

## PROGRAM

9:00 AM	Registration, Coffee and Refreshments
9:45 AM	Welcome Messages Idalia Ramos, University of Puerto Rico at Humacao Arjun Yodh, University of Pennsylvania
10:00 AM	An unexpected turn for twisted graphenes Eugene Mele, University of Pennsylvania
10:45 AM	Super-capacitors research work at PREM Jorge J. Santiago Avilés, University of Pennsylvania
11:30 AM	Opportunities at Penn's Property Measurement Shared Equipment Facility, Jay Kikkawa, University of Pennsylvania
12:15 PM	Lunch
1:30 PM	<i>Bio-Nano Hybrids for Programmable Ligand Detection</i> A.T. Charlie Johnson, University of Pennsylvania
2:15 PM	Trends in the Spatial-temporal Scales of Coarse-grain Molecular Dynamics Simulations, Preston Moore, University of Sciences in Philadelphia
3:00 PM	Thin Film Solar Cells with Printed CZTS Absorbers Irina Malajovich, Dupont & Co., Wilmington, DE
3:45 PM	Posters Setup
4:00 PM	Poster Session and Reception
5:00 PM	Closing









### ABSTRACTS

An unexpected turn for twisted graphenes, Eugene Mele, Department of Physics & Astronomy, University of Pennsylvania

Twisted graphenes are a family of multilayer graphenes in which the crystallographic axes of neighboring layers are rotated by angles  $\theta \neq n\pi/3$ . Experimentally the misalignment is associated with a suppression of the energy scale for coherent interlayer electronic motion relative to its known value for Bernal stacked graphenes and for related multilayer graphenes where  $\theta=n\pi/3$ . The microscopic origin and the consequences of this reduction is attracting significant theoretical interest. In this work we focus on the physics for small rotation angles, a regime where a continuum treatment is thought to be valid. We find that rotational anisotropy in the interlayer coupling Hamiltonian plays an unexpected role by selecting distinct electronic states for the coupled system. This talk will discuss the topological classification of electronic states in multilayer graphenes and their spectral signatures.

*Super-capacitors research work at PREM,* Jorge J. Santiago-Avilés, Department of Electrical & Systems Engineering, University of Pennsylvania

The structure of a modern super-capacitor reflects its function as an electrochemical device. They all possess current collectors, electrodes, electrolyte and a permeable membrane to separate the poles. it is also true that all electrical double layer (EDL) capacitors have a Faradaic component, perhaps as low as 5% of the total capacity. Similarly all the Faradaic capacitor also possess a EDL component of the same magnitude. In this talk we will describe some results in the design and fabrication of a suitable permeable membrane, the design and fabrication of the polymer-carbon composites for electrodes and the systematics of these materials characterization as part of working super-capacitors.

# **Opportunities at Penn's Property Measurement Shared Equipment Facility**, Jay Kikkawa, Department of Physics & Astronomy, University of Pennsylvania

I have been Director of the Property Measurement Shared Equipment Facility at the University of Pennsylvania since its inception in 2001. In this talk I will describe the range of measurement capabilities available to both internal and external users, and give potential users a concrete idea of what it is like to use the facility. In many ways this facility is ideal for exploratory research. I will highlight successful collaborative research projects from the last decade and the wide range of science enabled by data taken in the facility. Topics covered will range from thermal and electrical transport, to magnetism, to linear optics.







### ABSTRACTS

*Bio-Nano Hybrids for Programmable Ligand Detection*, A.T. Charlie Johnson, Department of Physics & Astronomy, University of Pennsylvania, USA

We have explored all-electronic chemical detectors based on bio-nano hybrids, where the biomolecule (DNA or protein) provides chemical recognition and a carbon nanotube (NT) or graphene transistor enables electronic readout. This sensor class represents a promising approach towards sensitive and selective detection of liquid- and vapor-phase analytes. NT or graphene transistors can be functionalized with proteins through an amide bond using a robust process based on carboxylated diazonium salts. Control of protein orientation is achieved through the use of a Ni-nitrilotriacetic acid (Ni-NTA) chemistry with affinity for the histidine tag on an engineered protein. We used this approach to create a nanoelectronic interface to olfactory receptor proteins (ORs) that were embedded in synthetic nanoscale cell membrane analogues. Olfactory receptor proteins (ORs) are the most numerous class of G-protein coupled receptors (GPCRs), a large family of membrane proteins that are important pharmaceutical targets. We have used similar methods based on an engineered antibody to demonstrate detection of a cancer biomarker at levels of 1 pg/mL, far more sensitive than methods used in the clinic today. Non-covalent functionalization of carbon nanotube transistors is achieved through self-assembly of monolayers of single-stranded DNA on the NT sidewall. The DNA is used not for its self-recognition properties but rather for its chemical recognition for small molecule analytes. This system represents a promising pathway to an "electronic bloodhound" capable of detecting arbitrary vapor analytes.

#### Trends in the spatial-temporal scales of Coarse-grain Molecular dynamics simulations, Preston Moore,

Department of Chemistry, University of the Sciences in Philadelphia

We will report on the trends of coarse-grain (CG) molecular dynamics (MD) simulation over the last 25 years. We find that a little over 4000 papers have been published using CG simulations, a number that has been greatly exaggerated in past reviews. However, we find that while the number of CGMD simulations continues to increase in an exponential rate and is become a standard simulation protocol. Further, we find that the spatial-temporal scale being simulated has only marginally increased in the last decade, indication that the spatial and temporal range are stable for CG simulations. Currently, the hardest/most time consuming part of CG simulations is now in obtaining initial conditions in which to run the simulations. Programs such as Wolffia (a PREM project) will be of great use and benefit to many scientist wishing to uses these methods.

