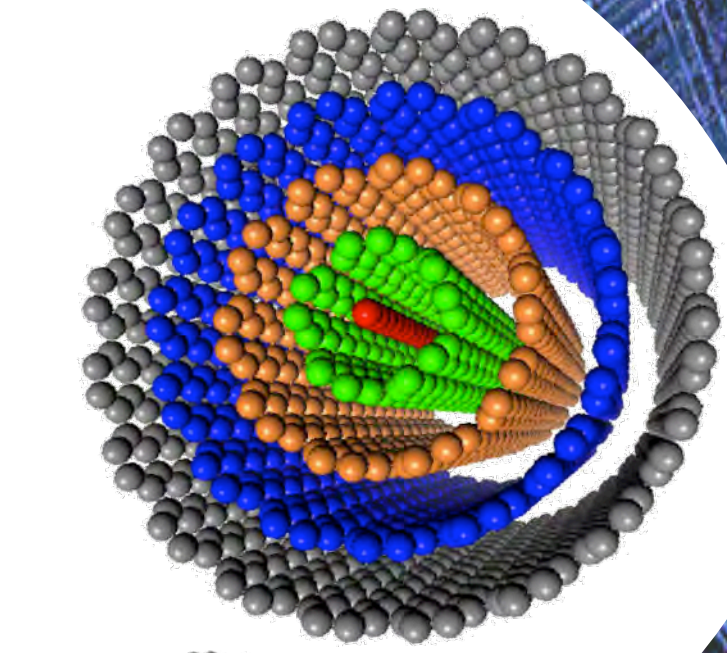
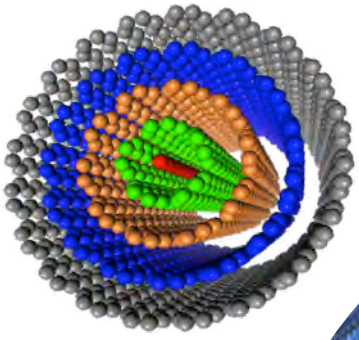
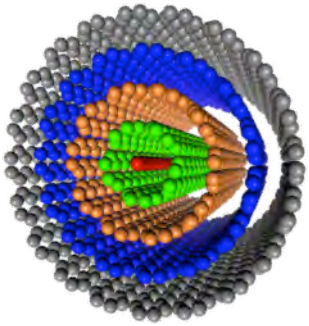
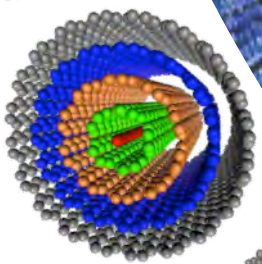
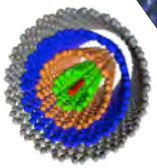
7th PREM Annual Meeting







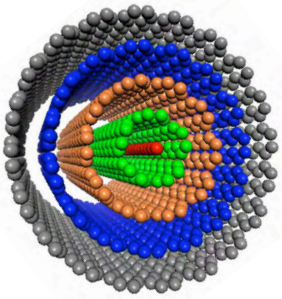




November, 19, 2010

Palmas del Mar, Humacao, P.R

7th PREM ANNUAL MEETING
November 19, 2010
Palmas de Mar, Humacao P.R.



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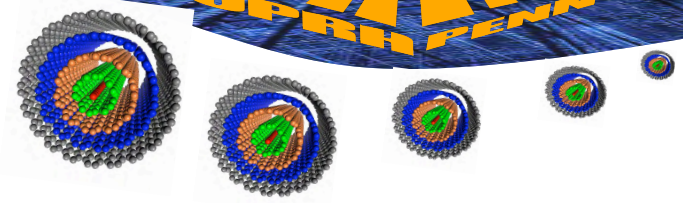


9:15 - 10:00 AM **Registration & Breakfast**

10:00 - 10:10 AM **Welcome Messages**
Idalia Ramos, PREM PI
Ernesto Esteban, UPRH Acting Academic Dean
Andrew McGhie, Associate Director PENN MRSEC
Arjun Yodh, PREM Co-PI, Director PENN MRSEC

10:10 - 10:25 AM **PREM UPDATE**
Idalia Ramos, **Andrew McGhie** and **Arjun Yodh**

10:25 - 10:30 AM **PREM Students UPDATE**
Katherine Carrasquillo, Yarely Dávila and Maritza Reyna

10:30 - 11:00 AM ***Deformation at the Nanoscale: New Mechanisms Revealed through In Situ Testing***, **Dan Gianola,** UPENN

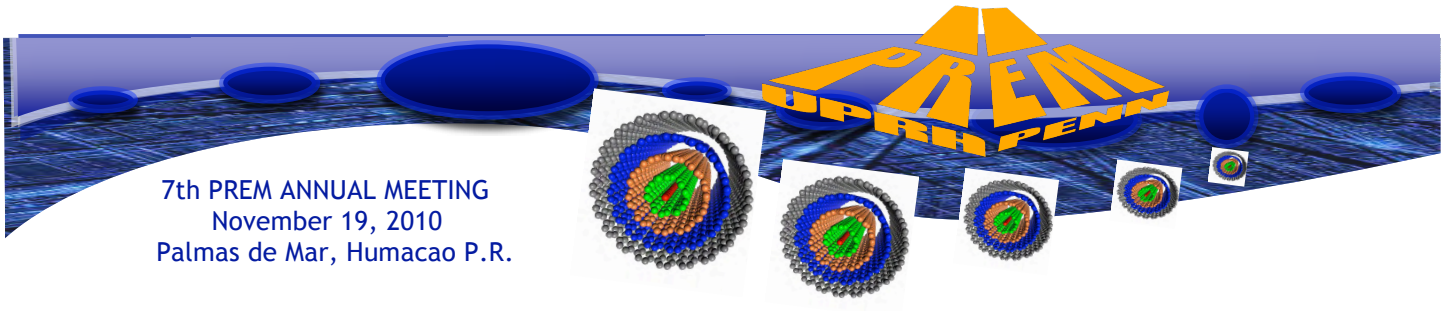
11:00 - 11:15 AM ***Fracture surfaces and actuators: mathematical models and their computational aspects***, **Pablo Negrón**, UPR-Humacao

