGcat** and **mECGi** hexadecamers, based on 1D and 2D NMR experiments. The balance between attractive and repulsive interactions is responsible for the self-terminating behavior and stability of this hexadecamers. Furthermore, this structure suggests a possible mechanism of formation for this supramolecule. In contrast, the **pAGi** and **mECGi**, in $CDCl_3$, self-assembles into an octamers, wile **3PyGi** self-assemble into a dodecamer.

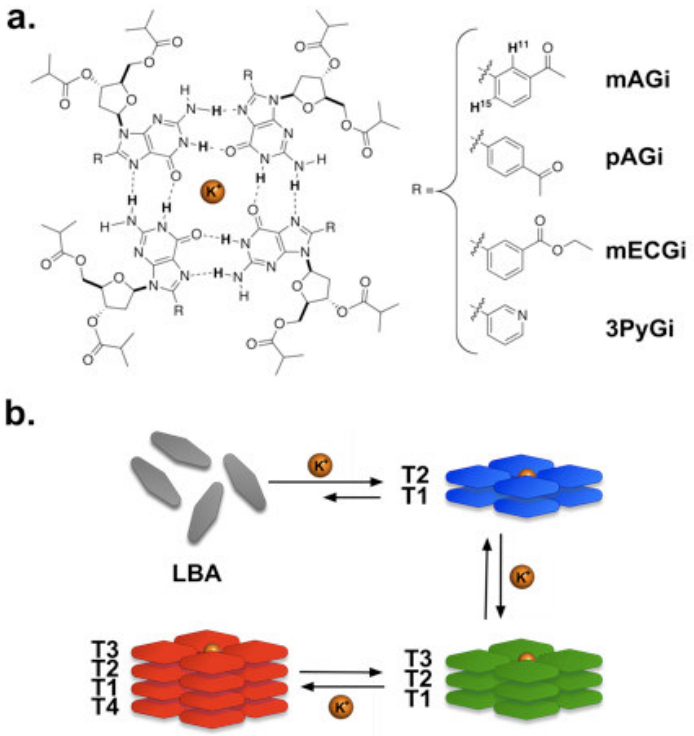


Figure 1: a) Chemical structure of a tetrad. b) Schematic of the formation of an octamer, dodecamer and a hexadecamer.

García Maldonado, María del Mar, UPR-RIO PIEDRAS; Hernández Borrero, Liz, Chemistry, University of Puerto Rico, Río Piedras Campus; Guadalupe, Ana R., Chemistry, University of Puerto Rico, Río Piedras Campus

[Chemistry 16]

Cyclic Voltammetry and UV-Visible Spectroscopy of Meldola's Blue at Different Ionic Strengths and pHs

Meldola's Blue, a commonly used pigment in textiles, papers, and paints, can also be used as a mediator in the design of biosensors for the detection of molecules such as NADH, pyruvates, hydrogen peroxide, glucose, and 3-hydroxybutyrate. The redox peaks of this dye can be observed in a window potential of -400 mV to -600 mV using a glassy carbon (GC) electrode versus Ag/AgCl 3M NaCl. We are interested in the use of Meldola's Blue as a recognition molecule for amyloid peptides in biological samples. In this work, we are reporting the electrochemical and spectroscopy characterization of Meldola's Blue in aqueous solution varying the pH and the ionic strengths. Cyclic voltammetry results showed an increase in current by augmenting the ionic strength of the solution using GC versus Ag/AgCl 3M NaCl. As well, the pH changes toward negative potentials with pH increments. These experimental results will allow us to understand the redox and spectral behavior of Meldola's

Blue in aqueous solutions and to establish a background signal to compare with future experiment in the presence of amyloid peptides.

Guzman, Rolando, UPR-RIO PIEDRAS; Cabrera, Carlos, Chemistry,UPR-Rio Piedras

[Chemistry 17]

PtCeHg/C Electrocatalysts Prepared by Impregnation Method for Direct Alcohol Electro-Oxidation

The most common alcohol for DAFCs is methanol (Direct methanol fuel cells,DMFCs), although ethanol has been recently gaining considerable attention due to its greater availability and higher energy storage capacity (per volume) than methanol. Recently, CeO2 on Pt supported carbon has been investigated as a possible anode material for DAFCs. In our investigation an impregnation method was developed for the preparation of CeO2-Hg on Pt/Carbon electrodes using cerium (III) nitrate and mercury (I) nitrate as the precursors and a glassy carbon electrode as the substrate. In order to achieve good dispersion of ceria and Hg on carbon, EDTA was used. Different CeO2 and Hg composition with Pt has been examined to optimize the catalyst material. The electrodes were characterized by using X-ray diffraction analysis, X-Ray photoelectron spectroscopy and scanning electron microscopy. The electrocatalytic properties of the electrodes were examined by using lineal sweet voltammetry, cyclic voltammetry, chronoamperometry and electrochemistry impedance spectroscopy. We performed electrochemical oxidation of methanol and ethanol, where it was observed that the catalytic material had better catalytic activity with ethanol.

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[Chemistry 18]

Modulating the Structure and Properties of Supramolecular Quadruplexes Using Metal Cations

G-quadruplexes (GQs) are formed through the self-assembly of guanine bases to form planar hydrogen-bonded tetramers that stack on each other, templated by a metal cation. The cation, the anion and/or the solvent can modulate the thermodynamic and kinetic stability of such GQs. We will present results on the formation of GQs made from a 8-Aryl-2'-deoxyguanosine derivative in the presence of various metal cations (alkaline, alkaline earth and transition metals).

Specifically, ESI-MS and NMR data indicates that the metal cation affects the molecularity, the fidelity, and stability (thermal & kinetic) of the GQs formed by **mAGi.** Supramolecules with high fidelity were observed with Na^+, K^+, Rb^+, Sr^{2+}, Ba^{2+}, with the latter two alkaline earth metal cations being superior in terms of the induced thermal stability. We are currently using this knowledge in the development of multifunctional nanodevices.

Mendez, Jessica, UPR-RIO PIEDRAS; Monteagudo, Alina, Chemitry, University of Puerto Rico; Griebenow, Kai, Chemistry, University of Puerto Rico

[Chemistry 19]

Covalent Immobilization of Modified Enzyme into Mesoporous Silica Particles for Drug Delivery Applications

The overall goal of this research project is to develop a novel nano particulate drug delivery system through the covalent immobilization of a bio-therapeutic agent into mesoporous silica nanoparticles (MSN). We activated MSN through functionalization with thiol groups. Characterization of the activated surface was performed utilizing XPS, dynamic light scattering, and SEM. The results demonstrated that the MSN were functionalized successfully and that the activation process decreased the size of the particles, but did not impact their morphology. Carbonic anhydrase (CA) was modified with a bi-functional cross-linker which allowed its immobilization onto the carrier by creating a redox-sensitive disulfide bond. We determined the level of modification of the enzyme and studied the impact of the modification on its residual activity and tertiary structure. Residual enzyme activity after modification was determined to be 76% and 72% for a 5% and 18% degree of modification of surface lysine residues, respectively. The CD spectra revealed that no significant changes in the tertiary structure occurred due to enzyme activation. Subsequently, the enzyme was covalently immobilized onto the MSN and we were able to demonstrate that the protein was released under typical intracellular redox conditions, but not under extracellular conditions. Future experiments will include characterization of the released enzyme from the MSN.

Montano, Rubenier, UPR-RIO PIEDRAS; Raptis, Rapahel G., Chemistry, UPR-Rio Piedras

[Chemistry 20]

Modification of [Fe8(ì4-O)4(pz)12Cl4] Towards Developing Luminescent Complexes

We propose the synthesis of artificial antennas to improve the efficiency of photovoltaic cells. These antennas need an electron donor and an electron acceptor. We use $Fe_8(\square_4\text{-}O)_4(\square\text{-}pz^*)_{12}Cl_4$ which has been demonstrated to be a

very good electron acceptor. This molecular cluster can accept up to four electrons, but the most important point to note here is the low energy needed to reduce the cluster. Two electrons are accepted at energy lower than the needed for fullerene to accept the first electron. We predict that more than one electron can be accepted using the available electron donors. For an electron donor we plan to use a porphyrin with a hydroxyl terminal since we can demonstrate that other ligands can substitute the chlorides from the Fe_8 cluster. We use a fluorescence marker (Fluorescein) which is simpler ligand than porphyrin to substitute the chlorides. Spectroscopic data indicate the presence of Fluorescein with the Fe_8 cluster suggesting the substitution of the terminal chlorides. These results show that Fluorescein hydroxyl terminal has preference coordination than chlorides when the incoming ligand is added in excess.

Negron, Luis, UPR-RIO PIEDRAS; Rivera, José M., Department of Chemistry ,University of Puerto Rico-Río Piedras

[Chemistry 21]

8-Aryl-2'-Deoxyguanosine dinucleosides for the Development of Robust Self-Assembled Dendrimers

Self-assembly offers a convenient strategy for the development of multifunctional nanostructures. Our group has developed a series of 8-aryl-2'-deoxyguanosine (8ArG) mononucleoside derivatives, which are useful in the construction of self-assembled dendrimers (SADs) in organic and aqueous media. Such dendrimers are composed of sixteen subunits held together by a combination of non-covalent forces such as hydrogen-bonds, ion-dipole, and pi-pi interactions, among others. Nonetheless, the equilibrium at low micromolar concentrations is shifted towards the monomeric subunits. For these systems to be useful for biological applications they must assemble at or below these concentrations. One strategy to achieve this is to increase the cooperativity in the assembly of these SADs. We aimed to do this by developing the corresponding 8ArG dinucleosides. The initial synthetic strategy relies on the dimerization of 8ArG mononucleoside derivatives via olefin cross-metathesis using a second generation ruthenium Grubbs' catalyst. We will present the detailed synthetic strategy and characterization of this new family of compounds. Additionally, we will show 1D/2D-NMR and other studies regarding the supramolecular structure and properties of these compounds. We expect that this new family of compounds will enable the construction of a wide variety of multifunctional supramolecular nanostructures useful for biological studies.

Pacheco, Yamaris, UPR-RIO PIEDRAS; Griebenow, Kai, Chemistry, UPR-Rio Piedras

[Chemistry 22]

Nanoparticulate Protein Formulations

This research intents to provide a suitable new methodology to prepare stable dehydrated protein nanoparticles suitable for long-term storage of proteins. Furthermore, the nano-particulate powders will be tested in various biotechnology applications relevant to the biopharma industry (e.g., sustained release formulation).

Model proteins with different stability and structure were employed, namely, the serine proteases subtilisin Carlsberg and α-chymotrypsin. Protein nanoparticles were formed by co-lyophylization of the proteins with the additive methyl-β-cyclodextrin at a fixed 1:4 w/w ratio. The excipient was removed from the powders by suspension of the powders in ethyl acetate. The spherical protein nanoparticles were analyzed by transmission electron microscopy (TEM), scanning electron microscopy (SEM) and light scattering, all of the techniques used to determine the particle size revealed an average diameter 114 $\pm$ 25 nm. The proteins secondary structure was analyzed using FTIR, which as presented does not affect the reactivity of the enzymes. The activity of the two enzymes was the same prior and after the procedure within less than two percent deviation. The data show that our methodology is effective in creating protein nanoparticles without inversely affecting protein stability.

Pagan, Miraida, UPR-RIO PIEDRAS; Sola, Ricardo, Chemsitry, UPR-Río Piedras; Griebenow, Kai, Chemsitry, UPR-Río Piedras

[Chemistry 23]

Chemical Protein Glycosylation: Method to Prevent Protein Instabilities on Biosensor Application

The development of small and robust sensors with low electrical power requirement will be essential to monitor astronaut physical fitness and condition in order to prevent and minimize adverse health effects that could result from space flight. Even though there are many advances reported recently using enzymes (e.g., alcohol dehydrogenase, glucose oxidase) as the principal sensing element to monitor specific biochemical analytes, an efficient methodology to prevent short lifetime and poor loading of the protein onto the sensor is lacking. These limitations are related to enzyme stability problems. Herein, we seek to improve the fundamental understanding of enzyme stabilization in order to increase the lifetime and performance of enzyme biosensors by employing the chemical glycosylation technique developed in our laboratory (for reviews see

Solá et al., 2007, 2009). Covalent chemical glycosylation consists in decorating the enzyme with glycans using our glycan chemistry which will increase protein thermodynamic stability and prevent unfolding by caging effects. Furthermore, covalent attachment of the modified protein to a nano-material with a large surface area will increase the enzyme loading and facilitate improved reaction kinetics. In order to study the effect of protein chemical glycosylation it used the model enzyme, Subtilisin. The central hypothesis of the research is that covalent chemical modification of the enzyme with glycans will reduce conformational motions (dynamics) and increase its thermodynamic stability thus positively affecting long-term stability (Solá et al., 2006, 2007, 2009; Pagán et al., 2009).

Pena, Sandra, UPR-MAYAGUEZ; Rivera ,Luis, Chemistry,UPR Mayaguez; Singh, Surinder, Engineering Science and Materials, UPR Mayaguez, Perales, Oscar, Engineering Science and Materials , UPR Mayaguez; Oyola, Oscar, Chemistry, UPR Mayaguez

[Chemistry 24]

Development of an Analytical Method for the Production and Measurement of Singlet Oxygen

Oxygen singlet processes are a matter of current interest, mainly due to the role that these reactions play in biological processes like photodynamic cancer therapy. Photosensitized generation requires only oxygen, light, and a photosensitizer. In this work singlet oxygen measurements were carried out by photooxidation reaction of selected photosensitizers (Rose Bengal and Methylene Blue) in the presence of different quenchers (diphenyl-1,3-isobenzofuranne, sodium azide and furfuryl alcohol). The reaction is monitored with the decrease in the intensity of absorbance of the quencher with time. Solvents used are water and methanol. In these conditions, the straight line obtained for $1/\Delta A=f(1/A)$ allows to characterize the formation of singlet oxygen, and to determine the parameters of β and photooxidation reaction constants. The β values obtained are 8.88x10-7 and 1.5x10-6 for Methylene blue and Rose Bengal respectively; and photooxidation reaction constants $2.14x10^{10}$ and $1.6x10^{11}$ M^{-1} s^{-1} for Methylene blue and Rose Bengal respectively, values in good accordance with the literature. Singlet oxygen quantum yields are around 0.50-0.80 for both photosensitizers.

Rivera, Luis, UPR-RIO PIEDRAS; Betancourt, José E., Chemistry, UPR Rio Piedras; Rivera, José M., Chemistry, UPR Rio Piedras

[Chemistry 25]

Discrete Hexadecameric Fluorescent Multifunctional Self-Assembled Dendrimers in Aqueous Media

Dendrimers, from the Greek word dendron meaning “tree”, are monodisperse polymers with unique globular shape where all repeating units or branching pattern emerge radially from a central core. Herein we describe the construction of water-soluble and discrete multifunctional self-assembled dendrimers (SADs) using dendronized 8-(m-acetylphenyl)-2'-deoxyguanosine (mAG) scaffold. Our laboratory has used the mAG scaffold for the self-assembly of supramolecules in water and for the synthesis of SAD in organic media. We will present the synthesis of dendrons of three different generations: mAGDX (OH)2, (X = 1, 2, 4) and the results of studies of their self-assembly properties in aqueous media at physiological pH. Their sizes were measured by Pulse Field Gradient-NMR (PFG-NMR) and Dynamic Light Scattering (DLS) experiments. The molecular weight to size ratios reflect the fractal geometry characteristic of dendritic systems. Differential Scanning Calorimetry (DSC) reveals that their thermodynamic stability decreases for the higher generations. The three generations assembled into relatively large supramolecules, hexadecameric guanine quadruplexes, similar to those previously reported by our group. Currently we are studying: (a) the ability of these SADs to encapsulate smaller molecules, and (b) the development of fluorescent congeners. We expect these and related systems to enable future applications in drug-delivery and biological imaging.

Rivera-Sánchez, María Del C., UPR-RIO PIEDRAS; Rivera, José M., Chemistry, UPR-Río Piedras

[Chemistry 26]

Supramolecular and Optical Properties of 8-Heteroaromatic-2\'-Deoxyguanosine Derivatives

Guanosine is a self-complementary nucleoside that forms planar tetramers known as G-tetrads. Further stacking of these, aided by the complexation of metal cations, yield G-quadruplex (GQ) nanostructures. Our main objective was to control the properties of self-assembled GQ nanostructures via intrinsic parameters (i.e. structural information in the subunits). This bottom-up approach should enable the reliable construction of functional nanostructures of well defined size and composition such as the unusual dodecameric GQs.
To modulate the formation of dodecameric GQ nanostructures we synthesized a library of lipophilic 8-heteroaryl-2'-deoxyguanosine derivatives (8HetGs). The

functionalization of the guanine base with heteroaroaryl groups (e.g. pyridyl, furanyl, thiophene) tunes the supramolecular and optical properties of the resulting GQ nanostructures. We studied those properties in the presence of organic media (chloroform and acetonitrile) using KI as the source of the metal cation template. More specifically, we used 1D/2D-NMR and ESI-MS to have a better understanding of their molecularity and fidelity. However, to explore the lower self-assembly concentration (lsac), and their optical properties we also used UV absorbance, and fluorescence. In conclusion, we achieved an optimum balance between the 8HetG subunits, repulsive (e.g. steric) and attractive (e.g. π-π, dipole-dipole) non-covalent interactions, that enable the high fidelity formation of stable and discrete self-assembled GQ-dodecameric nanostructures.

