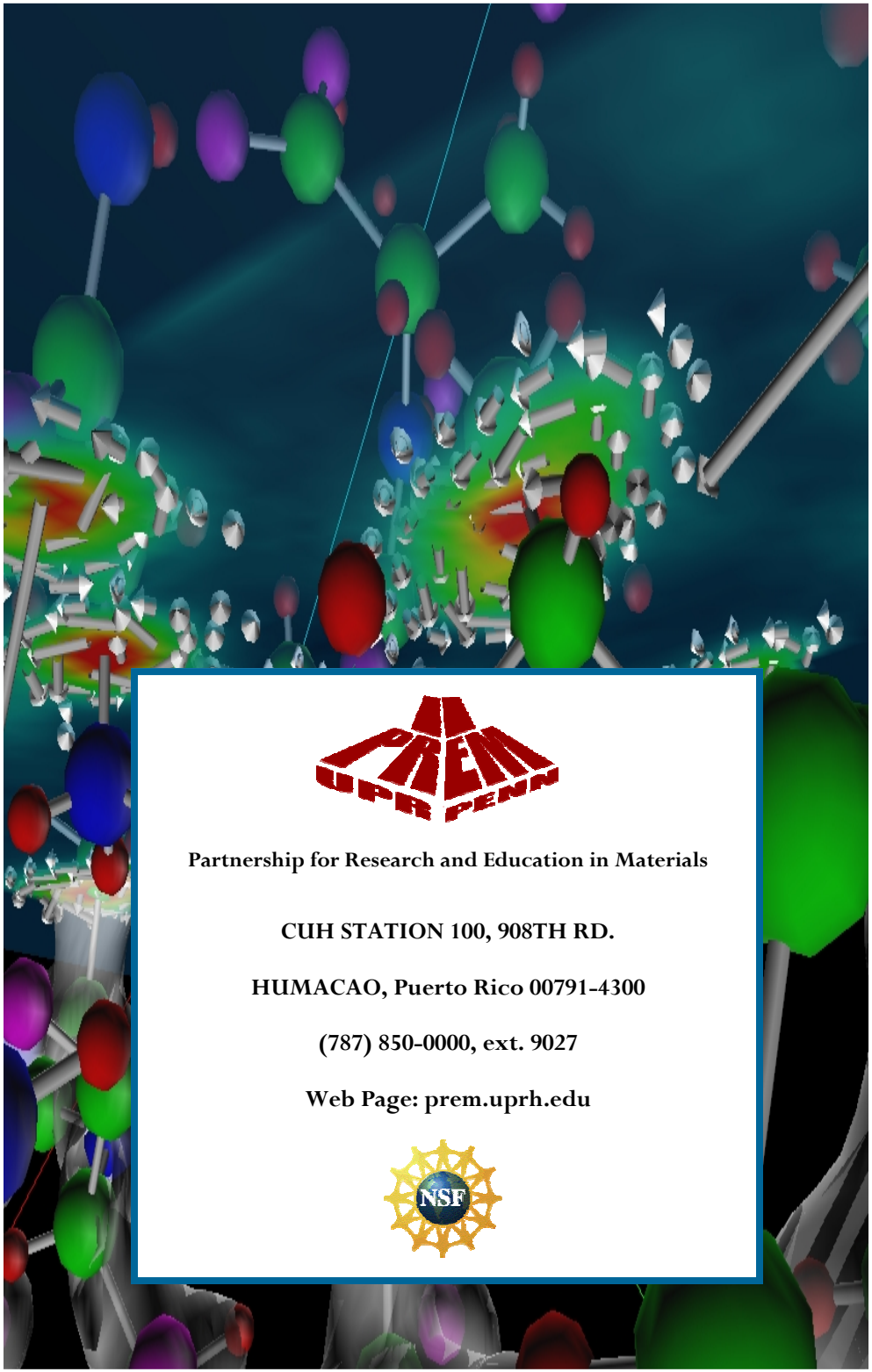

Partnership for Research and Education in Materials

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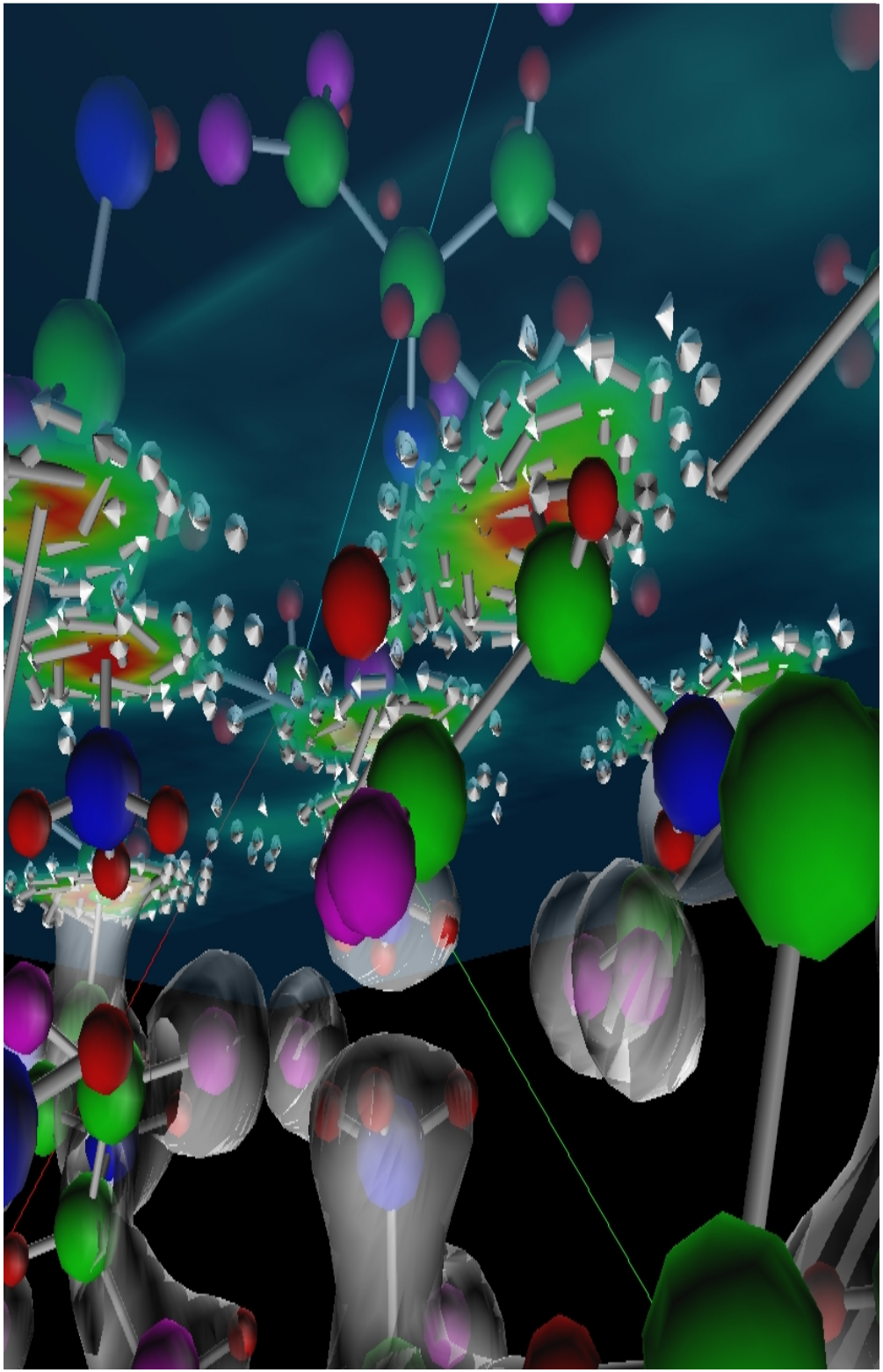
PREM

"Partnership for Research and Education in Materials"

4th Annual Meeting

UPR – Humacao

November 15-16, 2007



P13: ***Analytical solution of the ornstein-zernike equation for charged systems***

Melvin S. Arias and Lesser Blum
Department of Physics, University of Puerto Rico at Río Piedras

P14: ***Investigation on charged systems***

Domingo V. Pérez, Lesser Blum
Department of Physics, University of Puerto Rico at Río Piedras

P15: ***A graphical user interface to molecular dynamics simulation software for the study of CNT-Polymer hybrids***

Myrna Merced, Desirée Velázquez, Raúl Colón, José O. Sotero
Department of Mathematics, University of Puerto Rico at Humacao

P16: ***On the construction of state transfer matrices of closiple paths for modeling linear polymers***

Yesenia Cruz and José O. Sotero-Esteva
Department of Mathematics, University of Puerto Rico at Humacao

P9: Amplification of the whole genome of *Escherichia coli, Shigella flexneri and Salmonella enterica* by rep- PCR and multiple displacement amplification

Dianicha Santana[a], Esther Vega[b]
[a]Petra Mercado High Shool, Humacao
[b]Department of Biology, University of Puerto Rico at Humacao