11:15 - 11:30 AM **Break**

11:30 - 11:45 PM **Nanoparticle shape instability by Coulomb interactions,**
Natalya Zimbovskaya, UPR-Humacao

11:45 - 12:00 PM **Using GPUs for Molecular Dynamics Applications, *José Sotero***, UPR-Humacao

12:00 - 1:30 PM **Working Lunch**



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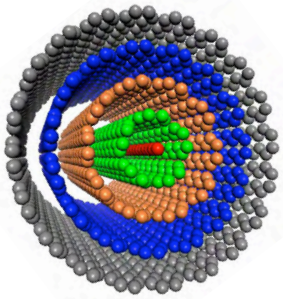
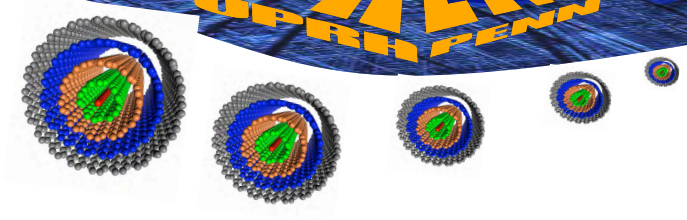
12:00 - 1:30 PM	**Working Lunch**
1:30 - 1:45 PM	***Devices based on Electrospun Poly(3,4-ethylenedioxythiophene) doped with (poly styrene sulfonic acid) Nanofibers and Nanoribbons*, Nicholas Pinto**, UPR-Humacao
1:45 - 2:00 PM	***Exploring Nanoscale Device Fabrication with Self-assembled Materials*, Josee Vedrine**, UPR-Humacao
2:00 - 2:15 PM	**Electrospinning of ZnO Gas Sensing Nanostructures, Victor Pantojas**, UPR-Cayey
2:15 – 2:30 PM	***Study of Inclusion Complexes between B-Cyclodextrin and Ferrocenyl Chalcones Derivatives*, Rocío Cardona**, UPR-Río Piedras
2:30 – 2:45 PM	**Break**
2:45-3:00 PM	**Posters Setup**
3:00 - 4:30 PM	**Students Posters Presentations**
4:30 - 5:30 PM	**Advisory Committee meets to write Report**
5:30 PM	**Closing**

Faculty Research Presentations





Deformation at the Nanoscale: New Mechanisms Revealed through In Situ Testing

Dan Gianola, UPENN

Experimentally approaching the theoretical strength of materials has been the holy grail of structural materials research and development. However, most engineering materials fail before reaching even a small fraction of this upper limit. This talk will present experiments on a new class of materials, the *ultra-strength*, which have the capability of withstanding specimen-wide mechanical stresses that approach the theoretical limit – the maximum achievable stress in crystalline materials – and represent a new frontier of materials design. Nanoscale "bottom-up" synthesis creates small volumes of materials and provides the high crystalline quality that allow for these mechanically extreme environments. However, the mechanisms that accommodate plastic deformation are not known, limiting our ability to tailor the properties of nanostructured materials in next generation technological devices that are subject to extreme mechanical and thermal duress.

Recent progress in the area of *in situ* electron microscopy (scanning and transmission) has allowed for quantitative interrogations of the deformation of nanoscale materials. Selected experiments will be presented to illustrate how these techniques have can directly correlate underlying physical phenomena with measured properties.

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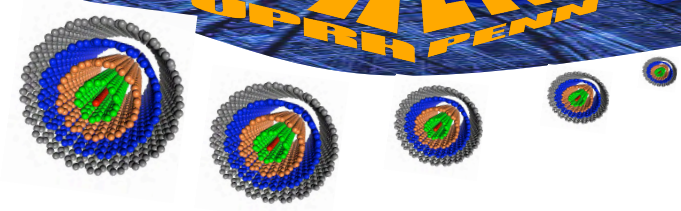

Fracture surfaces and actuators: mathematical models and their computational aspects

Pablo Negrón[1], Jey Sivaloganathan[2],
Jorge Santiago[3] and Eva Campo[3]
[1]UPR-Humacao, [2]University of Bath, UK,
and [3]UPENN

We discuss material instabilities of cavitation type for bodies under tension. We give a new characterization based on what we call the *volume derivative*, of the set of linear displacement boundary conditions for which energy minimizing deformations produce a hole inside an originally perfect elastic body. We show how this characterization leads to a numerical procedure for computing these critical hole producing three dimensional deformations and give numerical examples for specific materials.

Also we present a preliminary model based on the theory of nonlinear elasticity, of an actuator consisting of a mixture of a polymer with carbon nanotubes. Using a finite element method to solve the equilibrium equations for the resulting composite material, we compute the average deformation of a nanotube and corresponding average stresses when the specimen is put under axial tension and under the influence of an external energy source.

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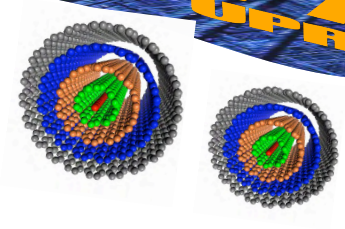
Nanoparticle shape instability by Coulomb interaction

Natalya Zimbovskaya[1], L. A. Somers[2],
A. T. Johnson[2] and E. J. Mele[2]
[1]UPR-Humacao, [2]UPENN

Metal atoms adsorbed on few-layer graphenes condense to form nanometer-size droplets whose growth in size is limited by a competition between the surface tension and repulsive electrostatic interactions from charge transfer between the metal droplet and the graphene. Under certain conditions a growing droplet can be unstable to a family of shape instabilities. This phenomenon was observed for Yb deposited and annealed on few-layer graphenes. A theoretical model to describe it is developed. The model describes the onset of shape instabilities for nanoparticles where their growth is limited by a generic repulsive potential and provides a good account of the experimentally observed structures for Yb on graphene [1].

[1] L. A. Somers, N. A. Zimbovskaya, A. T. Johnson, and E. J. Mele,
Phys. Rev B 82, 115430 (2010).