Rivera-Vélez, Nelson E., UPR-RIO PIEDRAS; Montañez, Efraín, Chemistry Department, University of Puerto Rico-Río Piedras; Scibioh, Aulice, Chemistry Department, University of Puerto Rico-Río Piedras; Cabrera, Carlos R., Chemistry Department, University of Puerto Rico-Río Piedras

[Chemistry 27]

Preparation and Characterization of Unsupported Iridium, and Platinum Oxides Nanoelectrocatalysts for the Oxygen Evolution Reaction by the Rotating Disk Slurry Electrode Method

We present preliminary results of Pt/Ir oxides nanoelectrocatalysts prepared by the Rotating Disk Slurry Electrode (RoDSE). This is a fast, clean, and cost efficient method of nanomaterial preparation for water electrolysis. Ir has been widely studied and is among the best working catalysts in the literature for the Oxygen Evolution Reaction (OER) and Pt for the Hydrogen Evolution Reaction (HER). Pt/Ir electrocatalysts have shown bifunctionality in the water electrolysis process. Iridium has been electrochemically deposited on Pt black nanoparticles by chronoamperometry. Linear sweep voltammetry (LSV) was used to characterize its performance for OER by measuring the onset potential and current density after preparing a Nafion® paste electrode on Glassy Carbon (GC). One of the samples was treated at 400℃ in order to obtain the oxidized material. In comparison to Pt black and unoxidized Pt/Ir, the oxidized Pt/Ir material showed a lower onset potential at 1.35 V vs. Ag|AgCl and higher current densities in 0.5M H_2SO_4 solution. In this presentation we will show details of the materials preparation method of Ir skin or adsorption on Pt nanoparticles.

Rivero, Kennett, UPR-RIO PIEDRAS; Chakraborty, Indranil, Chemistry, UPR Rio Piedras; Raptis, Raphael G., Chemistry, UPR Rio Piedras

[Chemistry 28]

Heterobimetallic Clusters Containing a Redox-Active Fe4O4 Cubane Core

The reaction between the simple indium complex *mer*-$InCl_3(pzH)_3$ and an iron salt in the presence of a base yields a mixed-metal cluster $[In_4Fe_4(\mu_4\text{-}O)_4(\mu\text{-}pz)_{12}Cl_4]$ (pz = pyrazolato anion, $C_3H_3N_2^-$) where the core is a Fe_4O_4 cube surrounded by four $[In(pz)_3Cl]$ peripheral units. This cluster represents the first example of a redox-active Fe_4O_4 magnetically isolated cubane in which every iron is in the ferric state and the periphery is redox-inert. Such complex offers the possibility of gaining a better understanding of the redox processes that occur in the parent cluster $[Fe_8(\mu_4\text{-}O)_4(\mu\text{-}pz)_{12}Cl_4]$, which can reversibly accept four electrons across a potential window of ~1.1 V. Substitution of the peripheral metals also minimizes some of the factors that affect the interpretation of the magnetic susceptibility studies. The energies of different electronic configurations have been computed using spin-unrestricted density functional theory. Calculations reveal weak antiferromagnetic coupling between the iron centers, mediated by the μ_4-O bridges.

Rodriguez, Idaliz, UPR-RIO PIEDRAS; Robles, Emily, Chemistry Department, UPR-RP; Raptis, Raphael G., Chemistry Department, UPR-Rio Piedras

[Chemistry 29]

Dendritic Redox-Active Fe4O4-Core Complexes

Encapsulated redox-active complexes are of great interest for biomimetic studies and application as memory and electronic storage devices. Studies have shown that encapsulation by covalent attachment of dendrons to a redox core causes changes in its electrochemical properties. The goal of this investigation is to synthesize supercomplexes based on caged redox-active $Fe_8(\mu_4\text{-}O)_4(\mu\text{-}4\text{-}Rpz)_{12}X_4$ (where pz is pyrazolate and X is -Cl, -NCS, $-OC_6H_4CHO$), in order to assess their potential as electrochemically operated, molecular memory devices. These Fe_4O_4-core iron complexes are very attractive from the standpoint of their electrochemical properties, since they show four consecutive, closely-spaced, reversible redox processes in cyclic voltammetry. Our recent efforts have been aimed at synthesizing Fe_4O_4-core dendrimers, either by reaction of dendrons at the X position of an $Fe_8(\mu_4\text{-}O)_4(\mu\text{-}4\text{-}pz)_{12}X_4$ complex, or by employing a dendritic pyrazole. Details on the synthesis and characterization of the compounds, based on dendron $(CH_2CHCH_2CH_2O)_2C_6H_3CO_2CH_3$, are shown.

Santana, Juan A., UPR-RIO PIEDRAS; Ishikawa, Yasuyuki, Department of Chemistry, University of Puerto Rico-Rio Piedras

[Chemistry 30]

Density-Functional Theory Study of O2 Adsorption on Platinum Electrode Under Electrochemical Conditions

The adsorption of O_2 on platinum electrode under electrochemical conditions has been studied by density functional theory methods to gain a thorough atomic-level understanding of the oxygen reduction reaction. The computational results reveal new insight into the interaction of O_2 and the OH-coverage platinum surface. Vibrational frequency analysis of adsorbates allows the assignment of recent experimentally detected infrared bands [*Phys. Chem. Chem. Phys.*, 2010, **12**, 621].

Santos-Figueroa, Gilmarie, UPR-RIO PIEDRAS; Gioda, Adriana, Department of Chemistry, University of Puerto Rico; Mayol-Bracero, Olga L., Institute for Tropical Ecosystem Studies, University of Puerto Rico

[Chemistry 31]

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

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 =~0.33 µm) 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.

Silva, Diana, UPR-RIO PIEDRAS; Rivera, José M., Chemistry, University of Puerto Rico-Río Piedras

[Chemistry 32]

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

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 hexadecameric 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) characterization in their monomeric and assembled states.

Torres, Zally, UPR-RIO PIEDRAS; Velazquez, Stephanie, UPR-Humacao; Barletta, Gabriel, UPR-Humacao

[Chemistry 33]

Thermal Stability of the Serine Protease Subtilisin Carslberg in Organic Solvents/ H©üO Mixtures

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 () of subtilisin C. was studied in acetonitrile/H_2O 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. 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. 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. 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 though.

Education

Caceres, Rita, UPR-RIO PIEDRAS; Ortiz-Zayas, Jorge, Instute for Tropical Ecosystem Studies; María E. Thiele, Escuela Intermedia Manuel Martín Monserrate, Santa Isabel

[Education 01]

Protecting the Puerto Rican Crested Toad: An Education and Outreach Program

The Puerto Rican Crested Toad (PRCT), the only endemic toad known in Puerto Rico, was the first amphibian to receive Species Survival Plan status (SSP). The SSP is both a captive breeding and conservation program administered through the American Zoo and Aquarium Association (AZA). One essential part of this program is to be able to do education and outreach activities that ensure the general publics participation in the activities related to the conservation of the PRCT. "Protecting the Puerto Rican Crested Toad" was an education and research program developed for middle school students from the Manuel Martín Monserrate School in Santa Isabel, Puerto Rico. The program included four parts: an introduction to field work and gathering data; characterization of the aquatic and terrestrial habitat available for the toad; a discussion of the data collected and data analysis; and student presentations of what they have learned to their fellow students and parents from their school and neighborhood. The objective of this project was to encourage students to recognize the importance of protecting a threatened species, their habitat, and at the same time encouraging science and research-based learning.

Morales-García, Flavia, UPR-RIO PIEDRAS; Otero-Montañez, James K., Escuela Secundaria Especializada en Ciencias, Matemáticas y Tecnología (CIMATEC), Municipio Autónomo de Caguas; Soto-García, Lydia L., Institute for Tropical Ecosystem Studies and Department of Chemistry, University of Puerto Rico, Río Piedras Campus; López-Alvarado, Iván J., Department of Physics, University of Puerto Rico, Río Piedras Campus, Mayol-Bracero, Olga L., Institute for Tropical Ecosystem Studies, University of Puerto Rico, Río Piedras Campus; Mayol, Ana R., Intitute for Functional Nanomaterials, University of Puerto Rico, Río Piedras Campus; Álvarez, Héctor J., College of Education, University of Puerto Rico, Río Piedras Campus

[Education 02]

Atmospheric Chemistry Research as a Tool to Augment Students' Scientific Inquiry

A fellow-teacher team from the NSF funded GK-12 program: *From Hectares to Nanometers: Multidisciplinary Explorations of Functional Nanosciences and Tropical Ecosystems* developed a series of inquiry-based interdisciplinary educational modules where they bring research into the classroom. *"One Universe, Many Worlds"* is our program's unifying theme by which GK-12 Program fellow-teacher teams compare the macro world with the nano world in order to understand the recurring patterns in nature. Therefore, in order to promote student research and scientific inquiry, the fellow-teacher team used the fellow's research topics and results in atmospheric chemistry to create a series of hands-on activities where student (n = 80) were able to perform basic atmospheric research. Then, the data obtained were used to suggest sources and solutions to the atmospheric pollution problem. The atmospheric chemistry activities where implemented at *Escuela Secundaria Especializada en Ciencias, Matemáticas y Tecnología* (CIMATEC) while the teacher was covering the topic of environmental pollution in the 7th grade life science course. Additional activities such as manipulative and in-class demonstrations are being developed to reinforce the environmental concepts given in class. As a result, the number of interdisciplinary projects submitted to the 2010 Scientific Fair increased in comparison to last year. Furthermore, there was an increase in the number of students presenting projects related to environmental issues. Pre- and post-tests were used to assess student's learning on the topics concerning the fellow's research. This poster will describe all the strategies used to incorporate and align atmospheric research in the 7th-grade life science curriculum.

Engineering

Anaya, Nelson, UPR-MAYAGUEZ; Been, Katherine

[Engineering 01]

Polymer-aided Alcohol Flushing to Enhance TCE remediation: Effect of Methanol Concentrations and Contact Times

In situ flushing for remediation of dense non-aqueous phase liquids (DNAPLs) contaminated soil and groundwater is done by the injection of an aqueous solution into the zone contaminated with them. The system is followed by down gradient extraction of groundwater and elutriate (flushing solution mixed with the contaminants) and aboveground treatment. Permeability is the principal cause which the flushing solution moves through a porous medium and, therefore, determines how effective the remediation is. The objective of the research is to evaluate a polymer-aided alcohol flushing by overcoming permeability contrast in the heterogeneous subsurface setting with different permeability. Trichloroethylene (TCE) was tested as the target DNAPL. The parameters measured were the pressure developed and the time reached the flushing solution, transport extent and concentration of the DNAPLs.

A series of subtasks were conducted to meet the objective. Presented will be the results from the one-dimensional, vertically oriented laboratory column designed for efficiency of alcohol flushing for TCE removal. Results indicate that a 5% (v/v) methanol solution as the in situ flushing agent increases the rate of TCE flushing due to solubility and/or mobility enhancement. A 10% methanol flushing showed similar results to the 5% methanol case. In addition, an increase of contact time enhanced overall TCE remediation effectiveness.

Avilés-Barreto, Sonia L., UPR-MAYAGUEZ

[Engineering 02]

Effect of Sulfonation Level and Counter Ion Substitution on the Water Swelling and Proton Conductivity of Poly(styrene-isobutylene-styrene) Membranes

In this study, poly(styrene-isobutylene-styrene) (SIBS), a triblock copolymer, was functionalized with sulfonic groups in order to obtain more selective membranes for gas sensors and fuel cell applications. Sulfonated SIBS was characterized using fourier transform infrared spectroscopy (FTIR) and elemental analysis (EA), to confirm and determine accurate sulfonation levels. Subsequently, the sulfonated polymer was neutralized with three +2 cations: Mg^{+2}, Ca^{+2} and Ba^{+2}; to reduce water swelling and create highly selective polymer-metal

nanocomposite membranes. Since the potential interconnectivity of the membrane's sulfonic groups is very important for the performance of these dielectric materials, the proton conductivity of the samples was measured. Results show that proton conductivity increases with sulfonation level until a maximum suggesting an optimum ion exchange capacity (IEC) level, while counter ion substitution decreases proton conductivity. Thermogravimetric analysis (TGA) were performed in order to evaluate the thermal stability, which increases with sulfonation level; while counter ion substituted membranes maintained the same degradation temperature. To complement the studies, absorption limitations and their effect on the membrane transport were investigated through water swelling experiments. Although water swelling increases with sulfonation, the effect of metal type will be further discussed.

Barajas, Ulises, UPR-MAYAGUEZ; Barajas, Ulises, Ingenieria Civil y Agrimensura, Universidad de Puerto Rico: UPR-Mayaguez

[Engineering 03]

Methodologies for the Analysis of Prestressed and Preflex Bridges Superstructures

This study provides a description of the analysis of prestressed and preflex beams applied to bridge superstructures. Considering the importance bestowed in these structures to properly withstand service loads, this study includes the following tasks: i) describe the analysis and load rating methods of prestressed beams based on AASHTO requirements; ii) to develop a methodology for the analysis and load rating of preflex beams based on AASHTO stress limits (including estimation of its nominal capacity); and iii) parametric study of pre-tensioned and preflex bridges with four different span lengths. Results show that AASHTO distribution factors are conservative in comparison to the values obtained from three-dimensional finite element models. In terms of the comparison between both systems, the composite preflex systems provide slenderer sections (in the order of 62%) than prestressed concrete AASHTO I-type sections. Contrarily, live load deflections in the pre-tensioned systems were smaller (in the order of 8%), but for no case AASHTO limits were exceeded.

Blagg, Amanda, UPR-MAYAGUEZ; Valentin, Ricky, Mechanical Engineering, UPRM; Perales, Oscar, General Engineering, UPR-Mayaguez

[Engineering 04]

Optimization of Electrospun Chitin Fibers for Arsenic Adsorption

Arsenic, a carcinogenic toxin, is introduced into groundwater by natural and industrial sources. Chitin, found in the structure of crustacean shells and fungi, can be functionalized with mercaptans to adsorb such heavy metals via sulfhydryl groups (-SH). Though it is biodegradable and has good mechanical

properties, applications have been limited because of its poor solubility in most solvents. In this study, chitin will be irradiated to decrease the molecular weight, dissolved in HFIP, and subsequently electrospun to increase surface area and therefore adsorption sites. The thermomechanical and structural properties of the fibers will be optimized by controlling solution parameters such as molecular weight and solution concentration; environmental parameters such as humidity and temperature; and processing parameters such as voltage, distance, and feeding rate. The morphological characteristics of the fibers will be analyzed with scanning electron microscopy (SEM) and the structure with X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR). The thermo-mechanical characterization of the fibers will also be presented and discussed.

Buitrago, Fabiola, UPR-MAYAGUEZ; Figueroa, Alberto, Civil Engineering and Surveying, UPR Mayaguez

[Engineering 05]

Statistical Analysis of Red Light Running Events at Signalized Intersections in Puerto Rico

One of the causes for crashes in signalized intersections is the phenomenon of Red Light Running (RLR), which is related to more than 100,000 crashes and approximately 1,000 deaths in the United States. RLR is also a significant problem in Puerto Rico where the crashes related to this cause is approximately 5,000 events annually. Various factors such as flow rate, number of cycles, phase termination, travel time, speed, approach grade, and yellow interval duration, have been theorized to contribute to RLR.
The objective of this study was to collect traffic behavior and intersection geometry data to identify relationships with RLR violations. Data was collected at nine signalized intersections located in the Western Region of Puerto Rico. The analysis of the data indicates a high occurrence of RLR events compared to results from other countries. The average RLR frequency in the studied intersections is four times higher than the values reported in the other studies reviewed. A statistical analysis showed that RLR events increase as the traffic flow rate at an intersection approach increases. Other variables that might be potential factors of RLR events, but where further data is needed to reach statistical significance, are vehicle speeds, roadway longitudinal grade, signal green time, and the ratio of green time to cycle time. Future analysis should include the collection of traffic control parameters, additional traffic operation parameters, such as deceleration rates, and human factors.

Calero, Carlos, UPR-MAYAGUEZ; Albert figueroa, Ingenieria Civil, UPR-Mayaguez

[Engineering 06]

Quality of Service Measures for Special Demand-Response Transit Services

The “Carros Públicos” is a special demand-response transit service developed for the Commonwealth of Puerto Rico. Outside of the San Juan Metropolitan Area, the “Públicos” is the only transit service available for the population, providing local service and connecting trips between metropolitan areas with population less than 250,000 inhabitants. This system is composed of private individual owners that operate their vehicles, sedans or vans, in particular routes with limited government supervision, primarily in terms of fare and route selection. Service is provided for urban, intermunicipal and regional trips. Although the system has terminals and stops, it does not have an established frequency of service or trip schedule. There is no established method for determining the quality of service provided by this system.

The objective of this research is to identify transit quality of service measures based on a user perspective that can be applied to the “Públicos”. To accomplish this objective, the study will survey system users to identify their preferences and perceptions toward transit service measures and operation characteristics of the transit system. The study will evaluate existing transit quality of service methodologies, such as the one in the Transit Capacity and Quality of Service Manual, to determine if these measures assess objectively the quality of service provided by the “Públicos” system.

Cameron, Ana Raquel, UPR-MAYAGUEZ; Alexandra Breban, Department of Chemical Engineering, University of Puerto Rico, Mayagüez; Aldo Acevedo-Rullán, Department of Chemical Engineering, University of Puerto Rico, Mayagüez

[Engineering 07]

Phase Behavior of Carboxylated MWCNT Dispersions in Liquid Crystalline Polymer Solutions: Rheology and POM

Nematic liquid crystalline polymers (LCP’s) are interesting anisotropic fluids due to their inherent orientational order (i.e. molecules tend to align in the same direction). Orientation enhances and allows for the control of the mechanical, electrical and thermal properties. Yet, physical properties may be affected by inclusion of particles. The effect can be positive or negative depending on the shape and aspect ratio of the particles, and not the same for all properties. Carbon nanotubes (CNT) are ideal candidates for the development of nanocomposites. In this research, we determinate the particle loading effect of

carboxylated-MWCNTs on the phase behavior of hydroxypropylcellulose matrices using both rheological and polarized optical microscopy measurements. We also evaluate the particle loading effect on the viscoelastic properties of these solutions.