P10: *Ferrocene chalcone derivatives as labels for DNA electrochemical sensors*

Rocío del A. Cardona, Aileen Díaz, Yesenia Enríquez, Ana R. Guadalupe and Ingrid Montes
Department of Chemistry, University of Puerto Rico at Río Piedras

P11: *Development of Polyvinylferrocene-ssDNA copolymer for electrochemical detection and isolation of an specific DNA sequence*

Ezequiel Paglia and Ana Guadalupe
Department of Chemistry, University of Puerto Rico at Río Piedras

P12: *Assesment of different amplification techniques as a source of DNA: assesment of diferent size amplification products as a probe*

Abigail Ruiz, Rosalmari de Jesus, Omayra Rivera, Giselle Gonzalez and Esther Vega
Department of Biology, University of Puerto Rico at Humacao

PROGRAM

Thursday November 15, 2007

10:00 AM - 4:00 PM Individual Interactions between Collaborators

10:30 AM - 11:30 AM Seminar: ***Quantum filamentary transport*** Raphael Tsu, University of North Carolina at Charlotte, Videoconference Room, UPRH

5:00 - 7:00 PM Welcome and Visit to ***Materia Extraña*** Exhibit, Casa Roig Museum, 66 Antonio López St, Humacao, P.R.

Friday November 16, 2007

Four Points by Sheraton Hotel, Palmas del Mar, Humacao, PR

9:00 - 9:30 AM Registration & Breakfast

9:30 - 9:40 AM Welcome Messages

9:40 -10:30 AM Presentation and Discussion: ***The Future of PREM***, **Idalia Ramos**, UPRH, **Andrew McGhie**, PENN, **Jorge J. Santiago**, PENN

10:30 - 12:00 PM **Faculty Presentations**

10:30 - 10:55 AM

Self assembly of transmembrane proteins into an ion channel within a lipid bilayer (See **Abstract O1)**, **Preston B. Moore**, USIP

P5: Study of electrospun undoped and antimony-doped in tin oxide nanofibers

Neliza León[a], Anamaris Meléndez[a], Idalia Ramos[a], Nicholas Pinto[a] and Jorge J. Santiago Avilés[b]
[a]Department of Physics, University of Puerto Rico at Humacao
[b]Department of Electrical Engineering, University of Pennsylvania

P6: Synthesis and characterization of porous SnO_2 nanofibers

Yu Wang[a], Idalia Ramos[a] and Jorge J. Santiago Avilés[b]
[a]Department of Physics, University of Puerto Rico at Humacao
[b]Department of Electrical Engineering, University of Pennsylvania

P7: Assembly and testing of Poly (3,4 propylenedioxythiophene)-based type I electro-chemical supercapacitors

Mariem Rosario-Canales[a], Michael J.Therien[a], and Jorge Santiago
[a]Department of Chemistry, University of Pennsylvania
[b]Department of Electrical Engineering, University of Pennsylvania

P8: Electrochemical DNA sensor for salmonella detection

Madeline Díaz Serrano[a], Joselyn del Pilar[a], Arelys Rosado[a], Esther Vega[b], Ana R.Guadalupe[a]
[a]Department of Chemistry, University of Puerto Rico at Río Piedras
[b]Department of Biology,University of Puerto Rico at Humacao

P1: ***Using electrospinning for the fabrication of rapid response gas sensors based on conducting polymer nanowires***

Richard Rojas[a], Idalia Ramos[a], Nicholas Pinto[a] and Alan Johnson Jr.[b]
[a]Department of Physics, University of Puerto Rico at Humacao
[b]Department of Physics, University of Pennsylvania

P2: ***Organic-inorganic Schottky diode based on few layer graphene***

Maria Abreu[a], Nicholas Pinto[a] and Alan Johnson Jr.[b]
[a]Department of Physics, University of Puerto Rico at Humacao
[b]Department of Physics, University of Pennsylvania

P3: ***Schottky diodes based on electrospun polyaniline nanofibers of varying diameter***

Rut Rivera[a], Nicholas Pinto[a] and Alan Johnson Jr.[b]
[a]Department of Physics, University of Puerto Rico at Humacao
[b]Department of Physics, University of Pennsylvania

P4: ***Synthesis and characterization of zinc oxide and palladium structures***

Adamari Rivera[b], Jean C. Calderón[b], Diego Rodríguez[c], Melvin Arias[c],Wilfredo Otaño[a], Víctor M. Pantojas[a], Carlos Ortiz-Rodríguez[a], and Jorge J. Santiago[d]