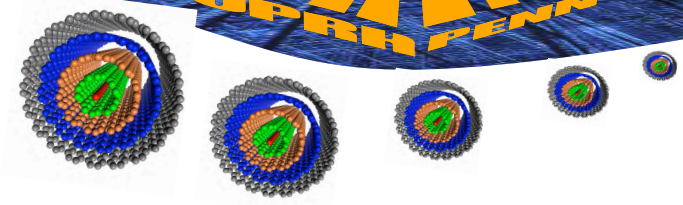


Using GPUs for Molecular Dynamics Applications

José Sotero, UPR-Humacao

Last year a method for computing the electrostatic potentials was tested using ACEPS, a graphical user interface (GUI). This tool approximates the electrostatic potentials by dividing the system in a grid. This methodology was compared with the exact computation in which all atoms are used. Results show that there is a minimum variation in the electrostatic potentials. This method was parallelized using the CUDA libraries to make the calculation using Graphical Processing Units (GPU). Tests using a GPU with 240 processing units showed an improvement in speed by a factor of 40 compared with the sequential version using CPU.

The focus of our group is now shifting to computation of properties of liquids at small scales. New code has been written and tested that take advantage of a GPU architecture that has reached the market recently. Existing code written by Preston Moore is also being modified to use this architecture. Test are being currently made to validate the results of the new software using widely used MD software as a benchmark. Current result show agreement of results as well as performance improvement of the new software over the standard general purpose MD software when used for this particular kind of application.



Devices based on electrospun poly(3,4-ethylenedioxythiophene) doped with (poly styrene sulfonic acid) nanofibers and nanoribbons

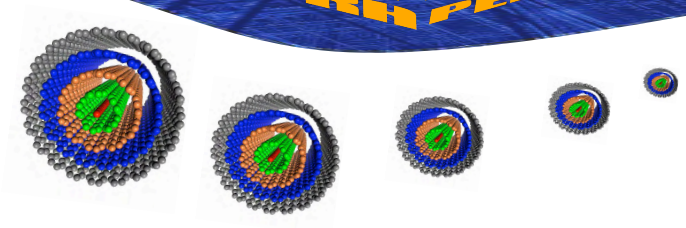
Nicholas Pinto, UPR-Humacao

The conducting polymer poly(3,4-ethylenedioxythiophene) doped with (poly styrene sulfonic acid)- PEDOT-PSSA is commercially available and commonly used as interconnects in devices, mainly in the form of thin films. Using the electrospinning technique, we have fabricated sub-10 nm fibers and ribbons of this polymer and have used it as the active material in several devices and sensors. Due to the large surface to volume ratio and small quantity of active material used in their fabrication, these sensors have a faster response time with larger amplitude changes when compared to similar alcohol sensors based on PEDOT-PSSA. By simply crossing nanoribbons of this polymer with SnO_2 we have fabricated Schottky diodes with tunable device parameters. Finally, by making composites of PEDOT-PSSA with PVDF-TrFE we wish to explore the possibility of making ferroelectric field effect transistors (FE-FET's). The latest results on these experiments will be presented.

Exploring nanoscale device fabrication with Self-assembled materials

Josee Vedrine, UPR-Humacao

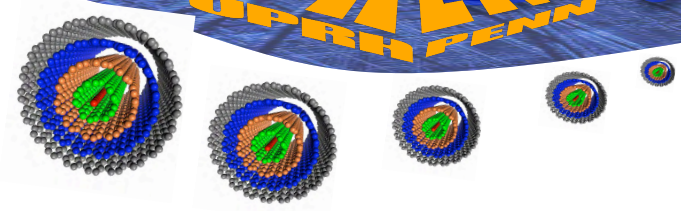
The process of self-assembly can allow devices to reach physical length scales in the 10's nm while offering a simplified and low-cost alternative from customary fabrication techniques. Our group is exploring a range of methods to fabricate devices using self-assembled organic materials. We have begun the fabrication process of basic components including nanocapacitors using a monolayer of polystyrene spheres as mask template, and nanoscale contacts for probing the material and electrical properties of films and compounds. AFM and SEM tools are used to analyze structures and process effectiveness



Electrospinning of ZnO gas sensing nanostructures

Victor Pantojas, UPR-Cayey

Metal oxides, such as ZnO, CuO, and FeO_x, are especially attractive as sensing elements synthesized in polycrystalline nanostructures. The properties of polyvinyl alcohol (PVA), a water soluble polymer, are been explored with the purpose of producing metal oxide fibers from PVA-containing solutions by electrospinning. The objective is to obtain faster and more sensitive gas sensors by reducing the dimensions of the sensing elements and by combining them with metal cluster additives. Zinc oxide fibers are formed by preparing a PVA solution containing zinc acetate which is electrospun and calcined in air. Zinc oxide shells are formed by deposing zinc by sputtering on top of a polymer mat previously electrospun on a silicon wafer with a top layer of silicon oxide. The samples are heated in air for two hours to gasify the polymer template and promote the oxidation of the metal resulting in the formation of ZnO shells. The thickness of the shell is controlled by simply adjusting the sputtering deposition time. A chamber was set up to test the sensitivity of the fiber to hydrogen gas.

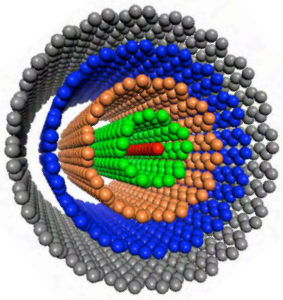


Study of Inclusion Complexes between B-Cyclodextrin and Ferrocenyl Chalcones Derivatives

Rocío Cardona, Myrna R. Otaño, Ingrid Montes and Ana R. Guadalupe,
UPR-Río Piedras