Chavez, Ermides, UPR-MAYAGUEZ; Lopez, Neshma, Department of Chemical Engineering, University of Puerto Rico Mayaguez Campus; Uwakweh, Oswald, Department of Engineering Science and Materials

[Engineering 08]

Mosbauer Spectroscopic Measurements of Mechano-Chemical Syntheses of ZnFe2O4

The mechano-chemical synthesis of single phase nanoparticles of $ZnFe_2O_4$ was carried out as a function of ball-to-powder ratio (BPR) in high energy ball milling (HEBM) process using stoichiometric amounts of solid precursors to yield the single phase spinel structured ferrite via the reaction: $ZnO + \alpha\text{-}Fe_2O_3 \rightarrow$ ZnFe2O4. The reaction occurred via rapid particle size reductions leading to the formation of metastable phases prior to completion. Substantively, the synthesis based on BPR = 40:1 was faster with the formation of non-magnetic nanoparticles due to superparamagnetism in comparison to the 20:1 case. While it took 5 hours for the BPR=40:1 to synthesize, it was 15 hours for the ball milling with BPR=20:1. The variation of the local Fe sites in both syntheses showed that BPR as a synthesis parameter is an important factor in the mechano-chemical syntheses of nanostructured ferrospinels.

Concepcion, Daniel, UPR-MAYAGUEZ; Hwang, Sangchul, Civil Engineering, UPRM; Juan Falcón, Civil Engineering, UPR-Mayaguez

[Engineering 09]

Engagement of UPRM Engineering in Sustainable Water Treatment Technologies

There are approximately 286 systems not served by the Puerto Rico Aqueduct and Sewer Authority (Non-PRASA) in Puerto Rico; of these, 95% percent do not comply with bacteriological standards (as of the year 2008). Of the Non-PRASA systems serving a population of less than 100, more than 60% do not receive any water treatment. Meanwhile, systems that serve a population between 101 and 3000 include some filtration and more than 80% use chlorine for disinfection purposes. The Río Piedras community in San Germán constitutes one of the latter Non-PRASA systems on the island. The Rio Piedras community possesses facilities to collect surface water from the Rio Cain and gravity head conducts this water to a horizontal flow pre-gravel filter followed by a slow sand filter coupled to a tablet chlorinator and a distribution tank with a capacity of 80,000 liters. A Non-

PRASA community water treatment system confronts several problems; but its main challenge is the scarcity of water quality assurance as well as the maintenance operations combined with technical assessment. The University of Puerto Rico at Mayagüez (UPRM) has a project agreement with United States Environmental Protection Agency (USEPA) at Cincinnati together with Shaw Environmental & Infrastructure, inc. to provide telemetry monitoring of water quality parameters at the community. Also a small scale Experimental Drum Filtration (EDF) unit developed at the USEPA T&E facilities at Cincinnati has been deployed at the Rio Piedras site in order to assess its performance on the field. While the EDF system has been deployed it has treated over 60,000 liters of water with minimal maintenance on a weekly basis over a period of 18 months. Water quality parameters such as: dissolved oxygen, pH, temperature, turbidity, residual chlorine, specific conductivity, water level and bacteriological parameters including Heterotrophic bacteria and Coliforms have been monitored during a period of more than 18 months on this community. Trained students fromthe Civil Engineering Department's Environmental Engineering Laboratory have involved in both telemetry monitoring of community-operated water treatment system and the EDF unit as part of their hands-on research experience, which integrates social work with practical training on sustainable water treatment technologies. The current water related environmental issues demands for a multidisciplinary approach to engineering education with emphasis on technical knowledge, diverse backgrounds teams and hands-on training experience. This venture has provided a unique opportunity for UPRM students to involve in community work and multidisciplinary teams. With a gravity-fed hydraulic design and the utilization of solar power, telemetry troubleshooting and instruments calibration as well as traditional physiochemical and microbiological water quality parameters has provided an excellent opportunity to assemble an interdisciplinary team in order to correctly attend the multiple scenarios that arise on field work. Eleven undergraduate and graduate students spanning four different engineering departments have collaborated on the project for over two years. The Departments involved so far have been Civil, Chemical, Mechanical and Electrical Engineering of UPRM.

Cortes, Natalia, UPR-MAYAGUEZ; De Jesús Padilla, Xavier F., Mechanical Engineering, University of Puerto Rico-Mayagüez; Calderón, Hermes E., Civil Engineering & Surveying, University of Puerto Rico-Mayagüez; Suárez, O. Marcelo, Engineering Science & Materials, University of Puerto Rico-Mayagüez

[Engineering 10]

Thermomechanical Characterization of AL-CU-MG Composites Reinforced with Diboride Particles

Aluminum-based composites have been evaluated for aerospace and transportation applications where light weight and appropriate strength at high temperatures are key requirements. The present work focused on the study of

mechanical response of a series of Al matrix composites at room and high temperature. The composite matrix contained 2.5 wt. % Cu and 1 wt. % Mg and was reinforced with different levels of boron (0, 1, 2, 3 and 4 wt. %) forming AlB_2 particles. The specimens, fabricated via gravity casting, were tested using a thermo-mechanical analyzer under constant compression loads to reveal the composite hardness and their response under creep conditions. Additionally, the composites were tested using a dynamic mechanical analyzer to corroborate their creep behavior. These experiments were conducted at 470ºC under an applied compression of 0.24 MPa. Our results indicated that even at 300ºC higher concentration of diboride particles helped the composite retain high hardness and effectively reduced the compressive creep strain compared to an unreinforced alloy with similar concentrations of Mg and Cu.

Cruz, Alvin, UPR-MAYAGUEZ; Díaz, Ruben, Mechanical Engineering, UPR-Mayaguez

[Engineering 11]

Single Particle Isolation by Pressure Difference in a µ-fluidic Channel

The increasing interest for dedicated analysis of single particles at microscopic scales, such as biological cells, has led researchers to create micro-fluidic systems capable of trapping particles in a liquid flow. The most common trapping mechanism is by physical obstruction which is simple but it has its limitation.

The present study evaluates the possibility of using a pressure difference trapping mechanism to overcome the limitations of the mentioned system. The proposed micro-fluidic device will be fabricated using soft lithography and consists of parallel canals link by small apertures that will function as traps. Two independent pressure driven flows are introduced across the channels and a pressure difference will emerge between the channels. The higher pressure fluid will pass from one channel to the other, thus trapping the particles.

Mathematical studies have been performed using COMSOL and these models showed that depending on the geometry of the channels a significant pressure difference can be achieve. Two types of experiment have been performed one with 2um fluorescent polystyrene beads and another with 20um polystyrene beads. The fluorescent beads have been used to study the directionality of the flow and the larger beads were used to study the behavior of the particles. Experiments showed that the 2um beads follow a similar behavior as the one predicted by the COMSOL models and the experiments with 20um beads demonstrated that the apertures were capable of trapping and retaining the beads and by changing the flow rates the beads were released to their corresponding flow.

Feliciano, Jeannette, UPR-MAYAGUEZ; Sodhi, Manbir, Industrial and Systems Engineering, URI

[Engineering 12]

Driver Eye Movements during merging maneuvers into Incoming Highway Traffic

A merge can be defined as a maneuver performed by a driver who must enter into to a faster moving traffic stream. Previous work on driver behavior when merging addresses lane change behavior, however this study looks at eye fixations as drivers merge into incoming highway traffic. When planning to merge, drivers use the acceleration lane to gaze at incoming cars. Since traffic and speed of the merge lane is less than that on regular lanes, drivers may feel safe spending more time looking backward or at the mirrors. Under these circumstances, gaze durations may be longer than for a single lane change.

Using field data collected as part of an ongoing study to examine the performance of drivers when using GPSs, eye movements of drivers where the subjects merge to the right lane of the US 1 south bound from a ramp in Narragansett Ave. E, Rhode Island were examined. US1 is a rural arterial road with 2 lanes in both directions. In order to gather data for this project, 19 test drives were performed. Because of ambient noise, only 14 drives could be used to determine the average glances and 9 to calculate their average duration. The primary reasons were bad eye data because excessive blinking and errors in calibration or synchronization.

Analysis of the data confirmed that the most common eye movement during merging to left incoming traffic was to glance to the left side mirror. This was done by 85.7% of the subjects. The back glance, whereby the driver turns his/her head to look at the incoming traffic stream, involves glances of the longest duration (842ms) and this was the second most frequent eye movement by the subjects. As expected – eye movements during the merge operation involved mean durations that were greater than for a single lane change (350ms). Taking into consideration whether the maneuver was preformed with or without incoming vehicles, the data was split to see the impact on the glance mean duration. It was observed that duration varies depending on the incoming traffic. Without incoming vehicles the glance mean duration (100ms) is less than the single lane change (350ms) and with incoming vehicles (367ms) it is greater. This research is one step for future research on merging maneuvers. These data could be a starting point to new research such as an analysis of crashes during the maneuver and to the length of the acceleration lane. The information also is useful for further traffic modeling.

Florian, Vivian, UPR-MAYAGUEZ; Acevedo, Aldo

[Engineering 13]

Surfactant Effect on the Solution Rheology and Casted Film Properties of Griseofulvin Loaded HPMC

The focus of this work was to study the effect of surfactant concentration and net charge on the processing and physical properties of biopolymer film loaded with an active pharmaceutical ingredient (API). Hydroxypropylmethylcellulose (HPMC) was chosen as the structural matrix. Three surfactants were studied: sodium dodecyl sulphate (SDS), cetylpyridinium chloride monohydrate (CPC) and lecithin, which are anionic, cationic and neutral, respectively. The API used was Griseofulvin, a poorly water soluble drug. Thermotropic gelation and steady-state rheology of aqueous HPMC solutions, water evaporation rate during film formation, film morphology, drug release profiles, and drug distribution were studied as a function of concentration and type of surfactant. An increase in the gelation temperature was observed when surfactant was added to HPMC solution. Evaporation rate did not show any significant difference with surfactant concentration, but it showed dependence with type of surfactant. Drug release showed to be dependent on both concentration and type of surfactant. Observations are discussed in terms of preferential association of the surfactant with drug or the polymeric matrix.

Gamez, Liliana, UPR-MAYAGUEZ; Martínez María, Department of Chemical Engineering

[Engineering 14]

PLATINUM CLUSTERS SYNTHESIS PROCESS STUDY BY X-RAY DRIFFRACTION

The preparation of platinum clusters includes both the loading of metal compound in or on the zeolite crystals and the treatment governing the final dispersion of the metal. The loading is usually designated to introduce the metal into the zeolite pore system. However for some applications one may wish to selectively obtain the metal on the external surface. This can be achieved by impregnating the zeolite with metal particles. Here, ion exchange in solution was used as route to introduce metal in the porous of framework. By the other hand, appropriate treatments are needed to obtain the highest metal dispersion, such as, dried, calcination and reduction. Nitrogen, Oxygen and Hydrogen respectively were used to carry out these stages. The samples were studied and compared at different heating rate and loading but the temperature conditions for the dried, caltination and reduction in all these were the same.
XRD was used to study the process under realistic conditions, i.e by means of an in situ reactor. These reactions were monitored with a tempeture control and the

diffraction patterns were recorded to obtain an indication of particle sizes, crystallographic planes, and Bragg relation to give the corresponding lattice spacing, which are characteristic for a particular compound. The X-ray diffraction signals showed that the (NH3)4(NO3)2 decomposition temperatures were between 200-250℃ and the crystallite sizes increase when the heating rate is increased in the calcination process, and when the loading was increased .
In these results, X-ray Diffraction had an important limitation, because clear diffraction peaks were only observed when the sample had sufficient long range order. For this reason is recommended improve that with a better technique.
Garcia, Glorimar, UPR-MAYAGUEZ; Oscar Perales-Perez, Department of Engineering Science and Materials, University of Puerto Rico, Mayagüez Campus

[Engineering 15]

Ag-based Nanofluids for High-Thermal Conductivity Applications

Metal-bearing nanofluids are receiving increased attention due to their expected enhanced thermal conductivity when compared with bare cooling fluids. Nanosize metals, e. g. gold, silver, copper or conductive carbon nanotubes are considered promising candidate materials to suspend them in typical cooling fluids. Our work is focused on the evaluation of silver crystal size and shape on the thermal conductivity of ethylene glycol, a typical cooling fluid. As the first step of our research, we have synthesized silver nanoparticles in ethylene glycol. Control of crystal size and shape at the nanoscale are attempted by suitable selection of the synthesis conditions and the presence of shape-control agents like Chloride salts. Synthesized nanocrystals were characterized by X-ray diffraction (XRD), Scanning electron microscope (SEM) and UV-vis spectroscopy.

Gorbea, Ivelisse, UPR-MAYAGUEZ; Valdes, Didier, Civil Engineering and Surveying, UPR Mayaguez

[Engineering 16]

Assessment of Land Use Transport Modeling Frameworks to Analyze Mass Transit Alternatives in Puerto Rico

Puerto Rico has particular socioeconomic, geographical, and population characteristics that present significant challenges in the development of its transportation system. It is a densely populated island (1,112 persons per square mile) where 94 percent of its population lives in urban areas (according to the 2000 US Census Bureau) in a limited geographical boundary of 3,425 square miles. Meanwhile, the transportation system operates with more than 4 million

registered vehicles, reflecting a high dependence toward the use of the private motor vehicle (87% modal share). Puerto Rico shows a trend of urban sprawl and transportation development that urges a new approach toward how transportation infrastructure and mass transit in Puerto Rico relates to land use issues in order to conform livable places. This study will review this relationship of transportation and land use examining transportation modeling studies that integrate land use variables comparing these approaches to similar studies in Puerto Rico.

Transportation is visualized in this study as part of the urban and regional development where the travel demand analysis or alternative analysis should include land use and socioeconomic variables in order to achieve better access, mobility, livable spaces and building environment for our citizens. Transport modeling frameworks will be examined as transportation planning tools for mass transit alternatives. The main objective of this study is to assess and learn from successful case studies that consider land use transport model frameworks in order to analyze how these land use variables were considered or could have been considered in alternative analysis studies in Puerto Rico. The first step in this study will define a land use model framework, by examining literature related to this subject through case studies, focused on transport modeling frameworks using land use variables. Similar studies of Puerto Rico will be then analyzed in the light of these case studies and how land use was considered in alternative analysis. Transportation models in the case studies will be examined with the objective to identify the assumptions or criteria behind the selection of land use variables, which land use variables were used, what systems or software, how the variables interact, the results of the modeling. At the end of the analysis, several variables will be selected to incorporate land use in transportation planning modeling using a robust framework for Puerto Rico.

Hidalgo-Hernandez, Ruth, UPR-MAYAGUEZ; Plaza, Nayomi, Mechanical Engineering, University of Puerto Rico-Mayaguez Campus; Suarez, O. Marcelo, Engineering Science and Materials, University of Puerto Rico-Mayaguez Campus

[Engineering 17]

Tribological Characterization of Al-Cu-Mg-B Composites Subject to Mechanical Wear

The tribological properties of a series of aluminum matrix composites reinforced with AlB_2 particles developed for machinery parts intended for aerospace and automotive applications were evaluated. This thesis encompasses the microstructure characterization of those composites and the assessment of their tribological response when subject to pin-on-disk wear test. SEM and EDS analyzes permitted to identify the phases present and correlate the composite microstructure with its mechanical and tribological behavior. SEM observations also allowed identifying the wear mechanisms involved during the pin-on-disks

tests against a 440 martensitic stainless steel ball. Wear coefficients were contrasted with Brinell and superficial Rockwell hardness. It was possible to establish the effect of chemical composition on the wear volume and wear coefficient for different composites compositions. This will then permit obtaining machinery parts with optimal performance, achieving high durability, high resistance and the reduction of maintenance costs.

Huertas-Miranda, Javier A., UPR-MAYAGUEZ; Marínez-Iñesta, María M., Chemical Engineering, UPR-Mayagüez

[Engineering 18]

Studies of the Combined Effect of Si/Al and Temperature on theTemplated Synthesis of Platinum Nanostructures in Mordenite

Zeolites are aluminosilicate crystalline structures with pores ranging between 0.4 to 1.4 nm. Depending on the zeolite framework, these pores can form one, two, or three-dimensional channels. These channels can be theoretically used in the templated synthesis of metal sub-nanostructures. In the case of zeolite frameworks with one-dimensional channels, such as mordenite, the pores can be used in the synthesis of metal nanowires. A synthesis process of metal nanostrucures using zeolites as templates will depend on many factors such as precursor compounds, zeolite framework, zeolite composition, and temperature. In the present work we are focused on the combined effect of zeolite composition and temperature on the template synthesis process. Metropolis Monte Carlo simulations and geometric minimizations using the *pcff* forcefield have been done to study the effect of the zeolite's silicon to aluminum ratio (Si/Al) and the temperature on the positioning of Pt metal atoms inside the mordenite (MOR) framework. It has been found that low Si/Al and low temperatures promotes the positioning of Pt atoms inside the main pore channels of the MOR framework, which is where metal nanowires could be formed. On the other hand, high Si/Al and high temperatures promotes the positioning of Pt atoms in the side pockets of the MOR structure. This suggests that there are in fact optimal conditions for the formation of subnanometer wires in zeolites.