Thin Film Solar Cells with Printed CZTS Absorbers, Irina Malajovich, Central Research and Development,

E. I. Dupont & Co., Wilmington, DE

New opportunities in the Photovoltaics market could arise if flexible thin film solar cells were built in a roll-to-roll process similar to newspaper printing. Reasons include reduced cost to manufacture and install, and reduced weight of modules. This presentation focuses on CZTSSe  $(Cu_2ZnSn(S,Se)_4)$ , a promising absorber for solar cells which has earth abundant low toxicity components and can be obtained from precursor printable inks. I will describe how we build CZTSSe thin film solar cells with efficiencies approaching 9% and discuss some of the challenges to improve cell performance.









#### POSTERS

- **P1 Carbon Nanotube Foams of High Surface area and Porosity**, <sup>1</sup><u>Peña Duarte A.</u> and <sup>2</sup>Puerta J.; <sup>1</sup>UPR-Mayaguez, <sup>2</sup>Universidad Simón Bolivar at Venezuela
- P2 The Effect of Carbon Nanotubes Dispersion on the Properties of Polymer Composite Nanofibers: Experimental and Computational Study, <u>Rosa S. M.</u>, Capel V.T., <u>Quiñonez R.I.</u>, Cuadrado W., Martínez F., Ramos I. and Sotero J. O.; UPR-Humacao
- **P3** Simulation of Ion Movement in Activated Carbon based Supercapacitors, <u>De Jesús A</u>. and Negrón P.; UPR-Humacao
- P4 Design, Fabrication and Implementation of a Sample Holder for Thin film Four Point Probe Electrical Characterization, <sup>1</sup><u>Pérez C. R.</u>, <sup>2</sup>Granda N., <sup>3</sup>Ortiz C. R., <sup>3</sup>Pantojas V. and <sup>3</sup>Otaño W.; <sup>1</sup>UPR-Río Piedras, <sup>2</sup>UPR-Mayaguez, <sup>3</sup>UPR-Cayey
- P5 Microgravity Effects on the Electrochemical Oxidation of Ammonia, Cabrera C., Morales C. and Poventud C.; UPR-Río Piedras
- **P6** Arrays of mirrors in the recollection of Solar Energy, <sup>1</sup><u>Velázquez J. O.</u>, <sup>2</sup>Negrón P.V. and <sup>3</sup>Montes E.; <sup>1</sup>Petra Mercado Bougart HS, <sup>2</sup>UPR-Humacao, <sup>3</sup>UPR-Cayey
- P7 Fabrication and study of Organic solar cells composed of P3HT/PCBM blend with Monolayers of P (VDF-TrFE), <u>Carrasco H. M.</u>, Marcano J. M., Pláceres J. C., and Vedrine J.; UPR-Humacao
- **P8** Development of a Fish Oil Oxidative Stability Test by Correlating Bromatological with Differential Scanning Calorimetry Measurements, <u>Rodríguez S.</u>, Escobar A. and Ortiz E.; University of Atlantico-Colombia
- **P9** Characterization of Electrospun AlN, GaN and AlGaN Nanofibers, <sup>1</sup><u>Robles Joshua L.</u>, <sup>1</sup>Sánchez F., <sup>1</sup>Barbosa X., <sup>1</sup>Meléndez A., <sup>2</sup>Santiago J. J. and <sup>1</sup>Ramos I; <sup>1</sup>UPR-Humacao, <sup>2</sup>UPENN
- **P10 CVD Graphene as a Glucose Sensor**, <sup>1</sup><u>Bonilla M.</u>, <sup>1</sup>Pinto N., <sup>2</sup>Lerner M., <sup>2</sup> Hee G. and <sup>2</sup>Johnson C.; <sup>1</sup>UPR-Humacao, <sup>2</sup>UPENN
- **P11 Pd alloys nanostructures for new and ultrasensitive hydrogen gas sensors**, <sup>1</sup><u>Vélez B.</u>, <sup>2</sup>Rodríguez D. and <sup>1</sup>Otaño W.; <sup>1</sup>UPR-Cayey, <sup>2</sup>UPR-Río Piedras
- P12 Electrospun fibers of [P(ND12OD-T2)]n on p-doped Si: Fabrication of a sub-micron p-n junction diode, <u>Rosado A</u>., and Pinto N.; UPR-Humacao
- P13 Biosensor for the detection of the ADP-Ribosylation of eEF2 by Pseudomonas Aeruginosa, <u>Enriquez Y.</u>, Navarreto M., Negrón, and Guadalupe A. R.; UPR-Río Piedras
- **P14** Electrospun fibers of PLA/P3HT blends for Devices and Sensor Applications, <u>Serrano W</u>. and Pinto N.; UPR-Humacao
- **P15** Amyloid β 1-40: fibril incubation, characterization and electrochemical studies, <u>García M.</u> <u>del M.</u>, and Guadalupe A. R.; UPR-Río Piedras
- **P16** ZnO and Mn doped ZnO thin films grown by DC pulsed and RF Co-sputtering, Camacho Berríos A<sup>1</sup>., and Otaño W.<sup>2</sup>, <sup>1</sup>UPR Rio Piedras, <sup>2</sup>UPR Cayey
- P17 Characterization of P<sub>3</sub>HT with Lithium Aluminum Hydride and Dimethyl Sulfate, <u>Marcano Bermúdez J. M.</u>, Fasoli E., and Vedrine J., UPR Humacao