Ferrocene derivatives have been extensively studied for a number of reasons. First, they exhibit the well-defined one electron redox of Ferrocene. Their redox process is electrochemically reversible or quasi-reversible. Their formal redox potential ($E^{o'}$) depends on the nature of substituents attached to the cyclopentadienyl rings. Through variety synthetic routes, derivatives can be made with tunable redox and spectroscopical properties. They have found applications in different fields such as biosensors, drug delivery systems, electrocatalyts, and optoelectronics, among others. A family of Ferrocene derivatives that have drawn considerable attention from scientists in recent years is that of the Ferrocenyl chalcones (FC's). These compounds not only possess the well known redox activity of Ferrocene, they also show intense colors. A FC is a compound where the Ferrocene is linked to an aromatic group through an enone moiety. Several derivatives of FC's have been synthesized and characterized structurally. More recently, studies on FC's have focused on their biological properties, in particular their potential antiplasmodial and anticancer activities. On the other hand, B-cyclodextrins (B-cyc) are cyclic oligosaccharides of seven units. They can form inclusion complexes with guest molecules by means of non-covalent interactions (hydrogen bonding, hydrophobic forces, and dipole interactions). The formation of such complexes can lead to an enhancement of the physical and reactivity properties of the guest. In previous work we have shown the electrochemical and spectroscopical properties of the Fc's, both in solution and when immobilized in polymeric matrix such as Nafion. In these environments the derivatives exhibit a quasi-reversible electrochemical behavior, and a shift in formal potential which depend on the electronic properties of the substituent's directly attached to the phenyl ring. We have interest in using these compounds for the detection of molecules of biological interest, such as glucose, that do not posses electrochemical response. To accomplish this goal, we propose the use of B-cyc in combination with our FC's. We expect that the formation constant (k_f) of the glucose molecules toward B-cyc is bigger than that between FC's and B-cyc, leading the removal of the electrochemical molecule of the cavity of the B-cyc and therefore increasing the current response. This current increment will directly related with the amount of glucose added. To achieve that goal it is necessary to calculate the k_f values of FC's-B-cyc complexes. Here will be presenting the chemical-physical studies of the interaction of selected FC's with B-cyclodextrin by ^{1}H-NMR, Cyclic Voltammetry, and Osteryoung Square Wave Voltammetry. Also, will present the first attempts on the development of a glucose sensor.

Poster Presentations



Detection of the Surface of a Liquid Nano - Droplet in a MD Simulation

P1

Fernando Berríos, Alexander Cruz, Mirgery Cuadrado,
& José O. Sotero Esteva,
Dept. of Computational Mathematics, UPR-Humacao

This work corroborates the existence of an intermediate layer of atoms between the liquid and gas phases in a nano - droplet as well as the correctness and increased performance of MD software that uses General Purpose Graphics Processing Units (GPGPU). The layering phenomenon is observed by means of a classical Molecular Dynamics Simulations (MDS). It has been observed recently in thin films of simulated liquid Argon. Measurements such as the surface tension depend on the detection of surfaces. Macroscopic models define surfaces as two-dimensional manifolds and establish relations between their geometric and physical properties, for instance, between curvature and surface tension. This 2D model of surfaces has been adapted to MDSs by extrapolating continuous surfaces from discrete data. The observation of an intermediate layer may lead to a new approach to defining the nature of surfaces of liquids at small scales.

The present simulation was performed using NAMD, NAMD for GPU, and a C++ program built exclusively for this simulation. A set of 10000 atoms was simulated using only non-bonded Lennard-Jones interactions with e and s parameter values consistent with Argon atoms. Performance comparisons were made using a single core of an I3 processor, a TESLA 1060 GPU and a TESLA 2050 GPU. The GPUs were programmed using CUDA extension of the C++ language. Trajectories of simulations were obtained with all three programs, both computing architectures, and simulated temperatures of 30, 70, 85, 100 and 140 degrees Kelvin. The total time of the run was recorded for each simulation. RDF graphs were computed for each trajectory. The speed of computations of NAMD-GPU increased by a factor of 2 when compared to the CPU NAMD. Results of our C++-CUDA code are consistent with NAMD's results. Direct observation of their graphical representation confirm that the atoms are distributed consistent with solid, liquid and gas phases according to the temperatures. RDF graphs of the trajectories of the liquid water droplet confirm the appearance of an intermediate shell between the liquid and gas phases.

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P2 Preparation of AlN nanofibers using Electrospinning

Xenia Barbosa[1], Idalia Ramos[1], Eva Campo[2], Jorge Santiago-Avilés[3]
[1]Dept. of Physics and Electronics, UPR-Humacao
[2]L.R.S.M., UPENN, [3]Dept. of E.E. and M.S.E.; UPENN

Aluminum Nitride (AlN) has important applications for the development of optoelectronics devices, ultrasonic transducers, surface acoustic wave devices and piezoelectric nano-actuators. In addition, AlN has become a very useful material as a barrier in superconductor-insulator – superconductor (SIS). We have attempted the fabrication of AlN nanofibers using electrospinning and a precursor containing aluminium nitrate nano-hydrate ($Al(NO_3)_3 \cdot 9H_2O$) and urea with cellulose acetate (CA) as the structural polymer. Both the precursor and the structural polymer were dissolved in a solution of acetone and dimethylacetamide (DMA). In electrospinning a high voltage source of 15 kilovolts (kV) is typically applied between the tip of a syringe containing a polymeric precursor and a grounded substrate, which is set at a specific distance to collect the fibers. Once the precursor was electrically charged, jets emerged from the syringe tip to the collector forming long and continuous nanofibers. After electrospinning, the nanofibers were subjected to a heat treatment under nitrogen (N_2) and ammonia (NH_3) atmospheres. Themogravimetric Differential Themal Analysis (TG-DTA) of the precursor solution showed chemical changes in the precursor solution as it was heated from room temperature to 600°C. This information was used to design the initial thermal treatment. The electrospun fibers were sintered in nitrogen (N_2) at 12ºC/min until a temperature of 900ºC was reached. Then, the atmosphere was switched to ammonia (NH_3) gas. Scanning Electron Microscopy (SEM) demonstrated the production of fibers with diameters ranging from a few nanometers to several micrometers. X-Ray Diffraction analysis confirms the production of α-Al_2O_3 fibers after heating for 90 minutes in ammonia. These results suggest electrospining is a promising technique in the production of AlN. Additional nitridation of electrospun fibers is expected by designing an appropriate heating treatment, namely by heating the fibers for longer periods and or at higher temperatures under an ammonia flow.