Mera, Daniel, UPR-MAYAGUEZ; Santiago, Nayda, Electrical and Computer Engineering, University of Puerto Rico, Mayaguez Campus

[Engineering 19]

Low Power Software Techniques for Real Time Operating Systems

Power consumption is an important constraint in embedded system running real time operating system (RTOS). Many approaches have been developed to reduce the power consumption in embedded systems at the hardware level, at the operating system level, and at the higher levels of abstraction. However, the

optimizations oriented to RTOS have been mostly directed to sophisticated embedded systems. This work presents an analysis the operating system level optimizations: dynamic frequency scaling, memory management strategies and low power modes and their significance in the power reduction of medium and small embedded systems running RTOS. Design of experiments techniques (DOE) allowed identifying the impact in power reduction of the system. We present experiments with optimizations applied to the FreeRTOS real time operating system on three different platforms: the LM3S811 and the MSP430F149 from Texas Instrument, and the ATmega323 from ATMEL using two different set of benchmarks.

Miranda, Felix Gabriel, UPR-MAYAGUEZ; Aldo Acevedo, Department of Chemical Engineering, University of Puerto Rico at Mayaguez

[Engineering 20]

Characterization Studies of Nematic Co-Polymer PHBA-PET Extruded Nanocomposites

Thermotropic liquid crystalline polymers are anisotropic materials with a high degree of molecular orientation when extruded. This property makes them suitable for the addition of nanoparticles since they can be oriented within the matrix in order to add and/or enhance polymer properties, resulting in a value-added composite. Nevertheless, particle shape and concentration may affect the liquid crystalline order causing an unwanted effect. In this work, we studied the effect of different particle shape such as anisotropic platelet-like clay nanoparticles, spherical nanosilica, multiwalled carbon nanotubes and halloysite nanoclays on the nematic thermotropic co-polymer, i.e. 60:40 poly(4-benzoic acid-co-ethylene teraphthalate) (PHBA-PET). Nanocomposite films were produced by direct melt blending using a Haake MiniLab2 twin-screw extruder. The rheological and thermal properties have been studied as a function of formulation parameters in a Reologica StressTech HR rheometer and a TA Q-2000 differential scanning calorimeter (DSC) while composite morphology has been studied using a JEOL scanning electron microscope (SEM).

Nieves, Alvin, UPR-MAYAGUEZ

[Engineering 21]

SnowFlake Expansion

The SnowFlake expansion project is a comparison of four US states and a US territory using various road safety metrics. It is based on previous studies that compared European countries to each other, and later compared a European country to a US state. These comparisons of different road safety metrics help to understand differences in road safety, laws, programs and how the road safety in

general has been improving over time. This project looks specifically at selected safety performances for Connecticut, Massachusetts, Rhode Island, Texas and Puerto Rico, primarily over the years 2004 to 2007.

Several different metrics can be used to assess various aspects of road safety, including fatalities per vehicle mile traveled (VMT), per capita, per kilometer of road infrastructure, and others. There are many similarities and differences that can be identified in the US regarding road safety in the different states based on these metrics. For example, in this study Texas and Puerto Rico had higher fatality rates on many of the metrics, while Massachusetts, Connecticut, and Rhode Island showed similar fatality rates for several, but not all of the metrics. The latter three states are also considered as a whole New England Region, and then again compared with Texas and Puerto Rico.

Polanco, Maximo, UPR-MAYAGUEZ

[Engineering 22]

Vehicle Headway Management on Rhode Island Highways.

This research comes as a second approach of a preliminary study. The preliminary study aimed to identify the leading causes of tailgating. This research aims to identify “tailgating” as one of the main issues on highways and possible means for tailgating treatments. Tailgating is the dangerous practice of following too close the vehicle in front, and as a driving behavior it is one of the major causes for the rear end crashes. To identify tailgating as one of the most important causes of rear end crashes a vehicle headway analysis was conducted, it consisted of a video analysis on specific segments of major Rhode Island highways. To identify effective means for tailgating treatments a questionnaire survey was conducted. The survey presented various tailgating treatments to identify the preferences of the drivers.Through the video analysis tailgating was confirmed as an issue in the Rhode Island Highways. The results of the survey indicated that the majority considered “tailgating” a serious offense. Between the few different tailgating treatments presented in the survey, most drivers preferred the horizontal bars treatment. They also indicated that properly designed dynamic overhead message signs using both graphics and words could help them better understand the proposed tailgating treatment systems.

Quinones, Leonel, UPR-MAYAGUEZ; Martínez-Iñesta, Maria M., Engineering Department, University of Puerto Rico Mayagüez

[Engineering 23]

Synthesis of Platinum Nanostructures in Zeolite Mordenite Using a Solid-State Reduction Method

The potential uses of nanowires are ample and include diverse areas such as drug delivery, cancer treatment, biosensors, reaction catalysis, and magnetic data storage. Specifically, integrated sensor devices based on platinum nanowires have been reported to provide higher sensitivity, improved signal-to-noise ratio (S/N), and a diminution of the threshold detection limit. Furthermore, platinum nanowires could play an important role as either interconnection elements or as active components in nanoscale electronic devices.

Platinum nanoparticles and nanowires have been synthesized for the first time in a porous template using a solid state reduction method. Tetrammine platinum nitrate was introduced into the pores of zeolite mordenite via incipient wetness impregnation and it was reduced using sodium borohydride in its solid state form. TEM and HRSTEM results were used to characterize the resulting nanostructures. It was found that with this method it was possible to obtain single crystal nanowires along the edges of the zeolite particle. It was also found that the molar ratio of the reducing agent to platinum atoms were critical parameters for the formation of either uniform nanoparticles or nanowires and that using a regular aqueous sodium borohydride solution it is not possible to obtain nanowires in this zeolite.

Ramos, Glorimar, UPR-MAYAGUEZ; Santiago, Paulette, Chemical Engineering, UPR-Mayaguez; Manzano, Roberto, Mechanical Engineering, UPR-Mayaguez; Suárez, O.Marcelo, Department of Engineering Science & Materials, UPR-Mayaguez

[Engineering 24]

Fabrication of Functionally Graded Aluminum-Based Targets for Sputtering Deposition of Hybrid Composites

New polymer/Al-based hybrid composites have been proposed for device fabrication, which require precise fabrication of sputtered Al-Si composite layers reinforced with AlB_2 and AlB_{12} particles because of their tunable elastic modulus. Nonetheless, precise bulk characterization of this sputtered material is lacking when silicon is added. To this purpose, specimens were manufactured via centrifugal casting and conventional vacuum casting (as control samples) using binary Al-Si and commercial Al-B master alloys. The microstructure and mechanical properties were investigated in Al-3wt.%Si alloys containing 2 and 3

wt.% boron (forming AlB_2 and AlB_{12} particles). The matrix grain size and volume fraction of the reinforcements were measured. Eutectic silicon was observed in the matrix as in un-reinforced Al-Si alloys. The centrifugally cast materials showed a functionally graded distribution of AlB_2 and AlB_{12} particles along the centrifugal direction due to the particle higher density. Higher superficial hardness and matrix microhardness were observed towards the centrifugal direction. Particle gradient concentration gradient allowed fabrication several sputtering targets in just one centrifugal casting process.

Reyes, Damian, UPR-MAYAGUEZ; Carrasquillo, Ronald, Chemical Engineering, UPR-Mayaguez; Marquez, Carmen P., Chemical Engineering, UPR-Mayaguez; Morales, Pedro, Chemical Engineering, UPR-Mayaguez, Cardona, Nelson, Chemical Engineering, UPR-Mayaguez

[Engineering 25]

Catalytic Performance and Stability of Bifunctional Materials for the Conversion of Cellulose into Renewable Biorefinery Feedstocks

This work presents the development of bifunctionalnanostructured materials for the catalytic conversion of cellulose into sugar alcohols that can be used as a sustainable source of renewable biorefinery feedstock. Mainly sorbitol and mannitol are obtained by the hydrolysis of cellulose to glucose followed by the corresponding reduction. Secondary products include sugars and ethylene glycol. Supported Ru catalysts were prepared by evaporative deposition on various ordered mesoporous silica (SBA-15) with different functionalities and compared to Ru/C and the corresponding supports. Ru/acidic SBA-15 displays the best catalytic performance. The catalysts were characterized using nitrogen adsorption, X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), and Thermogravimetric Analysis (TGA). The activity and selectivity of the bifunctional catalysts were studied by monitoring the cellulose conversion and production of sugars and sugar alcohols in a batch reactor. The effect of functionality loading, reaction time and temperature on conversion, selectivity, and catalyst stability will be discussed.

Rico, Zaida E., UPR-MAYAGUEZ

[Engineering 26]

Organizational Factors in Transit Services

Having great advances in technology and in financing instruments, why some transportation institutions are still unable to meet their Public Transit usage goals, even at apparently similar site conditions of successful systems? One aspect that varies among different institutions is their organization. The main objective of this research is to study if selected organizational factors have an effect on the

effectiveness of its transit institution. It is presumed that the system's effectiveness is proportional to its relative usage.

The methodology includes: literature review, preliminary statistical analysis using the National Transit Database (NTD) of 2008, survey development and execution, evaluation of collected data, developing conclusion and providing recommendations regarding the study approach and organizational factors.

This is an ongoing research; therefore, only preliminary analysis results are presented. Literature review includes three main sections: organizational theory, transportation relations theory, and recent organizational research in transportation. NTD data analysis includes correlation, regression, factor and combined effects. Survey will ask for information about internal environment and some capacity factors which are not well represented within NTD. A cluster analysis was used to select institutions to be surveyed based on UPT. Puerto Rico will be a study case.

The main expected contribution is to identify specific organization characteristics that are common among successful transit institutions and their possible relative level of impact. This project is part of a broader research that will aim to incorporate several variables from several institutions in order to produce a model that can describe relative impact of variables on usage.

Rivera, Lillian, UPR-MAYAGUEZ; Padilla, Ingrid, Civil Engineering, RUM

[Engineering 27]

Fate and Transport of DNT and TNT around an Improvised Explosive Device in an Urban Watershed Physical Model

Throughout history, the explosives had been used in different wars. Some of these are homemade bombs called Improvised Explosive Device (IED). These bombs are made with different dangerous chemicals which include DNT (2, 4-dinitrotolune) and TNT (1, 4-trinitrotoluene). These chemicals called Explosives Related Chemicals (ERC) are hazardous pollutants to the environment near the explosive device. Our research studies the fate and transport of DNT and TNT in the environment surrounding the explosive device. The transport of these contaminants is affected by the environmental conditions of the site where they are. The detection of trace of explosives in air and water is difficult due to their low vapor pressure and susceptibility to adsorption and degradation. In this project, an urban watershed physical model is simulated where explosive devices at the model scale are placed and exposed to field environmental conditions. The devices are placed in bags, simulating IEDs left near building structures. Air and rainwater samples are taken during the day under different rainfall, radiation and temperature conditions and analyzed for DNT and TNT detection. The air and

water samples were analyzed in a GC-ECD and HPLC respectively. The results show the concentration distribution of these chemicals in the urban setting relative to the location of the simulated IED and measured environmental conditions.

Rojas, Norberto Jose, UPR-MAYAGUEZ; Rojas, Norberto, Civil Engineering, UPRM; Lopez, Ricardo, Civil Engineering, UPR-Mayaguez

[Engineering 28]

Analytical Model of the Behavior of Reinforced Concrete Corner Joints With Substandard Reinforcing Details

The deficient seismic behavior of reinforced concrete frame buildings built prior to the 1970's has been evident in recent earthquakes. Damages observed is a clear indication of the serious structural deficiencies that some of these type of buildings may have. This can be attributed to the fact that seismic design requirements and construction practices at that time were not as strict as nowadays. These buildings pose a danger of partial or complete collapse and due to their vulnerability they are the principal seismic safety concern in the world. The critical part in these buildings are the connections. Its main role is to provide the connecting beams the capacity to dissipate energy through inelastic deformation. The reinforcing details of buildings built prior to the 1970's do no lead to a ductile response, implying that a premature failure of the joints can results in brittle failure of the structures. Thus the understanding of the performance of connections in old structures is essential. This research is oriented in develop, implement and verify an analytical model of a corner joint that can takes into account the biaxial loading of both beams and the axial load. This model should be able to model the loss of stiffness and the maximum capacity of the joint. Expected results include the development of a backbone curve that will be calibrated using available experimental test in the literature.

Sanchez, Matilde Luz, UPR-MAYAGUEZ; Isaza, Clara E., Facultad de Biologia, Universidad Autonoma de Nuevo Leon; Castro, Jose, Industrial Engineering and Welding Systems, Ohio State University; Cabrera-Ríos, Mauricio, Industrial Engineering Department, University of Puerto Rico-Mayaguez

[Engineering 29]

Biomarker Search as a Multiple Criteria Optimization Problem

Since their appearance, microarrays have become an extensively used tool for screening those genes that significantly change their relative expression between different states and, specifically, for the identification of biomarker genes. A

biomarker is a gene whose expression change can be taken as an indicator or a predictor of a particular state e.g. cancer. In the study of cancer, biomarkers have been discovered and used for many purposes including diagnosis and prognosis as well as prediction of recurrence of the illness among others. In the identification of potential biomarkers through microarray data analysis, albeit an active research area, it remains a challenge to have a method that is effective and, at the same time, independent of the users' ability and training. In this work, it is proposed that biomarker identificaction can be casted as a multiple criteria optimization problem. The solution to this problem i.e. the efficient frontier, can be approached through parameter-free algorithms that yield consistent optimization results. The first results on potential biomarker identification through the proposed optimization point of view are presented here.

Sierra, Sergio, UPR-MAYAGUEZ; Acosta, Giovanni, Chemical Engineering, UPRM; Rinaldi, Carlos, Chemical Engineering, UPR-Mayaguez

[Engineering 30]

Study of Fe-Co Nanoparticles Modified with Polyethylene Glycol Suspended in Polymer Melts

The surface modification of nanoparticles plays a very important role in their colloidal behavior. We want to study the effect on the graft polymer molecular weight in the rheological properties of different polymer melts. The Fe-Co nanoparticles will be synthetizes by thermo-decomposition, and their size will range between 15-30 nm. The particles will also be synthetized in a manner that they will exhibit Brownian relaxation.They will be characterized using Dynamic Light Scattering (DLS), a magnetometer and X-ray diffraction. The grafting polymer that will be used is polyethylene glycol (PEG). Four different molecular weight PEGs will be used as grafting substances. The polymer melts will also be PEG of different molecular weight to completely understand the effect of the molecular weight on the grafting substance as well as the medium on where they are suspended. All the PEG standards will be characterized using Differential Scaling Calorimeter (DSC), and their oxidation grade will be determined using NMR spectroscopy. The colloidal behavior of the particles suspended in the polymer melts will be studied using a magnetometer.

Soto, Denisse, UPR-MAYAGUEZ; Rinaldi, Carlos, University of Puerto Rico at Mayaguez

[Engineering 31]

Magnetorheology in Dilute Ferrofluids: Comparison of Direct Particle Simulations and Continuum Level Models, and Scaling Laws

Ferrofluids are suspensions of magnetic nanoparticles which respond to imposed magnetic fields by changing their viscosity without losing their fluidity. Prior work on modeling the behavior of ferrofluids has focused on using phenomenological suspension scale continuum equations. A disadvantage of this approach is that one such equation, the so-called Shliomis magnetization relaxation equation [Soviet Physics JETP, **34**, 1291, 1972], is subject of debate as its derivation is based on *ad hoc* arguments. An alternate expression, due to Martsenyuk *et al*. [Soviet Physics JETP, **38**, 413, 1974] is available, but its complexity prevents analytical solutions except in the simplest flow and magnetic field configurations. Yet a third magnetization relaxation equation derived from irreversible thermodynamics arguments has been proposed [Phys. Rev. E, **64**, 060501, 2001]. On the other hand, particle-scale simulations are emerging as an important tool in describing flows of ferrofluids. Simulations provide an alternative to study the applicability and limitations of suspension scale phenomenological equations in describing the flow of magnetic fluids under imposed magnetic fields. In this contribution, the rheology of dilute suspensions of spherical magnetic nanoparticles suspended in a Newtonian fluid and under applied shear and constant magnetic fields was studied through rotational Brownian dynamics simulations. Simulation results were compared with the predictions of suspension-scale models based on the two magnetization relaxation equations. Excellent agreement was observed between simulation results and the predictions of the MRSh equation. Good qualitative agreement was observed with predictions of the other two equations, although these models fail to accurately predict the magnitude and shear rate dependence of the magnetic field dependent effective viscosity. Finally, simulation results over a wide range of conditions are collapsed into master curves which provide the applicable scaling law relating magnetoviscosity, field strength, and shear rate.

Toro, Jaime, UPR-MAYAGUEZ; Cruz, Benjamin, University of Puerto Rico Mayaguez; Leonardi, Stefano, University of Puerto Rico Mayaguez

[Engineering 32]

DNS of Turbulent Channel Flow with V-Shape Turbulators

Modern gas turbines are extensively used in the aerospace industry for aircraft propulsion. The cooling system of the gas turbine blades plays a critical role in increasing the thermal efficiency and power output of advanced gas turbine. In fact, by increasing the heat transfer, the turbine blade can resist to an imping fluid with higher temperature. For instance, roughness elements (turbulators) are usually placed on the walls of the internal channels of a turbine blade to enhance the heat transfer. DNSs are carried out for passive heat transport in a turbulent channel flow with V-shape square ribs for w/k = 3, 8, 10, 15 (w being the pitch, k the height of the ribs turbulators). The angle of inclination of the lambda shape turbulators is 45 degrees. Numerical results show that V-shape square ribs are more efficient than square ribs in maximizing the heat transfer. The configuration

with w/k=3 presents the largest heat flux. The increase in the heat transfer is due to a secondary motion which is generated by the V-shape turbulators. Ejections at the location of the sidewalls transport the heat out of the cavity of the turbulators to the crest pane. Due to the ejections, two counter rotating vortices are produced above the square ribs transporting the heat out of the wall into the center of the channel. The distribution of the heat flux coefficient is not uniform in the channel and leads to temperature gradients at the wall.