[a]Department of Physics-Mathematics, University of Puerto Rico at Cayey

[b]Department of Chemistry, University of Puerto Rico at Cayey

[c]Department of Physics, University of Puerto Rico at Río Piedras

[d]Department of Electrical and System Engineering, University of Pennsylvania

10:55 - 11:20 AM

Research and outreach projects on combinatorics, graphical user interfaces and principal component analysis applied to the study of linear polymers (See **Abstract O2**), **José O. Sotero Esteva**, UPRH

11:20- 11:45 AM

On the dissipative effects in the electron transport through conducting polymer nanofibers (See **Abstract O3**), **Natalya Zimboskaya**, UPRH

11:45 - 12:10 PM

The critical boundary displacement for radial cavitation: new results and a numerical scheme (See **Abstract O4**), **Pablo Negrón**, UPRH

12:10 - 1:30 PM Lunch

1:30 - 3:00 PM Faculty Presentations

1:30 - 1:55 PM

Nanowire phase change non-volatile memory (See **Abstract O5**), **Ritesh Agarwal**, PENN

1:55 - 2:20 PM

Schottky diodes based on several layers of graphene (See **Abstract O6**), **Nicholas J. Pinto**, UPRH

2:20 - 2:45 PM

Formation of zinc oxide and palladium structures to be used in hydrogen sensor devices (See **Abstract O7**), **Wilfredo Otaño**, UPRC

2:45 - 3:10 PM

Assessment of different amplification techniques as a source of DNA: assessment of different size amplification products as a probe, **Esther Vega**, UPRH

3:10 - 4:30 PM Students Posters Presentations

4:30 - 5:30 PM Advisory Committee Meets to Write Report

5:30 PM **Closing**

Students Posters

O7: Formation of zinc oxide and palladium structures to be used in hydrogen sensor devices

Wilfredo Otaño[a], Víctor M. Pantojas[a], Carlos Ortiz Rodríguez[a], Adamari Rivera[b], Jean C. Calderón[b], Diego Rodríguez[c], Melvin Arias[c] and Jorge J. Santiago[d]

[a]Department of Physics-Mathematics, University of Puerto Rico at Cayey

[b]Department of Chemistry, University of Puerto Rico at Cayey

[c]Department of Physics, University of Puerto Rico at Río Piedras

[d]Department of Electrical and System Engineering, University of Pennsylvania

Different zinc oxide and palladium structures have been produced using electrospinning and/or dc sputtering. For ZnO, fibers and ribbons are prepared using electrospining while nanowires are prepared using dc sputtering. Pd structures such as nanoribbons, nanoshells, filaments, open tubes and wires are prepared by combining electrospining and dc sputtering. It will be presented how changing deposition conditions during the different stages of synthesis allows controlling crystallinity and important structure properties such as morphology, oxidation state and electrical properties. The control of these important characteristic-properties is expected to produce significative changes in the sensing capabilities of these materials. A computer-controlled vacuum chamber is being set-up to study the hydrogen sensing capabilities of ZnO and Pd structures, with partial support of NASA Ideas-ER program. Furthermore, results of preliminary studies of the catalytic properties of the Pd nanoribbons and nanoshells, being studied by cyclic voltammetry in collaboration with Dr. Carlos R. Cabrera (UPR-Río Piedras) and the IFN, will be presented.

Abstracts
Faculty Presentations

O1: *Self assembly of the transmembrane proteins into an ion channel within a lipid bilayer*

Preston B. Moore

Department of Chemistry & Biochemistry, University of the Sciences in Philadelphia

We simulate the self assembly of a transmembrane oligomeric ion channel from monomeric units using a novel coarse grain molecular dynamics model. The novel CG model has been parameterized using the experimental free energy of transfer of small molecules that represent the atomic moieties and thermodynamic properties. From the initial conditions of monomer transmembrane units within a lipid bilayer or bilayer mimetic consisting of a slab of octanol, we simulate the formation of a homo-oligomeric pentameter ion channel. We find that the self-assembly of the ion-channel occurs in a stepwise fashion instead of a concerted fashion. The structure and dynamics of the final oligomeric state is compared and contrasted to all-atom models in both DPPC lipid bilayer and a bilayer mimetic of octanol. We find good agreement between the Coarse Grain (CG) model's final structure and all-atom structures obtained previously as well as known experimental results.

O6: Schottky diodes based on several layers of grapheme

Nicholas J. Pinto

Department of Physics and Electronics, University of Puerto Rico at Humacao

In this work we extend our previous studies on Schottky diodes based on conducting polymer nanofibers to include few layer graphene. Few layers of graphene were removed from HOPG and from graphite rods and used in the construction of these diodes. N-doped Si/SiO_2 wafers were used in the fabrication of these diodes. The diodes were tested in vacuum as a function of temperature, air, nitrogen and in an ammonia environment. The diode rectification is affected in the presence of ammonia gas and could be related to the chemical doping introduced by ammonia that is believed to be n-type.