Study of Gallium Nitride nanofibers using Transmission Electron Microscopy

P3

Joshua L. Robles García[1], Lytzamed Santa[1], Anamaris Meléndez[1], Eva Campo[2], Idalia Ramos[1]
[1]Dept. of Physics and Electronics, UPR- Humacao
[2]L.R.S.M., UPENN

Gallium nitride is one of most important semiconductors for electronic applications because it has a wide bandgap, high heat capacity and high thermal conductivity. GaN can crystallize in the hexagonal or in the cubic crystal system. The crystal is formed by competition of grains growing in different orientations. In this work, GaN nanofibers were fabricated through an economic, simple and fast method called electrospinning. To prepare the precursor solution, Gallium nitrate was dissolved in dimethylacetamide (DMA) and mixed with a viscous solution of cellulose acetate dissolved in DMA and acetone. Initially, the electrospun fibers were sintered in Nitrogen at 400°C for one hour, to eliminate the polymer. Subsequently, the sintering process was repeated using ammonia at 900°C during five hours. X-Ray Diffraction analysis showed the characteristic peaks of hexagonal wurtzite GaN with 101 preferential orientation. The fibers were characterized using a JEOL 2010F Transmission Electron Microscope (TEM) to study the atomic planes of the nanofibers. The space between atomic planes in the selected areas was approximately 0.5nm, as measured from transmission electron microscope images. This result suggests TEM imaging of these nanofibers offers enough contrast to determine lattice parameters in the as-grown nanocrystals. During the experiment it was observed that the fibers are fragile and soft. They tend to crumble if not treated carefully. Future work includes enhancing the recipe to produce stronger fibers.

Characterization of Polyvinyl Alcohol (PVA) fibers using SEM

P4

Ericka Vélez
UPR-Cayey

The effects of solution concentration and electrospinning rate of injection on fiber diameter and morphology of electrospun poly(vinyl alcohol) (PVA) have been studied. A biodegradable polymer such as PVA is commonly used in biomedical applications because it is hydrophilic with good chemical and thermal stability, highly biocompatible, non-toxic, processed easily with high water permeability and it readily reacts with different cross-linking agents. The diameter and morphology of the fibers are evaluated after changing the amount of solvent which changes the viscosity of the PVA solution used for electrospinning. The fibers were evaluated by Scanning Electron Microscope (SEM). We show that, by changing the concentration of the PVA solution, we obtained fibers with diameter ranging from 1.4μm to 0.5 μm. The effect of changing the rate of injection from 0.6mL/hr to 0.3mL/hr on fiber diameter is also explored.

P5 Optimization of Pathogen-DNA Biosensor using Polymeric Films and Electrochemical Labels: Fc-labeled Sequences and Ru-Fc Intercalation Complex

Madeline Díaz[1], Arelys Rosado[1], Joselyn del Pilar[1],
Esther Z. Vega[2] and Ana R. Guadalupe[1]
[1]Dept. of Chemistry, UPR-Río Piedras
[2]Dept. of Biology, UPR-Humacao

Waterborne and foodborne diseases are one of the principal public health problems worldwide. Our particular interest is the development of nucleic acid biosensors (NAB) for the detection of pathogenic microorganisms in food and water samples. We have synthesized several PS films and anchored nucleic acid sequences with different lengths at gold and carbon surfaces. Non contact mode AFM and XPS were used to monitor each step of the NAB preparation, from polymer modification to oligos hybridization (conventional design).

The hybridization event has been detected electrochemically by the conventional method, which is modifying the target with Fc-NHS. We observed a small current at the potential for the Fc oxidation without signal amplification. A calibration plot was constructed using the 12K g/mol polymer modified glassy carbon electrode. A 15-mer probe was attached to the surface and hybridized with its complementary, Fc-labeled 15-mer target. We synthesized a $Ru(Fcphen)_2dppz$ complex to use as an electrochemical intercalator. The bimetallic redox complex was characterized by Square Wave Voltammetry (SWV) and we observed Fc and Ru oxidation signals at +720 mV and +1308 mV, respectively in DMF/ 0.1 M TBAP. Binding interactions of the complex with CT-DNA have been studied by UV-Vis, Fluorescence and SWV. Now, we are centered on testing the bimetallic label complexes in the polystyrene-modified surfaces as a label-free hybridization design. Currently, we expect to detect the DNA hybridization with the Ru-Fc complex and construct a calibration plot for the label-free design. Finally, we expect to produce a methodology for the construction of electrochemical biosensors based on the use of *Salmonella* DNA-functionalized polymeric films with spatial resolution, high reproducibility and high sensitivity.

P6 Study of Inclusion Complexes between B-Cyclodextrin and Ferrocenyl Chalcones Derivatives

Rocío del A. Cardona, Myrna R. Otaño,
Ingrid Montes, and Ana R. Guadalupe
Dept. of Chemistry, UPR-Río Piedras

See abstract at oral presentation number 8

Designing a New Generation of Electrochemical Biosensors for the Detection of *Pseudomonas aeruginosa* Exotoxin

P7

Yanira Enríquez, Yashira Negrón,
Rahul Singhal and Ana R. Guadalupe.
Dept. of Chemistry, UPR-Río Piedras

Pseudomonas aeruginosa (PA) is an opportunistic pathogen of clinical relevance. It secretes different virulence factors (such as enzymes and toxins) that are capable of causing infection. Exotoxin A (Exo A) is an extracellular toxin that PA produces and catalyzes the ADP-ribosylation of the eukaryotic elongation factor-2 (eEF2), inhibiting the RNA translational process and subsequently decreasing protein synthesis. We are interested in designing an electrochemical biosensor for the detection of Exo A. A free radical copolymerization of Styrene and NAS has been done in a range of 10:90 to 90:10 (Sty:Nas) molar ratios. The copolymer will be used to generate a film on carbon surfaces to anchor a ß-NAD^+ electroactive analog. Ferrocene-labeled NAD (Fc-NAD), NAAD (Fc-NAAD) and NADH (Fc-NADH) were prepared by attaching Ferrocene Succinimide (Fc-NHS) to the primary amine in the adenine moiety of each cofactor. The electrochemical analysis of the cofactors was done using the Epsilon analyzer. A three electrodes cell system was used with glassy C as the working electrode and Ag/AgCl (NaCl 3M) as the reference electrode. The Square Wave Voltammetry (SWV) analysis of the unpurified product showed the signal for Fc-NHS at 600 mV decreasing with time of reaction and a new band forming between 310-330 mV increasing with time of reaction for each cofactor. The band in 300-320 mV is tentatively assigned to the oxidation of Ferrocene in the new electroactive cofactor. The final product was purified using a column of Sephadex G-15.