Uribe, Victor, UPR-MAYAGUEZ; Alberto M. Figueroa Medina, Professor Civil Engieneering; Victor M. Uribe Florez, Ph.D Studen Transportation

[Engineering 33]

Behavioral Factors and Preferences Toward Transportation Transit Use of Residents in Urban Metropolitan Areas

The theory of mode choice in the transportation demand modeling process is one of the most significant elements due to the uncertainty in the selection of the variables that better represent the behavior of the population in an area of study. Although many theoretical choice models exist that determine the main variables as trip cost, household income, type of trip, etc., the user's behavior could be different for particular regions or countries. In other words, the behavior of the people in an area where there is a developed multimodal transportation system and a custom for using transit services will be different to other people in areas of limited or inexistent transit services.

The objective of this study is to identify the variables and parameters that explain the behavioral aspects individual traits and preferences of the urban population toward the transportation mode choice selection of work trips. A sample of residents from the San Juan Metropolitan Area of the Commonwealth of Puerto Rico will be selected for this study. An instrument, such as a survey or a focal group, will be developed in this study to obtain the information associated with the variables in the transportation mode choice selection. A binary logit model will be developed to explain the probability of transit use for work trips. This model could be useful for transportation planning models in order to understand better the actual behavior of the population and identify transit corridors for future transportation plans.

Vega, Ana, UPR-MAYAGUEZ; Valentin, Ricky, Ingenieria Mecanica , UPRM; Singh,Surrender, Ingenieria General; Velasco, Andres, Ingenieria Mecanica , UPRM, Blagg, Amanda, Ingenieria Mecanica , UPR-Mayaguez

[Engineering 34]

Electrochemical Response Of Carbon Supports For Biocatalityc Electrodes

Aligned Polyacrilonitrile (PAN) - multiwall carbon nanotubes (MWCNT) fibers were obtained at several concentrations of MWCNT (0.5 % wt, 1 % wt, 2 % wt, 5 % wt) and flow rates (50 µL/h, 70 µL/h, 100 µL/h). The diameter of these fibers ranged from 1 µm to 4 µm. The oxidation of MWCNT was proven using UV spectroscopy. Conductivity/resistivity measures were also conducted. Cyclic voltammetry tests were carried out revealing that the fibers obtained at 100 µL/h and 2% CNT exhibit a better performance in the test electrolyte (PBS 0.2M) compared to the other samples.
An experiment design analysis was conduced under a split plot model, this show that the concentration of CNT in the fibers has a higher incidence than flow rate over the electrochemical performance of the fibers.

In the same way fibers obtained under the conditions above mentioned were carbonized and then characterized.
A comparison between the carbonized fibers and the non carbonized fibers, will be done, in order to determinate their viability to be used like supports for electrodes in biofuel cells based on the electrochemical response and morphological characteristics.

Environmental Sciences

Alamo, Luis, UPR-MAYAGUEZ; Román, Félix R., Department of Chemistry, University of Puerto Rico at Mayaguez, PR; Perales-Perez, Oscar, Department of Engineering Science & Materials, University of Puerto Rico at Mayaguez; Santos-Santori, Lizette, Scientific Research Center, Pontifical Catholic University of Puerto Rico, Ponce, PR, Morales, Daisy, Scientific Research Center, Pontifical Catholic University of Puerto Rico, Ponce

[Enviromental Sciences 01]
]
Quantification of Organic and Inorganic Species in the Air particulate at Guayama, Puerto Rico

A PM 2.5 Single Filter Sampler System was used to take air samples at Guayama that is located in the southern region of Puerto Rico. The samples were extracted with pentane to analyze Volatile Organic compounds (VOCs) and Polyaromatic hydrocarbons (PAHs) using a GC-MS. Microwave digestion of samples was realized to extract metals and an ICP-MS was used to quantify them. Non VOCs and PAHs were found in all samples. The metals analyzed were Na, Mg, Al, K, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Ag, Cd, Sb, Pt, Au, Hg and Pb. K and Se were not detected. The metal concentrations were below than the standard levels established by Environmental Protection Agency (EPA).

Delgado, Diana, UPR-RIO PIEDRAS; Arce-Nazario, Rafael; Restrepo, Carla

[Enviromental Sciences 02]

Understanding Exotic Vine's Spread Through Network Analysis

The spread of invasive species has become a worldwide concern due to their potential effect on the health of organisms, ecosystems, and societies. One promising avenue to examine their patterns of spread is through their representation as networks whereby patches of an invasive species and dispersal among them are depicted as nodes and edges, respectively. Here we used this approach to examine the spread of invasive vines in the island of Puerto Rico. Unlike most invasive species, vines have the ability to disperse into new areas by climbing onto structures that provide them their needed support. We hypothesize that the topology of vine networks has to mirror that of the structures that they use. Centering on the Rio Grande de Arecibo drainage we followed a two-step approach to explore this hypothesis. First, we mapped vine

patches by running several supervised classifications on IKONOS satellite images collected in 2002. Second, we described the topology of the network using the software Pajek. Patches with an area ≥ $3m^2$ where considered in the analysis and identified as nodes. The nodes were linked by edged if they were ≤ 200m in proximity. Preliminary results have identified 88 patches in an area of $49.4km^2$. These patches vary in size ranging from $2{,}014m^2$ to $41{,}188m^2$.

Sanchez, Diana, UPR-MAYAGUEZ; Roman, Felix, Chemistry, UPR Mayaguez Campus; Perales, Oscar, Department of Engineering Science and Materials, UPR Mayaguez Campus

[Enviromental Sciences 03]

Se(IV) and Se(VI) Removal from Aqueous Solutions using Dried Sludge and Modified Ca-Alginate Beads as Sorbents

Selenium is an essential mineral for mammals at low concentrations, although when it intake exceeds of 1mg/kg is associated with toxic acute or chronic health effects in humans. This study addresses the development of a green, simple and cost effective process capable to remove both Se species from water using dewatered sludge and ferric chloride as coagulant, and as an alternative process use modified ca-alginate beads as sorbent. The expected sorbent capability of the dewatered sludge was based on the presence of silicates and oxides bearing iron and aluminum, as confirmed by XRD analyses, which could interact with selenium species by ionic exchange or formation of low solubility compounds. In contrast, the alginate beads are non toxic and capable to remove divalent cations. In our experiments the Ca-alginate beads were modified using iron as a doping agent in order to enhance it sorption capability. Experimentally, the Se concentration varied from 100 ppb to 1000 ppb. Results show a 100% removal of Se(IV) at pH 6.0 using 10g/L of sludge and 10 ppm of $FeCl_3$ as a coagulant. Instead, the complete removal of Se(VI) species from initial 100 ppb was achieved only, after reducing the Se(VI) to Se(IV) with elemental iron (1 mg/L) at pH 2.5 and 10g/L of sludge. In contrast, the removal efficiency of the iron Ca-alginate beads using 5g/L were of 48% for Se(VI) and 100% for Se(IV). Results show that both sorbents could be used for the removal of selenium ions at trace levels from aqueous solutions.

Torres, Irimar, UPR-MAYAGUEZ; Adel Gonzalez, University of Puerto Rico at Mayaguez; Christian Castro, University of Puerto Rico at Mayaguez; Lynn Williamson, University of Wisconsin Madison, Heather Allen, University of Wisconsin Madison; Lilliam Casillas, University of Puerto Rico Humacao; Carlos Rios-Velazquez, University of Puerto Rico at Mayaguez

[Enviromental Sciences 04]

Generation of Large-Insert Metagenomic Libraries from Tropical Hypersaline Microbial Mats on the Dry and Rainy Seasons and their Screening for Antibiotic Resistance

The generation of metagenomic libraries to access microorganisms' genetic traits has led to the discovery of gene products with potential biomedical applications. Some extreme environments, such as microbial mats, harbor high biological diversity for which they are valuable sources of novel activities. Our research is focused on generating large-insert metagenomic libraries from a young (Fraternidad) and a mature (Candelaria) tropical hypersaline microbial mat on the dry and rainy seasons and their screening for antibiotic resistance. High molecular weight environmental DNA was obtained by an indirect extraction method and fragments of more than 25 Kbp were cloned into the fosmid pCC1FOS and packed *in vitro* by lambda particles which transfected the appropriate host strain. Four metagenomic libraries were generated with 30,000 (Fraternidad) and 32,000 (Candelaria) clones from the dry season, and 1,400 (Fraternidad) and 1,200 (Candelaria) clones from the rainy season. The inserts sizes ranged from 25-50 Kbp. The four libraries sub-pools were screened for resistance to tetracycline 10 µg/ml, gentamycin 16 µg/ml and carbenicillin 32 µg/ml. There were clones resistant to gentamycin in a Candelaria dry season sub-pool and to carbenicillin in all the sub-pools of the tested libraries. Some resistant clones were isolated for further molecular analysis which includes fosmid extraction, restriction enzyme digestion of fosmids and retransformation of an isogenic bacterial strain with recombinant fosmids in order to verify if the resistance phenotypes that have been found are encoded by an environmental insert.

Alvarez, Derry, UIA-BAYAMON; González, Barbara, Ciencias Naturales y Matematicas, UIA-Bayamón; Ruiz, Oscar, Ciencias Naturales y Matematicas

[Enviromental Sciences 05]

Development of a Bio-Hydrogen Production System in Algae Chloroplasts

Currently, hydrogen is produced from natural gas using energy derived from the combustion of fossil fuels. Our proposed approach is to genetically engineer the chloroplast genome of the unicellular green alga *Chlamydomonas reinhardtii* to produce pollution-free H_2 during oxygenic photosynthesis. Such an alga system

may be produced and the H_2 that evolves from the cells can be collected and used to help supply our energy needs. The objective of this research project is to develop a transgenic alga via the chloroplast genome capable of producing hydrogen (H_2) in a clean and cost-efficient way. To achieve the objective the following activities will be undertaken; 1) the development of a multigene expression vector for alga chloroplast transformation, 2) the transformation and selection of chloroplast transgenic algae, 3) the molecular characterization of transgene integration and expression, and, 4) the characterization of the hydrogen production capabilities of the transgenic algae. We are proposing to develop chloroplast transgenic algae that can express the mouse myoglobin (*Mb*) and chloroplast hydrogenase (*HybA1)* genes. Myoglobin will serve as an oxygen (O_2) sequestering agent in the chloroplast; reducing the inhibitory effect of oxygen over the hydrogenase. Over-expression of the chloroplast hydrogenase will ensure efficient H_2 formation. The research plan will allow us to make direct comparisons between the transgenic algae and control algae to establish the functionality of the pathway. Additionally, this approach can be used to genetically engineered other green alga species if desired.

Escobar, Zalleris, UPR-MAYAGUEZ; Lugo, Yahaira, Ingenieria Civil, UPR-Mayaguez; Hwang Sangchul, Ingenieria Civil, UPR-Mayaguez

[Enviromental Sciences 06]

Influence of Manufactured Coal Ash Agreggates Used for Daily Covers on Landfill Leachate Characteristics

Covering daily solid wastes after a day operation is a standard practice at most landfills. Use of alternative materials could conserve landfill space and soil resources while also meeting environmental (i.e., leachate characteristics) and operational requirements. Coal ash aggregates (CAAs) are solidified agglomerates of fly and bottom ashes produced during the coal combustion process for electricity production. CAAs can reduce toxicity of leachate from both organic and inorganic substances and enhance the rate of waste decomposition by providing the necessary water content for landfill microorganisms and to maintain an optimum pH for methanogenic microbial activity. In addition to saving soil resources, CAAs would physically conserve landfill space by providing greater overburden pressure landfill closure and facilitating post-closure management due to smaller post-closure settlement.

The purpose of this research is to evaluate the potential of the CAAs as ADC materials achieving resource recovery, enhancing biological decomposition and leachate characteristics, and subsequently inducing early settlement of landfills. Biochemical decomposition and settlement have been simulated using laboratory-scale physical landfill models (PLMs) in a temperature-controlled environmental chamber. For settlement monitoring, the PLMs were constructed with a side-wall window of transparent plexi-glass. Artificial solid wastes were

made based on the typical waste characteristics in Puerto Rico. Results show that using CAAs as an ADC has the following advantages: lower concentrations of chemical oxygen demand, biological oxygen demand, and nitrogen and phosphorus compounds in leachate. The PLM with CAAs also achieved more settlement indicating better biodecomposition in the presence of CAAs as ADC materials.

Herrera, Gloria, UPR-MAYAGUEZ; Castañer, De Choudens Jeylisse, Chemical Engineering; Hernández, Samuel P., Chemistry

[Enviromental Sciences 07]

Photocatalytic Degradation of Explosives Using Iron Oxide as Photocatalyst

Iron oxide nanoparticles were synthesized through a hydrothermal method. Raman and infrared spectra were used to characterize the oxide nanoparticles. SEM images were acquired to determine particle sizes. The photocatalytic degradation of TNT, DNT and RDX using a UV irradiation at 365nm as a light source and iron oxide as a photocatalyst, was investigated. The effects of various parameters of TNT degradation rate photocatalyzed by iron oxide were examined. Among the parameters studied were the concentration ratio of TNT to oxide added and the irradiation time. Another technique used to characterize the chemical composition the nano-oxide was X-ray diffraction. An amount of nano-oxide was transferred to aqueous solutions of the contaminant in a known concentration. The quantitative analysis of pollutant degradation was carried out using high-performance liquid chromatograph equipped with diode array UV detector. The concentration of TNT was observed to decrease as a function of time. This can be attributed as oxidative degradation of the organic compound by iron oxide. The best results observed were for RDX degradation where the oxide decreases its concentration in around of 80 per cent. The experiment was simultaneously carried out with the TNT – iron oxide mixtures without UV irradiation in order to compare the results and of studying the effectiveness of the catalyst.

Irizarry, Ivelisse, TURABO UNIV; Sharon A. Cantrell, Universidad del Turabo

[Enviromental Sciences 08]

Bacterial Endophytes of Coccoloba Uvifera in Cabo Rojo, Puerto Rico

Plants contain microorganisms called endophytes that live within their tissues without causing signs of disease. In the present study, bacterial endophytes of the coastal tree *Coccoloba uvifera* (sea grape) were characterized near a hypersaline solar saltern and a beach site in Cabo Rojo, Puerto Rico in September, 2008 (wet season) and March, 2009 (dry season). It is hypothesized

that the frequency of colonization and bacterial diversity will differ in both ecosystems sampled between the wet and dry seasons. Two trees were selected at a site nearest the solar saltern and two trees in Playa Sucia. On each sampling, four healthy leaves from each tree were obtained. Leaves were surface sterilized and ten fragments measuring 2mm x 2mm were chosen randomly from each leaf. The fragments were inoculated on 50% Tryptic Soy Agar until colonial growth was observed. DNA was extracted from pure isolates of different morphotypes and characterized by 16S rDNA sequencing. Sixty one cultures were genetically sequenced and they were characterized as 42 different strains within 14 genera of endophytic bacteria. Endophytes belonging to the Gammaproteobacteria have been found with higher frequency, but members of Betaproteobacteria and Bacilli have also been encountered in this study. Some commonly encountered genera are *Stenotrophomonas* sp*, Pseudomonas* sp*, Bacillus* sp*,* and *Burkholderia* sp. Chi-square statistics demonstrated that the frequency of colonization differed significantly between the trees studied in the salterns and Playa Sucia on both seasons sampled indicating that location and seasonality can affect populations of bacterial endophytes.

Rivera, Héctor, UPR-RIO PIEDRAS; Mayol-Bracero, Olga L., Institute of Tropical Ecosystems Studies, UPR Río Piedras; Ogren, John A., Earth System Research Lab, NOAA; Sheridan, Patrick, Earth System Research Lab, NOAA, Andrews, Elisabeth, Earth System Research Lab, NOAA

[Enviromental Sciences 09]

Physical and Radiative Properties of Aerosol Particles across the Caribbean Basin: A Comparison Between the Clean and Perturbed African Dust and Volcanic Ash Air Masses

Aerosol's optical and physical properties were measured during years 2007 and 2008 at Cape San Juan, a ground-based station located at the northeastern tip of Puerto Rico. The three cases investigated were classified according to the origin of the air masses: clean (C), African dust (AD), and volcanic ash (VA). The instrumentation used included a sunphotometer to determine volume size distributions and aerosol optical thickness (AOT), a 3-wavelength nephelometer to determine the scattering coefficient (σ_{sp}), and a 3-wavelength particle/soot absorption photometer (PSAP) to measure the absorption coefficient (σ_{ap}). The average volume size distributions were bimodal for the C (peaks at 0.14, and 4.25 µm radius), AD (peaks at 0.11 and 2.00 µm radius) and for VA (peaks at 0.19 and 2.75 µm radius) case. Fine and coarse modes maxima for AD occurred at radii smaller than for VA, confirming the different origins of those particles. The average values for the total σ_{sp} were higher for AD (82.9 Mm^{-1}) and VA (33.7 Mm^{-1}) compared to C (16.6 Mm^{-1}). A similar pattern was observe for the AOT, with maximum values at 500 nm with 0.92, 0.30, and 0.06 for AD, VA, and C, respectively. The observed increase in the values of the Angstrom exponent (å) is indicative of a decrease in the size of the particles associated to VA (å= 0.27)

and AD (å =0.89) when compared to C (å =0.24). The volume size distributions and thus the mass were dominated by the coarse mode (> 1.0 µm) especially for the AD case. Results have shown that AD as well as VA has a significant impact on the physical and radiative properties across Puerto Rico and the Caribbean. The hemispheric backscatter fraction and some calculations of the aerosol forcing per unit of optical depth will be presented.