O5: *Nanowire Phase Change Non-volatile Memory*

Ritesh Agarwal

Department of Materials Science and Engineering, University of Pennsylvania

I will discuss our efforts in studying reversible crystalline to amorphous phase transitions in chalcogenide nanowires (GeTe, $Ge_2Sb_2Te_5$), which are becoming important materials for Phase Change Memory (PCM) devices. Of the different memory device concepts being currently explored, PCM devices based on Ge-Sb-Te alloys are very promising for scalable device size, high-speed operation with nonvolatile random accessing capability. However, the top-down nature of thin-film device fabrication and etching-induced material damage leads to scalability problems at sub-100 nm size. Therefore, there is great interest in developing new materials and processing techniques to overcome this barrier. Self-assembled nanowires devices are particularly promising owing to their sub-lithographic sizes and unique geometry that is free of etch-induced damage. Reversible phase transitions in single-crystalline nanowire devices scaled down to 20 nm sizes are observed with dramatic reduction in switching currents and power consumption. Size-dependent spontaneous recrystallization dynamics demonstrates non-volatile data retention capabilities at 20 nm length scales. Our results show that nanowires are promising candidates for scalable nonvolatile memory applications and studying intrinsic properties of current-induced phase transitions in nanoscale systems.

O2: *Research and outreach projects on combinatorics, graphical user interfaces and principal component analysis applied to the study of linear polymers*

José O. Sotero Esteva

Department of Mathematics, University of Puerto Rico at Humacao

This project is following bifurcations of the work being done at PENN on carbon nanotubes (CNT) properties and applications in three different areas: testing new quantitative metrics or novel implementations of known metrics that can be used to study the conformation of linear polymers on CNT or other fibers, developing graphical user interfaces for the setup and simulation of such hybrid systems, and a combinatorial approach to the study of linear polymer properties. Based on a script developed last year a collection of classes written in Python programming language for the representation of linear polymers has been developed. It has been incorporated into the VMD molecule visualization software along with a graphical user interface that lets the researcher setup polymer-CNT hybrids and run MD simulations with little knowledge about the underlying software and/or data file formats. A researcher with experience with MD simulations may still benefit with the software for it's ease of use for setting up the files needed. Eventually it will incorporate the trajectory analysis graphs that are best suited to the analysis of this type of systems. As a mathematical modeling tool we are exploring techniques used by Pólya seven decades ago, and still being used in recent literature, to study linear polymers.

O3: ***On the dissipative effects in the electron transport through conducting polymer nanofibers***

Natalya Zimbovskaya

Department of Physics and Electronics, University of Puerto Rico at Humacao

Here, we study the effects of stochastic nuclear motions on the electron transport in doped polymer fibers assuming the conducting state of the material. We treat conducting polymers as granular metals and apply the quantum theory of conduction in mesoscopic systems to describe the electron transport between metallic like granules. To analyze the effects of nuclear motions we mimic them by a phonon bath, and we include electron-phonon interactions in consideration. Our results show that the phonon bath plays a crucial part in the intergrain electron transport at moderately low and room temperatures, suppressing the original intermediate state for the resonance electron tunneling, and producing new states which support the electron transport. Also, the temperature dependence of magnitudes of the peaks in the electron transmission corresponding to these new states is analyzed. Natalya A. Zimbovskaya, J. Chem. Phys. **126**, 184901 (2007).

O4: ***The critical boundary displacement for radial cavitation: new results and a numerical scheme***

Pablo Negrón[a], Jeyabal Sivaloganathan[b]

[a]Department of Mathematics, University of Puerto Rico at Humacao

[b]Department of Mathematical Sciences, University of Bath, UK.

We study radial solutions of the equations of isotropic elasticity in two dimensions (for a disc) and three dimensions (for a sphere). We describe a numerical scheme for computing the critical boundary displacement for cavitation based on the solution of a sequence of initial value problems for punctured domains. We give examples for specific materials and compare our numerical computations with some previous analytical results. A key observation in the formulation of the method is that the strong—ellipticity condition implies that the specification of the normal component of the Cauchy stress on an inner pre--existing but small cavity, leads to a relation for the radial strain as a function of the circumferential strain. In addition we get sharper asymptotic estimates on radial cavitated solutions and on the cavity size vs displacement curve, and give a characterization in the phase plane of the nonconstant solutions of the corresponding Euler-Lagrange equations for radial solutions in terms of the curves of constant normal component of Cauchy stress.