The SWV analysis of the final product showed one band at 320 mV for Fc-NAD, 320 mV for Fc-NAAD and 324 mV for Fc-NADH. The Cyclic Voltammetry (CV) analysis was done at different scan rates (50, 100, 200, 500 and 1,000 mV/s) and our new product shows chemical reversibility and electrochemical pseudo-reversibility. Our work is now focused on the full characterization of each cofactor. Our goal is the successful modification of the electrode surface with Fc-NAD and the electrochemical monitoring of the ADP-ribosylation process mediated by Exo A in vitro.

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P8 Fabrication of semiconducting ZnO thinfilms and nanofibers

[1]Yarely C. Davila, [2]Nicholas J. Pinto;
[1]Department of Biology,
[2]Dept. of Physics and Electronics; UPR-Humacao

The inorganic compound ZnO has been known for several favorable properties, one of them being its high electron mobility. We have fabricated fibers and thin films of this material using electrospinning. A solution was prepared using polyvinylpyrrolidone (PVP) as the base polymer, and mixing it with Zinc acetate (anhydrous) in deionized water. The fibers were fabricated through the electrospinning method which consists of an electric field between the polymer solution and a collector plate. The samples were collected on silicon substrates and sintered at 450°C in air for forty-five minutes. A TEM grid was placed over preselected fibers and used as a shadow mask and 100 nm of gold were deposited by vacuum evaporation to create contact pads over the fibers. External contacts were made with silver paint and gold wires. Current-voltage (I-V) measurements on the fibers and films demonstrated *n*-doped behavior when a back gate bias was applied. This is very important as we plan to fabricate diodes and other electronic devices and sensors using this material. The fibers and films were also characterized using X-Ray diffraction (XRD) and energy dispersive X-Ray spectra (EDAX) confirming the presence of Zn.

P9 Fabrication of Titanium Dioxide Nanofibers for UV Light Protection

[1]Jennifer M. Reyna Liriano and [2]Nicholas J. Pinto
[1]Petra Mercado Bougart, High School
[2]Dept. of Physics and Electronics,
UPR-Humacao

In this investigation, nanofibers of titanium dioxide (TiO_2) were produced by the process of electrospinning. Titanium (IV) propoxide precursor was first electrospun into nanofibers and then heated in air at 450°C to obtain nanofibers of TiO_2. The fibers were caharacterized using XRD, SEM-EDAX and electrical measurements. Titanium dioxide has many applications as in cosmetics, as a photo catalyst and as pigment (it is considered the whitest white). In protecting from the UV light, it is used in solar screens as an active ingredient, because of is high refractive index which goes from n = 2.488 (anatase) to n = 2.609 (rutile). In order to test the TiO_2 as a UV light filter, a SnO_2 nanofiber will be used and the current passing through it monitored as a function of time. The purpose of realizing this experiment is to see if the TiO_2 nanofibers would prevent the UV light from reaching the SnO_2 sensor and how it would respond when the UV light is on or off.

Tunable Schottky diodes fabricated from electrospun crossed SnO_2/PEDOT-PSSA nanoribbons

P10

[1]Katherine V. Carrasquillo, [1]Nicholas J. Pinto
and [2]Ritesh Agarwal
Dept. of Physics and Electronics,UPR-Humacao
Dept. M. S. E., UPENN

Hardware in most solid state devices contains at least one interface between a *p*-type and an *n*-type semiconductor. Such hetero-junctions form the basic building block in logic circuits that are at the heart of microprocessors and are typically fabricated from all inorganic Si based materials. In the past two decades however, devices fabricated from organic-inorganic semiconductors that are not Si based, or from all organic semiconductors have been the focus of much research. Semiconducting *n*-doped metal oxides are attractive for use in devices and of particular interest is tin oxide (SnO_2) as it is stable in air and is optically transparent with a band gap of ~3.6 eV. *p*-doped poly(3,4-ethylenedioxythiophene) poly(styrene sulfonate)-PEDOT-PSSA is a conducting polymer that is also stable in air with a band gap of ~1.6 eV and widely used in flexible devices. The simplest and easiest polymer based device to fabricate is a hybrid organic/inorganic diode in which a junction of a *p*-doped polymer with an *n*-doped inorganic semiconductor is formed. We report on the electrospinning technique to fabricate Schottky diodes in air, by simply crossing *n*-doped SnO_2 and *p*-doped PEDOT-PSSA nanoribbons. The devices operate equally well in an ambient environment and in vacuum. An important feature of our device architecture is the complete exposure of the nano-junction to the surrounding environment (unlike other architectures where the junction is covered by the electrical contact pads) making them attractive candidates for sensor applications. By using doped Si/SiO_2 substrates in the fabrication process, the diode parameters can be tuned via a back gate voltage, an attribute that is novel to our devices. The diode on state current also increases in the presence of UV light enabling it to rectify ac signals. Turning off the UV light slowly restores the device to its original condition making it useful as a photoelectric sensor as well. Electrospinning is therefore an economical and facile technique to fabricate a wide range of multifunctional devices based on individual organic/inorganic nanofibers or nanoribbons.

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P11 Engineering of Hybrid Organic-Inorganic Solar Cells

Earl Goodwin[2], Melissa Dávila Santana[1],
David Kim[2], Danielle Reifsnyder[2],
Josee Vedrine-Pauleus[1],
Chris B. Murray[2] and Cherie Kagan[2]
[1]Dept. of Physics and Electronics, UPR- Humacao
[2]Dept. of E.E./M.S.E., and Chemistry, UPENN

The application of organic-inorganic heterostructures would allow alternative photovoltaic solar cells that convert energy into current, low fabrication costs, and fabrication on flexible substrates. In this work we explore the combinations of P3HT (poly-3-hexyl-thiophene) with PCBM (penyl-C61-butyric acid methyl ester) or P3HT combined with QDs (quantum dots) to fabricate hybrid hetero-junctions. Our experimental results show that the solution containing P3HT:PCBM with chlorobenzene as solvent improved device efficiency, and the consequence of thickness on the efficiency yield of our hybrid solar cell devices.