Sandra, Correa, UPR-MAYAGUEZ; Jean K. Rivera, UPRM; Nancy M. Soto, UPR-Mayaguez

[Enviromental Sciences 10]

Caribbean plants using for Remediation of Aqueous Medium

The Caribbean plant *Spermacoce Assurgins* also know as Juana la Blanca, collected from soils in Puerto Rico, was used in this study for phytoremediation in an aqueous medium. The medium contained organic contaminants as 2,4,6-trinitrotoluene (TNT). This plant was selected on the basis of availability and sufficient power of endurance for cultivation at the site. This study presents the kinetics of absorption of TNT by Juana la Blanca in aqueous medium after several days of sampling. The analysis of medium extracts of TNT was made using HPLC-UV and was confirmed by GC/MS. The results demonstrated that the plant is tolerant to 35 ppm of TNT and absorption occurs in 48 hours. The TNT was transformed in amino derivates and DNTs. Juana la Blanca was germinated and micro-propagated in a greenhouse under controlled environmental conditions such as temperature and humidity.

Keywords: *Spermacoce Assurgens,* HPLC-UV, GC/MS, Phytoremediation, TNT.

Sierra, Maria del Pilar, UPR-MAYAGUEZ; Figueroa Matias; Nolberto, Chemical Engineering, UPR Mayaguez

[Enviromental Sciences 11]

Comprehensive Utilization of Coffee Processing Waste: A Feasibility Study

Coffee production, one of the major agricultural commodities in Puerto Rico, is facing serious challenges with regards to environmental policy compliance. Only 6% of the coffee cherries constitute the portion produced as coffee powder, while the remaining is obtained as by-products such as coffee husk/pulp and caffeine containing wastewater with high concentration of organic carbons. Direct discharge of coffee processing waste has already caused serious environmental problems. US coffee farmers are lagging behind foreign production partly because EPA is regulating the waste disposal, which significantly increases the cost of the product; while in many foreign countries, there is no restriction at all. Our research addresses these challenges by providing the biological technical

solutions as well as a demonstration of our vision for the next generation of coffee farms, which will still be profit oriented, but environmental friendly, energy independent and sustainable. We propose to convert coffee husk/pulp to animal feed, after microbial pretreatment to detoxify contaminants, while the coffee processing wastewater will be treated together with animal manure wastewater to provide biogas energy to support the coffee farm. With the reinforcement of fundamental scientific development, microbial community in the habitat with high concentration of caffeine will be revealed, which will provide future guidelines for producing other valuable bio-products from coffee processing waste. The work shown here represents a feasibility study for the implementation of an integrated approach in the utilization of coffee processing waste.

Geosciences

Ruidiaz, Cyd, UPR-MAYAGUEZ

[Geosciences 01]

Reef Characterization and Coral Identification in a Unit of the Lares Limestone (Late Oligocene) Exposed in Road Pr-111, Between Salto Collazo and the Intersection with Road PR # 445.

Reef characterization has been made in one unit of the Lares Limestone of Oligocene age in north Puerto Rico. This unit is part of the 4th parasecuence of nine proposed by Ortega (2009) in the Lares Limestone. The unit is exposed laterally for 120 m in road PR-111. Preliminary data indicates that this unit represents patch reef facies that extends for 30m laterally, were 3 main facies were identified: 1) branching coral facies, 2) Head coral and platy coral facies, and 4) Calcareous silt. The branching coral facies are in-situ corals that are predominated by *Pocillopora guantanamensis* and *Porites portoricensis*. This facies also include isolated mounds of head corals. Branching coral is the major frame builder of the patch reef. The head coral facies is predominated by in-situ corals of *Solenastrea bourbonni, Montastrea cannalis, Stylophora sp., Goniopora imperatoris, Goniopora hilli, Goniastrea canalis, and Stephanocoenia sp.*, with occurrence of encrusting algae in some areas. The calcareous silt facies contains fragments of red algae, oysters and bivalves, with isolated head corals. This facies is often intercalated with the branching coral facies. This unit changes laterally to a calcareous shale with occasional patches of the branching coral facies and isolated mounds of head corals. This research helps understand better the Lares Limestone in terms of lateral facies changes and parasequences. Also, this research aids to understand the coral reef development in the late Oligocene in Puerto Rico.

Life Sciences

Acevedo, Jean Marie, UPR-MEDICAL SCIENCE CAMPUS; Ortiz-Correa, Zacha, Biology, Ciencias Naturales; Díaz-Ríos, Manuel, Anatomy and Neurobiology, Medical Sciances Campus

[Life Sciences 01]

Localization of Choline Acetyltransferase-Like Immunoreactivity in Interneurons of the Mouse Spinal Cord

The basic motor patterns driving rhythmic limb movements during locomotion are generated by neuronal networks called central pattern generators (CPGs), located within the spinal cord. Networks of interneurons control the rhythmic activity of flexor and extensor motor neurons on both sides of the body to generate locomotion. It has been suggested that ipsilateral excitatory ventral interneurons (IINs), whose axonal projections do not cross the midline, are involved in the maintenance of rhythmic activity of flexor and extensor motor neurons to generate the normal alternating motor pattern between antagonistic muscle groups within each limb (intralimb coordination). Additionally, another population of spinal neurons known as the commissural interneurons (CINs), which have axons crossing the midline of the spinal cord, has been shown to be implicated in the control of left-to-right alternation of both limbs during locomotion (interlimb-coordination). It has been recently suggested that interneurnons which are using acetylcholine as their neurotransmitter (cholinergic interneurons) make synaptic contacts into motorneurons and regulate their excitability via activation of muscarinic receptors, and that this system is used during motor behavior. Additionally, previous studies have used immunohistochemical techniques to localize the presence of cholinergic neurons in the rat spinal cord. In this study we are localizing the presence of cholinergic interneurons throughout the lumbar segments of the mouse spinal cord with the use of an antibody directed toward the enzyme choline acetyltransferase (ChAT), a known marker for cholinergic neurons. Additionally, by using an axonal retrograde tracing technique we wanted to identify ipsilateral interneurons (IINs) that could be using acetylcholine as their neurotransmitter. This study will provide further information into the anatomical organization of the spinal locomotor network and its potential neuronal members. Supported by: NIH Grant RCMI-UPR-MSC G12RR-03051, NIH Grant P20 RR016470, NIH Grant R25-GM061838 and The Craig Nielsen Foundation.

Agosto, Ibis, UNE; J. Barreto-Estrada, UPR-RCM; Roig-Lopez, JL, Science and Technology, UNE; Ortiz-Pineda, P, Science and Technology, UNE, Brito-Vargas P, Science and Technology, UNE; Vizcarrondo-Martinez G, UNE; Fernandez M., Science and Technology, UNE

[Life Sciences 02]

Microarray Expression Profile of the Hypothalamic Neuroendocrine Cell Line GT1-7 Under Exposure to Class I Androgen Analog Testoterone Propionate

Hypothalamic cell line GT1-7 has been used to elucidate cellular and molecular mechanism of the expression and secretion of the neuroendocrine protein gonadotroping releasing hormone (GnRH). Our interest is to use GT1-7 cell line to unravel the androgenic regulation on GnRH expression and how the neuropeptide Y signaling pathway maybe involve in this regulation. As first objective we want to analyze how the general expression profile of the GT1-7 cell line change under different androgenic environments. In this work we exposed the GT1-7 cell line to the androgenic analog of the Class I testosterone propionate for 24 hrs. The mRNA from three independent cultures and treatment were pool and used on GCAT mouse micro arrays chips (MEEBO 25,000 genes). The microarray chip was analyzed with Magic Tool software from the GCAT consortium. Bioinformatics analysis shows 209 up and 194 down regulated genes. Of the up-regulated genes 40 genes were associated with signaling pathways (GO Category), some already reported in hypothalamic neurons and GnRh responsive cells such as Adcy4 and Ptpn11. However a significant part of the signaling pathways genes identified are associated with energy and metabolic homeostasis functions including glucose regulation. These preliminary data suggest that class I androgen may regulated genes involved in metabolic processes.

Conde-Costas, Carlos, UPR-RIO PIEDRAS; Ortiz-Zayas, Jorge, Biology, UPR-Rio Piedras

[Life Sciences 03]

Nitrogen Dynamics in a Tropical Cave Stream

The ongoing global change in the amount of nitrogen cycling in the biosphere forecast serious impacts to the structure and functioning of aquatic ecosystems. Excessive inputs of nitrogen can eutrophy freshwater ecosystems and represents a major threat to estuaries and coastal waters, where nitrogen is usually the limiting nutrient to algae growth. Karst landscapes occupy about 20 percent of the earth's land surface and are characterized by subsurface drainage where linkages between groundwater, cave and surface streams are very strong. The way that nitrogen is transported and transformed along cave streams will have a

direct and significant influence in the quality of karst surface streams and basin ecological processes. Nitrogen dynamics along a tropical cave stream that receives a constant input of nitrogen-rich organic material in the form of bat guano is currently investigated at El Convento Cave-Spring System, Guayanilla, Puerto Rico. Preliminary findings suggests an efficient removal of nitrogen from the water column in the surveyed cave stream, while the documented relative composition of nitrogen forms suggests an optimum and efficient nitrification and denitrification process. The detected relative stability between nitrate inputs and outputs suggest that nitrogen export is favored over retention and that nitrogen cycling is sustained at a near equilibrium condition.

Figuerola, Cielo, UPR-RIO PIEDRAS; Meléndez-Ackerman, Elvia, Institute for Tropical Ecosystems Studies, University of Puerto Rico at Río Piedras

[Life Sciences 04]

Evaluation of Potential Demographic Differences in the Subpopulations of the Mona Island Iguana Cyclura Cornuta Stejnegeri Across Different Forest Types in Mona Island, Puerto Rico

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 an oceanic island with a subtropical dry forest climate. The largest habitat type of the island is the limestone rocky “plateau” (93%). Another unique habitat type are the forest depressions located in the plateau (1%). 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 microhabitats and 3) assessing the differences in the utilization of the habitat by the Mona iguana between microhabitats. 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, microhabitat 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.

Fumero, Jose J., UPR-RIO PIEDRAS; Elvia J. Melendez-Ackerman, Institute for Tropical Ecosystem Studies

[Life Sciences 05]

Effects of Nectar Robbing Bananaquits on Flower Nectar, Pollinator Behavior and Plant Reproductive Success of Pitcairnia angustifolia

Animal visitors that remove nectar without pollinating flowers are considered nectar robbers that may have direct and indirect effects on the reproductive success of their host plants. In this work, I studied the effects of nectar robbers on nectar production, pollinator behavior, pollen movement, pollen export potential, and components of female reproductive success of the bromeliad *Pitcairnia angustifolia.* Under natural conditions this bromeliad is visited by four different animal species including a robber-like pollinator and a secondary robber. My results showed that natural levels of nectar robbing were high in natural patches of *P. angustifolia* and that natural variation of the proportion of robbed flowers per inflorescence was not a good predictor of female reproductive success (i.e. fruit set, seed mass, seed set). Nectar robbing simulations did not stimulate increases in nectar production nor concentration in contrast to other species where this phenomenon is known to occur. Overall, nectar robbing had negative effects and was found at different levels; first, I found that nectar removal was not followed by an increase in nectar production; second, nectar robbery seems to change hummingbird behavior from a legitimate pollination to a robber lowering its visitation rates. I found that robbery was a poor predictor of female reproductive success most likely because of high levels of nectar robbing. Overall results suggest that high levels of nectar robbing maintain condition of pollination limitation that results in natural selection favoring larger inflorescences.

Laguna, Jessenia Yaris, UPR-RIO PIEDRAS; Cruz Muñoz, Ambar Roselyn, 1Department of Biology, University of Puerto Rico-Rio Piedras; Castro, Edgardo, 1Department of Biology, University of Puerto Rico-Rio Piedras; Santos Soto, Iván, 1Department of Biology, University of Puerto Rico-Rio Piedras; Soto, Yarelis, 1Department of Biology, University of Puerto Rico-Rio Piedras; Colón Cesario, Melissa, 2Department of Biology, University of Puerto Rico, Humacao; Peña de Ortiz, Sandra, 1Department of Biology, University of Puerto Rico-Rio Piedras

[Life Sciences 06]

DNA Recombination, Remote Memory and Hippocampal Synaptic Plasticity.

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.

Malavé, Josué, UPR-MAYAGUEZ; Malave, Josue, University of Puerto Rico, Mayaguez; Carlos Rios Velazquez, University of Puerto Rico, Mayaguez; Rebecca Fry, Massachusetts Institute of Technology, Leona D. Samson, Massachusetts Institute of Technology

[Life Sciences 07]

Development of a High-Throughput System to Globally Monitor the Dynamics of Sub-cellular Localization of a Saccharomyces cerevisiae Proteome Upon Exposure to an Alkylating Agent

Exposure to a variety of toxic agents can cause serious damage on the DNA and the cellular machinery, activating specific mechanisms to ensure cells recovery and survival. In order to understand how cells deal with environmental disturbances different approaches have been collected, merged, and analyzed computationally. Here we describe a high-throughput system using a whole *Saccharomyces cerevisiae* genome *gfp* fusion library to analyze the global proteome dynamics after addition of the DNA damaging agent Methyl Methane Sulfonate (MMS). Growth curves, and cell counts were performed to determine the optimum physiological phase and inoculums size in which a detectable change in cells is obtained using 0.02% of MMS. The response of a *gfp* tagged mutant of a known and unknown MMS altered-cellular-localization protein in *S. cerevisiae*: Ribonucleotide Reductase (Rnr2) and Glutathione transferase (Gtt) were used respectively to validate the monitoring system. The re-localization of the *gfp* tagged proteins was confirmed (before and after fixing with formaldehyde) using the compartment-specific fluorochromes Hoechst and Texas-Red, and several microscopy approaches including fluorescent, and high resolution microscopy (Delta Vision). Quantification of the whole *S. cerevisiae gfp* library to such changes in a 96 well plate arrangement is being completed using a Bio-imaging Cellomics microscope. At least two compartments can be analyzed in yeast using this system: nucleus and cytoplasm. The response to MMS was best detected when the treatment was done in early-log growth phase (6 – 8 hrs; OD_{600} 0.3 - 0.5), and 1 – 2 x 10^6 cells/ml, were used.

Martinez-Rivera, Noraida, UPR-RIO PIEDRAS; Torres-Vazquez, Irma, Biological Imaging Group, University of Puerto Rico-Rio Piedras; Serrano-Velez, Jose L., Biological Imaging Group, University of Puerto Rico-Rio Piedras; Rosa-Molinar, Eduardo, Biological Imaging Group, University of Puerto Rico-Rio Piedras

[Life Sciences 08]

Immunohistochemical Characterization of a Gonadotrophin-Releasing Hormone 1 (GnRH-I) Neuronal System within the Ventral Spinal Cord in the Sexually Dimorphic Internal Fertilizing Teleost Fish, Gambusia

Gonadotrophin-releasing hormone 1 (GnRH-I) is expressed by a restricted population of neurons present in the hypothalamus and has been found to regulate and coordinate reproduction and copulatory behavior in vertebrates. Using immunohistochemistry, we have discovered a GnRH-I neuronal system within the ventral spinal cord of the sexually dimorphic internal fertilizing adult male Western Mosquitofish, *Gambusia affinis*. GnRH-I-immunoreactive (ir) cell bodies and fiber tracts with a rostrocaudal orientation were observed within the adult male *Gambusia* ventral spinal cord. The fiber tracts were relatively dense and formed bundles surrounding the central canal. In addition, short, varicose GnRH-I-positive processes with a radial orientation were present throughout the gray matter. These fibers were particularly abundant ventromedially and formed a diffuse network that branched laterally to end in the vicinity of spinal motor neurons. The presence of GnRH-I-immunoreactive cell bodies and fibers within the ventral spinal cord suggests that GnRH-I may influence the plasticity and activity of a subpopulation of spinal motor neurons within the rapid copulatory circuit (RCC) involved in controlling the adult male *Gambusia* rapid copulatory behavior and sperm deposition. NMR was supported by AGEP fellowship. This research was supported by NIH grants NS-39405 and MH-086994.

Nogueras, Carlos J., UPR-RIO PIEDRAS; Daniel Caballero-Rivera, Jessica Oyola-Cintrón; Orestes Quesada, José A. Lasalde-Dominicci

[Life Sciences 09]

C418W-nAChR as a Model to Study the Role of Lipid-Protein Interactions in Channel Clustering and Postsynapse Stability at the Neuromuscular Junction

Several studies have demonstrated that the stability of the neuromuscular junction (NMJ) at the postsynaptic membrane is achieved through the clustering of nicotinic acetylcholine receptors (nAChRs) which co-localize with lipid rafts. However, little has been done to elucidate the effects of lipid rafts' environment upon nAChR activity and proper functioning. For this purpose C418W-nAChR, a slow channel congenital myasthenia syndrome (SCCMS) causing agent, is a perfect model.

It has been demonstrated that the peak current of the recently discovered C418W is decreased upon physiological membrane cholesterol enrichment in *Xenopus laevis* oocytes. These observations suggest that lipid-cholesterol interactions between the mutant and the surrounding bilayer might regulate the channel's function resulting in its phenotype. Western blot analysis for C418W and WT-nAChR transfected HEK-293 cells were used to assess the role of cholesterol levels in the diffusion of nAChRs in the absence of raft synaptic components MuSK and rapsyn.