P12 Electrical response of electrospun PEDOT-PSSA nanofibers to organic and inorganic gases

Nicholas J. Pinto[1], Anamaris Melendez and Idalia Ramos
Jong H. Lim[2], Alan T. Johnson Jr.
Dept. of Physics and Electronics, UPR- Humacao,
Dept. of Physics and Astronomy, UPENN

Electrospun isolated nanofibers of poly(3,4-ethylenedioxythiophene) doped with (poly styrene sulfonic acid)-PEDOT-PSSA were used to sense vapors of several aliphatic alcohols. Due to the large surface to volume ratio and small quantity of active material used in their fabrication, these sensors have a faster response time with larger amplitude changes when compared to similar alcohol sensors based on PEDOT. Increasing the size of the alcohol molecule leads to longer response times, which is attributed to slower diffusion of the larger molecule into the polymer. The sensors were annealed in air at 70C and used to sense NH_3, HCl and NO_2 gas. The response time for NH_3 was faster than HCl, and the sensors showed a large initial response to NO_2 at room temperature which is very desirable, as some NO_2 gas sensors only operate at elevated temperatures. Electrospinning is a simple and inexpensive method of preparing PEDOT-PSSA nanofibers making it an attractive technique to fabricate polymer based low cost, rapid response and reusable gas sensors.

Temperature dependence of the electrical conductivity of Sb-SnO_2 nanofibers

P13

Maritza Reyna, Idalia Ramos, Nicholas J. Pinto
Dept. of Physics and Electronics, UPR-Humacao

Antimony-doped tin oxide (ATO) can be used for a variety of applications including the development of gas sensors, energy storage devices, and transparent electrodes. In previous work, ATO nanofibers were fabricated using the electrospinning method, which consists of producing nanofibers from a polymeric precursor solution using an electromagnetic field generated with a high voltage source. The polymeric solution was composed of tin (IV) chloride mixed with propanol and 2-propanol, and cellulose acetate dissolved in a mixture of acetone, dimethyl acetamide and antimonium (III) chloride. Using this method ATO nanofibers with sizes ranging from 200 nm to 600 nm and a bandgap of 4.4 e.V were produced. The XRD spectra of the nanofibers showed the characteristic peaks of Sb: SnO_2 with rutile structure. In this research, the temperature dependent electrical properties of single ATO nanofibers were studied following a cycle of cooling from 295 to 15 K and then heating from 15 to 295 K. These measurements were done in cold finger (close cycle helium refrigerator) in a vacuum. The conductivity measured at room temperature is 4.3 S/cm. Compared to the literature this conductivity is in the higher end of the accepted range. The conductivity decreases monotonically from 295 to 15K. As the temperature increases an anomalous peak is observed in the range of 250 to 300 K. This anomaly has been attributed to the chemi-absorbed molecules on the surface of the fiber and could be reduced by improving the vacuum conditions.

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P14 Electrospun Polymer/Carbon Nanotubes Nanocomposites for Photoactuation

Sabrina Rosa[1], Jean P. Crespo[2], Idalia Ramos[3], and Eva M. Campo[4]
[1]Petra Mercado H.S., [2]Dept. of Biology, UPR-Humacao, [3]Dept. of Physics and Electronics, UPR-Humacao, [4]L.R.S.M., UPENN

Research studies demonstrate that the photomechanical properties of carbon nanotubes (CNT) are important in the development of optical actuators. The integration of CNTs into polymers combines the good processability of polymers with the functional properties of CNTs. The understanding of photoactuation in these CNT/polymer composites can contribute to the development of nano-optical-mechanical systems for applications that include intracellular motors, artificial muscles, and tactile displays for the general public. CNT/polymer nanocomposites were fabricated in the form of fibers using the electrospinning technique. Electrospinning is a simple and economic method that can produce fibers with micro and nano dimensions in seconds. The precursor solution for electrospinning was prepared by adding Multiple Wall Carbon Nanotubes (MWCNT) to a combination of Poly(methyl methacrylate) (PMMA) and Polydimethylsiloxane (PDMS) in Dimethylformamide (DMF) and Tetrahydrofuran (THF). Before adding them to the precursor, the CNTs were dispersed in a Sodium dodecyl sulfate/water solution. Scanning Electron Microscopy (SEM) analysis of the electrospun mats shows the production of long and continuous fibers with diameters in the range of hundreds of nanometers. Atomic Force Microscopy (AFM) images of the fibers confirm the presence of CNTs in the fibers. Initial experiments show the photomechanical response of the fibers when exposed to visible light. Additional tests are being conducted to understand the mechanisms of the composites response to light stimulation and the effect of using different polymers and CNTs concentration.

Synthesis of ZnO nanostructures for hydrogen sensing applications

P15

Sara Armaiz[1], Gabriela Berríos[1], Natalia Vázquez[2], Diego Rodríguez[3], Carlos Ortiz[4], Víctor M. Pantojas and Wilfredo Otaño[4,5].
[1]Dept. of Chemistry, UPR-Cayey, [2]Radians High School, [3]Dept. of Physics, UPR-Río Piedras, [4]Dept. of Physics-Mathematics, UPR-Cayey and [5]I.F.N., UPR.

Zinc Oxide is a multi-functional material with potential applications in different areas including sensors, electronics and energy cells. It is a semiconductor, piezoelectric, transparent in the visible and with high excitonic energy promising interesting electro-mechanical and electro-optical applications. A great effort has been applied to the formation of nanoscale materials to take advantage of effects taking place in the surface of this material. In this work, the results obtained in the fabrication of different ZnO structures, such as nanowires and nanoshells, will be presented. The different morphological structures are being prepared using a combination of electrospinning and/or sputtering techniques followed by a heat treatment in air. The samples were characterized using scanning electron microscopy, x-ray diffraction and energy dispersive spectrometry. Hydrogen sensing was tested using a home-made two contact resistance system. A mask was used to create gold contacts on top of the samples. 300 sccm of Ar with 1% hydrogen was used to test the sensor prototypes. The current versus time curves obtained and their relation with morphological features will be discussed.

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Hydrogen Gas Sensors Based on *PEO* Electrospun Nanofibers and *Pd* Sputtering Techniques.

Diego Rodríguez[1], Carlos Ortiz[2],
Víctor M. Pantojas[2] and Wilfredo Otaño[2,3]
[1]Dept. of Physics, UPR-Río Piedras, [2]Dept. of Physics-Mathematics,
UPR-Cayey, [3]I.F.N., UPR

Palladium nanomaterials are potential candidates for robust high surface-to-volume ratio structures to be used for the development of ultra-sensitive hydrogen sensors. A new family of highly sensitive Pd nanostructures has been developed in the NAMAS Laboratory at UPR Cayey. The samples were prepared by the electrospinning technique. A polyethylene oxide (PEO) mat of fibers was electrospun on top of an oxidized silicon substrate followed by sputtering deposition of Pd. Other mats of fibers were prepared using a mask such that they were deposited on the middle of the wafer with the Pd on top of the fibers. The samples were characterized by SEM, AFM, XRD and TEM. The chemical gas response was studied using the conductivity changes generated in the palladium-PEO samples in the presence of hydrogen. A home-made chamber where two needles are in contact with gold pads deposited on top of the samples is used for the electrical measurements. It was found that the density of mat (aligned or densely random mat) is a determining factor in the behavior of the electrical conductivity of the sample. Percentage changes were obtained in resistance of over 50%. In some particular cases (samples prepared with three layers of *PEO-Pd*) the heat treatment improved the response of the sample in the presence of gas. The SEM analysis revealed new details of the nanoshells morphology. In addition, the samples synthesized showed special features in the limiting case of percolation theory when the thickness was close to 10nm.

Preparation and Characterization of Iron and Iron oxide Polymer Embedded Nanoparticles with Potential for Sensing and Environmental Application

P17

Nelson Granda[1] and Wilfredo Otaño[2,3]
[1]Dept. of Chemistry, UPR-Mayaguez, [2]Dept. of Physics-Mathematics, UPR-Cayey, Cayey, Puerto Rico, [3]I.F.N., UPR

Electrospinning technique has been recognized as an unequaled process for preparation of continuous polymer-based fibers at nanometer scale with promising application in diverse areas. In this work, we report preliminary results about preparation and incorporation of iron and iron oxide nanoparticles (NP) into electrospun polymer nanofibers. Iron NP were prepared by reduction of aqueous Fe(III) with sodium borohydride and then incorporated into polylactic acid (PLA) and poly(ethylene oxide) (PEO). However, the electrospinning process was more favorable for the Iron NP/PEO system. Interestingly, it was found that the iron oxide NP were generated by the spontaneous oxidation process of electrospun fibers prepared using a solution comprising $FeCl_3$ and poly(vinyl alcohol) (PVA) or PEO. Raman analysis of the material was consistent with the α-FeOOH iron oxide. In addition, Scanning electron microscopy (SEM), Energy-dispersive spectroscopy (EDS), and X-ray diffraction (XRD) were used to characterize the materials. Studies of the applicability of the fibers as sensors as well as for reduction of nitroaromatic pollutant compounds are in progress.

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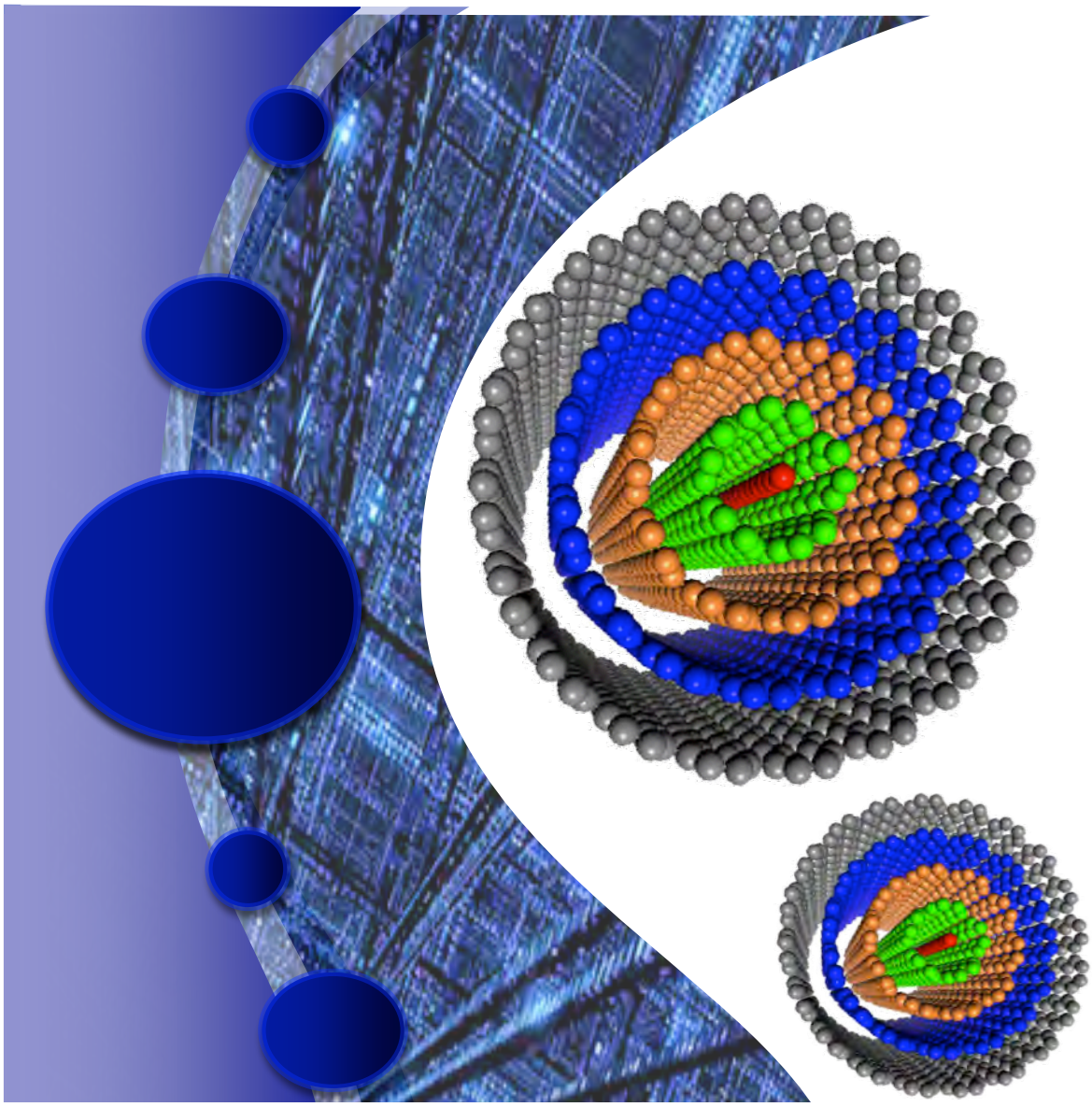

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