Our results suggest that C418W mutant's strong affinity for cholesterol induces a significant aggregation of the channel into CAV-1/FLOT-2 rafts in comparison with WT, this without the help of the AChR-clustering machinery.

Ocasio Torres, María, UPR-RIO PIEDRAS; Ocasio Torres, María E, Biology, UPR-RP; Sabat, Alberto, Biology, UPR-RP; Giray, Tugrul, Biology, UPR-Rio Piedras

[Life Sciences 10]

Long Rostrum as a Defense Mechanism for Xiphocaris Elongata

Amphidromous shrimp *Xiphocaris elongata* possess a short rostrum in headwater streams where predatory fishes cannot access, but have a long rostrum below waterfalls where predators are present (Covich et al. 2000). The objective of our investigation was to examine if the long rostrum exhibited by some *X. elongata* reduces their susceptibility to predation by catadromous fish *A. monticola*. We videotaped attacks by six *A. monticola* individuals on long and short rostrum shrimps. 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 ($p=0.001$) for the same amount of consumptions. Long rostrum shrimps were also rejected significantly more than short rostrum individuals ($p=0.001$). *A. monticola* attacked first shrimp with short rostrum ($p<0.0001$). Handling time was significantly higher in long rostrum shrimps than short rostrum shrimps ($p=0.005$). This study suggests that long rostrum is an effective anti-predatory strategy in *X. elongata*.

Ruiz, Francheska, UPR-RIO PIEDRAS; Tremblay, Raymond, University of Puerto Rico Humacao

[Life Sciences 11]

Population Dynamic of Eleutherodactylus Antillensis in Two Habitat Types

Eleutherodactylus antillensis is found from sea level to the highest peaks in Puerto Rico which makes it a species which is likely plastic in its ability to adapt to varying environments. Population studies and demography studies have been

used in many fields and studies that range from conservation and evolution to genetic and pathology studies. Some of the main parameters that are needed to fully understand a population dynamic includes: population size, recruitment, survival, recapture probability and growth rate. In this study we aimed to determine if the survival and recapture probabilities of this species population dynamics vary among four different populations that vary by habitat type. Ceiba and Vieques offer a unique opportunity to study this species ability to adapt to varying environments as both posses subtropical dry and humid forest. We collected data for seven months in the municipal towns of Ceiba and Vieques in dry and humid forest making the total study sites four. The program MARK was used to calculate survival and recapture probabilities. We used the Cormack-Jolly-Seber (CJS) to determine if survival and recapture probabilities varied between the four different study sites. After running the different models separating by sex, habitat type and municipality, we found that the model that best separated the populations was the model that separated populations by municipality. We then ran the models again only separating by municipality and found that the best model was the one that were the survival probability varies by site but not in time and the recapture probability varies by time and not by site.

Ruiz, Hector, UPR-MAYAGUEZ; Ballantine, David, Marine Science, UPR-Mayaguez

[Life Sciences 12]

Dynamics of Shelf Edge Coral Reef-Associated Macroalgae at La Parguera, Puerto Rico

Percentage cover of coral reef associated algae increased significantly at two shelf edge sites in southwest Puerto Rico (42.8 % to 75.3% at Weinberg Reef and 67.4% to 81.8% at El Hoyo). While the increase was driven largely by increase in cover of *Lobophora variegata,* percent cover of the individual spatially dominant algal species was highly variable temporally. The variability was apparent even at the subquadrat level ($0.0625m^2$) for which adjacent subquadrats demonstrated little concordance in species cover over subsequent sampling periods.

Santos, Sylmar, UPR-RIO PIEDRAS; Ramirez, Alonso, Biologia, Universidad de Puerto Rico - Rio Piedras

[Life Sciences 13]

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

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, with 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 analyzing otolith increments for age determination. In addition, standard length, liver and body weight are going to be measured to determine fish body condition (hepato-somatic index). Juvenile dispersal will be assessed using migration traps along the watershed. Overall, the proposed research will provide critically needed information to further understand and manage fish communities in tropical island streams.

Seda Miró, Jasmine, UPR-MAYAGUEZ; Rosado, William, Marine Sciences, UPR-Mayaguez; Govind, Nadathur, Marine Sciences, UPR-Mayaguez

[Life Sciences 14]

Genetic Variation and Phenotypic Heterogeneity in Response to Cobalt(II) Among Strains of the Marine Yeast Debaryomyces Hansenii

Variation in phenotypic characteristics may be an indication of genetic heterogeneity; however, the direct association between genetic variations and their functional roles among strains of the same species remains to be elucidated. In this study, several strains of the marine yeast *Debaryomyces hansenii* were evaluated for phenotypic differences in sensitivity and tolerance to metal toxicity (cobalt(II)). The genetic heterogeneity of the *FET3* gene, which is associated with iron transport, riboflavin production and cobalt toxicity, was also studied in these strains. Comparative sequence alignments of ribosomal and "housekeeping" genes between the sensitive strain CBS767 ^{T} and the tolerant strain J26 revealed larger sequence variations in mostly conserved genes, suggesting a larger divergence than previously anticipated among strains of the same species. Expression levels of the *FET3* gene in CBS767 ^{T} and J26 were also analyzed. These genetic variations may be implicated in the functional role of genes associated with the organism's response to environmental stress.

Soler-Figueroa, Brenda María, UPR-MAYAGUEZ; Otero-Morales, Ernesto, Marine Science Department, University of Puerto Rico, Mayaguez

[Life Sciences 15]

Pyrodinium Bahamense var. Bahamense and Ceratium Furca var. Hircus Growth Rates and Bloom Dynamics at Bahía Fosforescente, La Parguera

The impetus for this research is the growing concern by the scientific community, public and federal management agencies over the ecological status of Bioluminescent Bays (BB) in Puerto Rico. For decades, these ecosystems have intrigued researchers due to the high and almost complete dominance of the bioluminescent dinoflagellate *Pyrodinium bahamense* var. *bahamense*. However, in recent years decreases in the abundances of this species have been observed at Bahía Fosforescente and instead, high concentrations of the non-bioluminescent dinoflagellate, *Ceratium furca*, have been found. The goals of this research are: 1) gain a better understanding on the effects of environmental factors over *P. bahamense* and *C. furca* populations and growth rates 2) identify species variability on short-time scales and 3) determine if *P. bahamense* and *C. furca* compete for nutrients. Daily field measurements of *P. bahamense* and *C. furca* cell densities and several environmental factors (i.e., temperature, salinity, nutrient concentration and rainfall) will be performed at the bay during two time periods (i.e. dry and wet season). Also, laboratory experiments will be made to determine the effects of temperature, salinity and nutrient concentration on unialgal batch cultures and the effects of nutrient concentrations in mixed cultures. Expected results: 1) understand the physiological requirements of the species and their tolerance to temperature, salinity and nutrient concentration 2) evaluate the effect of environmental factors on species population dynamics 3) evaluate how environmental changes, due to natural events or anthropogenic activities, affect the abundance of both species in the bay.

Soto, Kristina, UPR-MAYAGUEZ; De Jesus-Cruz, Moises, Biology Department, University of Puerto Rico- Mayaguez; Casillas-Martinez, Lilliam, Biology Department, University of Puerto Rico- Humacao; Visscher, Pieter T., Marine Science Department, University of Connecticut, Rios-Velazquez, Carlos, Biology Department, University of Puerto Rico- Mayaguez

[Life Sciences 16]

Purple Non-Sulfur Anoxyphototrophs Bacteria isolated from Tropical Hypersaline Microbial Mats of the dry season at the Cabo Rojo Salterns of Puerto Rico

Purple non-sulfur anoxyphototrophic bacteria (PNSA) are a diverse group of microbes with versatile physiological traits. As part of the microbial community present in tropical Hypersaline Microbial Mats (THMMs), they are exposed to seasonal changes, such as pluvial precipitation, as well as oxygen and sulfur

variations. We are interested in studying the diversity of this group in THMMs. This research seeks to isolate and characterize the PNSA present in young and mature mats from two sites at the Cabo Rojo Saltern THMMs during the dry season, and compare the results to data obtained during the rainy season. To identify PNSA, mats were dissected and the three layers were separated and cultured in liquid and solid media. All samples were incubated anaerobically in the presence of light and colonies showed the characteristic reddish bloom. The colonies were characterized microscopically, biochemically and molecularly. During the dry season, 13 PNSA were isolated; 6 and 7 from mature and young mats, respectively. All the isolates were gram-negative straight and spiral rods of variable sizes. Spectral and molecular analysis suggests the presence of characteristic bacteriochlorophylls peaks. Amplicons from all the isolates were obtained using specific primers for *puf*M. and 16S rDNA. The 16S rDNA *in silico* analysis suggest the presence of one *Rhodothalassium,* two species of *Rhodobacter, one Rhodospirillum sp.* and various unidentified members of the *Rhodospirillaceae* family, including several unidentified members of the PNSA similar to *Vibrio sp.*

Mathematics

Almodóvar, Edgard, UPR-RIO PIEDRAS

[Mathematics 01]

Statistical Analysis of Egg Eclosion from Clutch Size of Eretmochelys imbricata

Previous estimates of survival rates of sea turtle eggs to adulthood depend upon the assumption that their populations are neither increasing nor decreasing in numbers. The assumption is made in spite of the fact that recent interest in sea turtle demography stems from the belief that populations are in decline. Presented are estimates of the survival rate of eggs from initial clutch size with region as a factor from the population of hawksbill turtles, *Eretmochelys imbricata*, at its present observed rate of decline. Results indicate that the proportion of eggs surviving decline with a greater number in clutch size. The methodology may be used to assess gross survivorship from egg to adulthood in increasing or decreasing populations of this species, and others, in which adults and eggs are more easily studied than are juveniles.

Cardona, Gloriell, UPR-RIO PIEDRAS; Pérez, María-Eglée, Department of Mathematics, University of Puerto Rico Rio Piedras

[Mathematics 02]

Relationship Between Climatic Variables and The Incidence of Dengue in Ponce, Puerto Rico from 2003 to 2009

This research is focused on relating the incidence of dengue with climatic variables in Ponce, Puerto Rico. Previous studies have demonstrated that climate can limit vector-borne diseases from spreading but it can also favor the transmission dynamics. In addition, laboratory evidence suggests that the extrinsic incubation period in Aedes aegypti has a direct relationship with temperature. In order to perform an exploratory analysis of the possible relationships between climatic variables and the incidence of dengue, a preliminary research was done for the years 2003-2007. A data base was created using information available in the Internet for those years of the cases of dengue in Ponce and certain climatic variables: maximum temperature, minimum temperature and precipitation. The statistical software R was used to analyze the data using descriptive techniques for time series as graphs, cross correlations and decompositions in trend plus seasonal component. The results of this research showed the highest increment of the vector activity in the odd years, and temperature variables seem to be associated with the number of cases. However, no relationship between precipitation and incidence was found. In order to study further this cases pattern, the cases and climate data of 2008 and 2009 will be incorporated.

Pinero, Fernando, UPR-RIO PIEDRAS; Janwa, Heeralal, Department of Mathematics-UPR-Rio Piedras

[Mathematics 03]

Norm-Trace Codes and Subfield Subcodes For Deep Space Communications

This poster introduces concepts of Coding Theory and its relevance to NASA, in particular to Deep-Space Communications. We also introduce Algebraic Geometry Codes (AG Codes), Subfield Subcodes and Norm-Trace Codes and discuss their importance in Coding Theory and Communications.

Physics

Bobea, Milena, UPR-RIO PIEDRAS; Torres, Guillermo, Department of Physics - University of Puerto Rico, Rio Piedras Campus; Palai, Ratnakar, Department of Physics - University of Puerto Rico, Rio Piedras Campus

[Physics 01]

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.

Carpena, Jennifer, UPR-RIO PIEDRAS; Fonseca, Luis, Physics Department, UPR-Rio Piedras; Valentin, Luis, Physics Department, UPR-Rio Piedras; Yang, Dachi, Physics Department, UPR-Rio Piedras

[Physics 02]

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□ and Pd nanowires. 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.

Correa, Margarita, UPR-RIO PIEDRAS; Kumar Ashok, Physics and Institute for Fuctional Nanomaterials, University of Puerto Rico; Katiyar Ram, Physics and Institute for Fuctional Nanomaterials, University of Puerto Rico

[Physics 03]

Study of Dielectric and Ferroelectric Properties of Perovskite Thin Films Grown by Pulsed Laser Deposition technique

We have fabricated $PbSc_{0.5}Nb_{(1-x)/2}Ta_{x/2}O_3$ $0 \leq x \leq 1$ ferroelectric thin films on single crystalline 100 MgO substrate with a $La_{0.5}Sr_{0.5}CoO_3$ layer as a bottom electrode by pulsed laser deposition technique. Films were single phase perovskite with in-plane orientation along 100 direction. Although, these films have a disordered macrostructure each of them showed striking features on their microstructure, dielectric and polarization properties depending of the concentration of Nb and Ta ions. Those films with $x \leq 0.5$ exhibited frequency dispersion at low frequencies range -100 Hz to 50 KHz- with the maximum of transition temperature -T_m shifted towards lower frequency for about 40 degrees, while for higher frequencies T_m suffers an exaggerated shift. The polarization hysteresis loops of these films were slim in the vicinity of the DPT and become well saturated and well defined on decreasing temperature. High Resolution Transmission Electron Microscope studies of these films illustrated small polar nanoregions surrounding by bigger disordered regions. In the case of films with higher x values $x>0.5$, the frequency range of the frequency dispersion was high -1 to 1000 kHz- with a T_m shift of about 50 degrees. However, their polarization hysteresis loops were slim without significant change with temperature at the same time their HRTEM show mainly an ordered microstructure which may support the invariant nature of polarization hysteresis. We also found a systematic shifting of T_m to lower temperature side for each film respect to their bulk counterpart that is due to the compressive strain in films.

Dussan, Sandra, UPR-RIO PIEDRAS; Ashok Kumar; Ram Katiyar, Physics, UPR-Rio Piedras

[Physics 04]

Multiferroic properties of artificially PZT/LSMO bi-layers

A Multiferroics material combines or more functional properties i.e. ferromagnetism, ferroelectricity and ferroelasticity. The recent finding of multiferroic composite and layered nanostructure with the coexistence of ferroelectric and ferromagnetic materials have attracted the attention of various researchers due to its potential applications in highly sensitive magnetic field sensors and multistate memory devices. Early experimental analysis on heterostructures comprising a ferro-or piezoelectric and a carrier-mediated magnet suggest the possibility of artificially engineered multiferroics in which the coupling is mediated through an electrical field effect at interface. We present here the results of our progress on the synthesis and characterization of $PbZr_{0.52}Ti_{0.48}O_3/La_{0.67}Sr_{0.33}MnO_3$ (PZT/LSMO) bi-layers thin films. The samples were grown on MgO (100) and $LaAlO_3$ (100) substrates using Pulsed laser deposition technique. The XRD patterns of PZT/LSMO heterostructure compared with the pure PZT and LSMO thin films grown at the same conditions evidenced that all picks present correspond to pure structure without secondary phases, confirmed by their respective Raman spectra. Room temperature M-H results exhibit well-shaped magnetization hysteresis loops, good saturation and high coercivity. Preliminary results evidenced the existence of electrical and magnetic properties into heterostructure.

Galvez, Marco, UPR-MAYAGUEZ; Montes, Gina, Mechanical Engineering, University of Puerto at Mayaguez; Perales, Oscar, Engineering Science and Materials, University of Puerto Rico at Mayaguez

[Physics 05]

Progress on the Synthesis and Characterization of Nanostructured Multifunctional Materials: BiFeO3 and ZnO

Pure and doped Bismuth ferrite (BiFeO□) nanoparticles and ZnO films and powders were produced to study the effect of the composition and crystal size on the structure and the corresponding functional properties. BiFeO□ ferrite was synthesized in ethylene glycol media and thermally treated at different temperatures to investigate the development of the ferrite phase. Observed magnetic behavior of this ferrite was dependent on the crystallite size and the Cobalt levels in starting solutions. Depending on synthesis conditions, the formation of BiFeO□/Co ferrite nanocomposites could be suggested. In turn, pure and Co- or Sc-doped ZnO films and powders were synthesized through a

modified sol-gel approach, where different types of agents to improve the viscosity in precursor acetate solutions in ethanol were evaluated. Films thickness of around 100nm was produced by this way. TG-DTA analyses suggested annealing temperatures of above 400ºC were required for effective development of the oxide phase. The average crystallite size, estimated from XRD analyses, varied from 19.5nm to 29nm when ZnO films were annealed for 1 hour at 450°C or 550°C, respectively. The magnetic response of powders and films changed from diamagnetic to weakly, but noticeable, ferromagnetic depending on the Co- and Sc-contents (in the 0.0 at%-1.0 at% range) and annealing temperature.

Li, Fengyu, UPR-RIO PIEDRAS; Zhao,jijun, School of Physics and Optoelectronic Technology,Dalian University of Technology; Wang,Lu, School of Physics and Optoelectronic Technology,Dalian University of Technology; Chen,Zhongfang, Department of Chemistry, University of Puerto Rico

[Physics 06]

Ab Initio Studies on Water Clusters

Using MP2 and CCSD computational results as reference, the performance of a series of density functionals and basis sets were evaluated for small water clusters H_2O_n (n=1-10), and the M06-L/6-31+G(2d, 2p) method is recommended as compromise of accuracy and efficiency. This method was then used to refine the medium-size water clusters H_2O_n (n=11-25), whose lowest-energy configurations were screened by Mont Carlo search algorithm using TIP4P and TIP5P empirical potentials. These studies result in some lower-energy minima in the potential energy surface, and would give some implications on the size-dependent structural evolution of the water clusters.

Lopez, Ivan Joel, UPR-RIO PIEDRAS; Dolidze, Vladimir, Department of Physics, UPRRP; Rivera, Manuel, Department of Physics, UPRRP; Rodriguez, Fabiola, Department of Chemistry, UPRRP, Martinez, Shirley, CIMATEC; Otero, James, CIMATEC; Aliev, Fouad, Department of Physics, UPRRP

[Physics 07]

Molecular Dynamics in Complex Systems

By studying the molecular dynamics of complex systems one can learn the intricacies of the physics and chemistry, which occur at the solid/liquid interface of a wide range of materials. Implementing various techniques allows one to obtain valuable information on various phenomena, raging form protein folding to phase and glass transitions, that may lead to breakthroughs in condensed matter physics, materials scienceand technology. We present the results of our current research on the molecular dynamics of polymer nanocompositesand confined

liquid crystals by various methods: Broadband Dielectric Spectroscopy(BDS), Differential Scanning Calorimetry (DSC), Dynamics Light Scattering (DLS), and Brillouin Light Scattering (BLS). We also present an educational module, as part of the GK-12 program, designed to bring the concepts that are implemented in our research laboratories to middle school children in the public school system.

Medina, Olga, UPR-RIO PIEDRAS; Nocua, Jose Eneider, Fisica, UPR-Rio Piedras; Gomez, Ramon, Biologia, UPR-Bayamon; Montano, Daniel, Fisica, UPR-Rio Piedras, Avalos, Javier, UPR-Bayamon; Morell, Gerardo, Fisica, UPR-Rio Piedras; ,

[Physics 08]

Bacterial Behavior of Pseudomonas Aeruginosa on Micro and Nano diamond surface

Nanotechnology leads to the synthesis of new types of nanomaterials that have great potential to enhance the quality of human life, such as nanodiamond. The medical industry can greatly benefit from coatings designed to reduce the bacterial viability on implants and medical tools. We studied the survival of pseudomonas aeruginosa bacteria, a common nosocomial pathogen, on nanodiamond (NCD) and microdiamond (MCD) coatings grown by chemical vapor deposition in comparison to copper (Cu) and silver (Ag), known bactericides, and stainless steel (SS) and polyethylene (PE), widely used in households and hospitals. The results indicate that nanodiamond inhibits P. Aeruginosa, similar to Ag and Cu. On the other hand, P. Aeruginosa remains alive on SS, MCD and PE for days. Nanodiamond, besides making excellent hard coatings, is a fully biocompatible material because it is completely made of carbon, the element of life. Hence, biomedical applications and biomedical devices can take advantage of its extraordinary self-sterilizing properties.

Mendez, Hector G, UPR-MAYAGUEZ

[Physics 09]

Development of Pt Nanowires as Electrochemical Gas Sensors

Very small Pt and Pd nanowires have shown a mechanism for the electrochemical detection of H_2 that is the inverse from that of the bulk material, the resistance decreases with H_2 adsorption. Here we propose to study the sensing capabilities of Pt and Pd nanowires ranging from 10 to 20 nanometers in diameter, synthesized using zeolites as templates. These nanowires are formed through a solid-state reduction method developed at our laboratory. These nanowires were deposited on a silicon based interdigitated electrode with platinum electrodes. Due to Pt nanowire agglomeration issues, the resistance of Pt inside zeolites formed into films was also tested. The zeolite films with

platinum nanowires, show a percent difference in resistance of 188% over the zeolite alone, showing that these films show potential as a hydrogen sensing system.

Montalvo, Stephanie, UPR-RIO PIEDRAS; Valentin, Luis, Physics, UPR - Rio Piedras; Hernández, Janiece, Chemistry, UPR - Rio Piedras; Resto, Oscar, Physics, UPR - Rio Piedras

[Physics 10]

Transition Metal Silicide Nanorods for Spintronics Applications

Spintronics is a technology that uses the spin of the electron, its magnetic moment, and the electronic charge for the development of new ultra compact and fast devices. Transition metal silicide nanorods are new materials with great potential for spintronics applications. This is due to their simple integration into conventional silicon base electronics and their 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- and micro-scaled rods and tubes. When the material is in the nano-scale, the electrical and magnetic properties might show significant differences from their bulk counterparts. We have synthesized nanorods of $CrSi_2$ and we are planning to synthesize nano- and micro-rods of Fe-silicide, and $Cr_xFe_ySi_z$. We plan to explore selective doping of the nanostructures using ion implantation and investigate the subsequent modifications of their electronic and magnetic properties that will allow us to develop magnetic-semiconducting interfaces. ZnO nanowires grown by CVT will be implanted with Cu and Cr ions to evaluate this technique for the formation of room temperature magnetic semiconducting phases.

Nocua, Jose, UPR-RIO PIEDRAS; Morell, Gerardo, Physics, UPR Rio Piedras

[Physics 11]

High-yield Synthesis of Stoichiometric Boron Nitride Nanostructures

Boron nitride (BN) nanostructures are very important materials in engineering applications, which include the strengthening of structural materials to make lighter components. Using borazine ($B_3N_3H_6$) as precursor and chemical vapor deposition, BN nanostructures were deposited on cooper substrates. Their morphology was examined by scanning electron microscope and transmission electron microscopy, while their chemical composition was studied by energy dispersive spectroscopy, Fourier transform infrared spectrometry and X-ray photoelectron spectroscopy. The results indicate that the nanostructures obtained are hexagonal and rhombohedral or a mixture of the two, with a 1.1:1 atomic ratio of boron to nitrogen. The onset of deposition occurs at 2300^{o}C

temperature of filament for five seconds deposition time, at 2.4 Torr pressure. By this temperature, H bonds break and radicals join together to form stoichiometric BN nanostructures.

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[Physics 12]

Structural Evolution of ZnO Thin Films wth the Deposition Duration

ZnO thin films have been prepared on Si (100) substrate by direct current (dc) and radio frequency (rf) magnetron sputtering respectively. Thermal annealing was performed at up to 800 ºC in atmosphere for 2hrs in order to improve the qualities of ZnO thin films. The effects of deposition duration on the crystallization behavior of the films have been investigated. The structural properties of ZnO thin films via dc and rf sputtering techniques were compared. Experimental results indicated that the structural and crystal properties of the films synthesized by dc sputtering do not appear largely change following an increasing of deposition time, whereas rf sputtering deposition yields high quality of single crystalline structure of film at first 10 minutes of disposition. Thickness of the file is around from 200nm to 600nm. Following an increase of deposition time from 5minutes to 10 minutes, the ZnO varied from monocrystalline structures to polycrystalline structures. Furthermore, large nano particles are observed on the surface of the surface.

Rivera, Adriana, UPR-RIO PIEDRAS; Wu, Javier, Department of Physics, UPR-RIO PIEDRAS; Palai, Ratnakar, Department of Physics, UPR-RIO PIEDRAS

[Physics 13]

Growth and Characterization of Ga1-xYbxN Nanostructures Thin Films

Rare-earth nitrides (REN) are emerging materials for novel microelectronics applications because of their interesting optical and electronic properties, from metallic or semi-metallic to semiconductor. Heterostructures of nitrides have applications such as high power microwave devices, high frequency and high field effect transistors, light-emitting diodes (LEDs), and high electro mobility transistors.

The optical and electronic properties of rare-earth nitrides have not been widely investigated. In order to improve on the performance of these materials further studies of the optical and electrical properties of the nitride layers are required. The present work is interested in further development of rare-earth nitrides, and

GaN:RE doped materials for higher brightness, superior durability and color capability, in order to advance its commercial application.

Nanostructures of Ga1-xYbxN have been grown using plasma assisted Molecular Beam Epitaxy. X-Ray diffraction, atomic force microscopy, Hall effect, photoluminescence, cathodoluminescence, and magnetoelectric properties have been investigated for better understanding of optical and electronic properties.

Sajjad, Muhammad, UPR-RIO PIEDRAS; Zhang Hongxin, Physics, UPR; Peng Xiaoyan, Physics, UPR; Peter X. Feng, Physics, UPR-Rio Piedras

[Physics 14]

Synthesis of BN Nanostructure on Si and Mo substrates by Short Pulse Laser Plasma Deposition Technique

The synthesis of Boron Nitride nanostructure (BNNS) have great interest in material technology due to its applications and numerous properties i.e good thermal conductivity, high hardness, low thermal expansion, good thermal shock resistance, high electrical resistance, microwave transparency and chemically inertness. There are several phases of BN, synthesized in different experimental conditions. In present work, we report BN nanostructure i.e nanorods, nanoballs and nanosheets.

Short pulse laser plasma deposition technique is used to nucleate BN nanostructures on the Si and Mo substrates at different temperatures, ranging from 300°C to 700°C. Initially, BN thin film layer is deposited on substrates surfaces and then with increase of temperature, stress increases and this layer is transformed into nanostructure i.e nanorods and nanoballs. Scanning Electron Microscopy is used to revels micro level information of BN nanostructures. EDX spectra showed fewer percentage of impurity i.e 1.45At% of oxygen in the BN structure. X-Ray diffraction (XRD) is used to study the different phases of BN. The small intensity peak appeared at 26° shows the presence of h-BN whereas large intensity peak at 42.5° degree shows c-BN phase. Raman spectroscopy was used to study the sp^3 bonding for c-BN and sp^2 bonding for h-BN. Both Raman and XRD results are in good agreement in analysis of BN nanostructure.

Sanchez, Dilsom Alberto, UPR-RIO PIEDRAS; Kumar, Ashok, Katiyar, Ram S.; Physics Dept, UPR Rio Piedras

[Physics 15]

Evidence of Multiferroic Properties at Room Temperature of Single-Phase Pb(Zr0.53Ti0.47)1-x (Fe0.50 Ta0.50)xO3 Thin Films

Magneto electric (ME) multiferroic (MF) materials that couple with the magnetic and magnetic fields possess a rich variety of macroscopic, mesoscopic and microscopic properties. For example, it is possible to manipulate the electrical state of a multiferroic material through a magnetic field or vice versa, which is not only appealing scientifically, but also makes the multiferroic materials promising for a wide range of applications, including electrically controlled microwave phase shifters or ferromagnetic resonance devices, magnetically controlled electro-optic or piezoelectric devices, broadband magnetic field sensors, and magnetoelectric memory cells.

Single phase MF thin films of Pb(Zr0.53Ti0.47)1-x (Fe0.50 Ta0.50)xO3 (PZFT) (x= 0.10, 0.20, 0.30, 0.40) highly oriented were fabricated by pulse laser deposition technique. Surface topography of these films showed well defined grain with average grain size (~ 20 -100 nm), that increases with increase in Ta and Fe compositions. The surface roughness (~ 2-8 nm) also increases with increase in Fe and Ta compositions. X-ray diffraction pattern confirmed (100) orientations of these films without any pyrochlore/impurity phase. All of these films indicated low leakage current, low dielectric loss, and high dielectric constant. The dielectric constant maximum temperature shifted to lower temperature with increase in iron and tantalum concentrations. The magnetization vs. applied magnetic field (M-H) curves showed well defined hysteresis with remanent magnetization (Mr ~ 0.004- 0.13 emu/gm) and very small coercive field (900 Oe). These films displayed very high polarization ~ (90-75 µC/cm2) at room temperature and therefore these may be suitable for high density non volatile memories.

Tovar, Faiver, UPR-RIO PIEDRAS; Mosquera-Vargas , Edgar, Physics Department and Institute for Functional Nanomaterials, Universidad de Puerto Rico-Rio Piedras; Marin, Carlos, Engineering Department and Institute for Functional Nanomaterials, Universidad de Puerto Rico-Mayaguez

[Physics 16]

Vapor-Liquid-Solid Synthesis and characterization of Selenium-filled Single-Walled Carbon Nanotubes.

Selenium-filled single-walled carbon nanotubes (Se-SWCNTs) have been studied by analytical transmission electron microscopy (TEM) and micro-Raman spectroscopy. TEM imaging, EELS and EELS mapping confirms the incorporation of selenium into nanotube channels. The behavior of the radial breathing mode and the G-band was detected by Raman spectroscopy and indicates the strong influence of incorporated selenium inside SWCNTs.

Urcia-Romero, Silvana, UPR-MAYAGUEZ; Perales-Pérez, Engineering Science and Materials; Gutierrez, Gustavo, Mechanical Engineering

[Physics 17]

Effect of Dy-Doping on the Structural and Magnetic Properties of Co-Zn Ferrite Nanocrystals for Magnetocaloric Applications

Nanoparticles for magnetocaloric applications should combine small coercivity, low demagnetization temperature and high pyromagnetic coefficients while keeping the magnetization as high as possible. The strong dependence of the magnetic properties of Cobalt-Zinc ferrite with specific dopant species enables this material to be considered a candidate for magnetocaloric applications. Hence, pure and Dy-doped $Co_{0.7}Zn_{0.3}Fe_2O_4$ cobalt-zinc ferrite nanocrystals have been synthesized by conventional and flow-rate controlled coprecipitation routes. This modified approach allows the control of ferrite crystal growth at the nanoscale and tuning of the corresponding magnetic properties. The magnetic properties of the produced nanocrystals were determined as a function of their structure, nominal dopant concentration and crystal size. X-ray diffraction, transmission electron microscopy, and Raman spectroscopy analyses suggested both, the actual incorporation of the dopants into the host ferrite lattice and the promoting effect on crystal size of the flow-rate at which the reactants are contacted. The average crystallite size varied from 13nm (no control of flow-rate) to 28nm when the ferrite was synthesized at 1mL/min. Doping caused the maximum magnetization to decrease from 60emu/g (non-doped ferrite) to 55emu/g when the ferrite was doped with 1 at % of Dy. The maximum magnetization of the Dy (y = 0.01) Co-Zn ferrite went up to 62emu/g with synthesis under flow-controlled conditions. The presence of 1 at % Dy in the ferrite caused the demagnetization temperature to decrease from 350^{o}C (non-doped ferrite) to 320^{o}C. The demagnetization temperature further decreased down to 308^{o}C when the ferrite powders were synthesized under flow-rate controlled conditions.

Valentin, Luis, UPR-RIO PIEDRAS; Hernandez Mayra, Chemistry UPR Rio Piedras; Fonseca Luis, Physics UPR Rio Piedras, Resto Oscar, Physics UPR Rio Piedras

[Physics 18]

Fabrication of Transition Metal Silicide and Oxides Nano- and for Thermal Sensors Applications

We report the fabrication of novel micro and nano structures of chromium silicide. The nano- rods and tubes were grown on a p-type Si wafer. We synthesise this nanostructure using quartz reactor. We maintainthe temperature near 1000 ^{o}C for 20minutes.The characterization of the nano- and microtubes included:

HRTEM spectrum an mapping, electron diffraction, X-ray fluorescence and XPS spectroscopies. Details of the morphology and composition of the structures will be presented

Velazquez, Rafael, UPR-RIO PIEDRAS

[Physics 19]

Study of growing microcrystaline Diamond on CrN coated Stainless Steel substrate

Ferro-materials has a disadvantage with carbon materials due to can not grow a carbon film on the surface. This condition is a common phenomenon in ferro-materials due to the ferro-materials absorbed carbon atoms inside the lattice, making this a interesting area to be research. As a proposed solution, to decrease or eliminate the possibility of carbon absorption in the surface a material should be between both surfaces. The ferro-material used was stainless steel, and it had CrN film. This pretreatment was performed previously to the samples submitted. In this research we will try to grow Microcrystalline diamond (MCD) and nanocrystalline diamond (NCD) on the stainless steel sustrated coated with CrN film.Microcrystalline diamond (MCD) and nanocrystalline diamond (NCD) films (including materials referred to as tetrahedral amorphous carbon, ultra-nanocrystalline diamond, and nanostructured diamond) are highly hard materials, in general. This situation precludes from taking advantage of the many superlative properties of diamond that make it suitable for protective and tribological coatings (i.e. hardness, chemical inertness). Various techniques are used for Microcrystalline diamond (MCD) and nanocrystalline diamond (NCD) grow. The employed technique was Chemical vapor deposition (CVD) System to grow the stainless steel substrate coated with a CrN thin film in a (MCD) film. Such a diamond/substrate interface represents an important advantage in the efforts to integrate these two dissimilar materials*. The samples were examined by a number of complementary techniques for characterization such as Raman, XRD and SEM to make sure we have a good quality Diamond surface and structure.

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[Physics 20]

Defects and Edge Reconstructions of Few-Layer Graphene

Few-layer graphene were produced on transition-metal templates by using super-short-pulse laser produced plasma deposition techniques. Unusual

structures within clean few-layer graphene patches were observed and studied. Some unique spherical shapes with diameter around 100 nm were distributed in the interior of few-layer graphene, which could be caused by the residual stresses during the fast cooling process. The edges of the few-layer graphene are not ideally smooth and shows a fractal-like “coastline” morphology, which could be caused by the crack phenomenon during the growth process. An unusual edge reconstruction was also observed: a double layer folded back on itself, representing four layers. It is not yet clear how the folding negotiates its bonding with the few-layer graphene; presumably all the upper layer are held in place simply by van der Waals bonding with atoms in the underlying few-layer graphene, and thus it would constitute a double folded layer. Wrinkles were found within the few-layer graphene, which is likely due to the presence of nanoparticles underneath the few-layer graphene causing distortion. These results can provide valuable information for understanding the growth mechanism of graphene, which may facilitate its controllable synthesis and offer unique opportunities for engineering novel nano-devices with complex topologies.

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