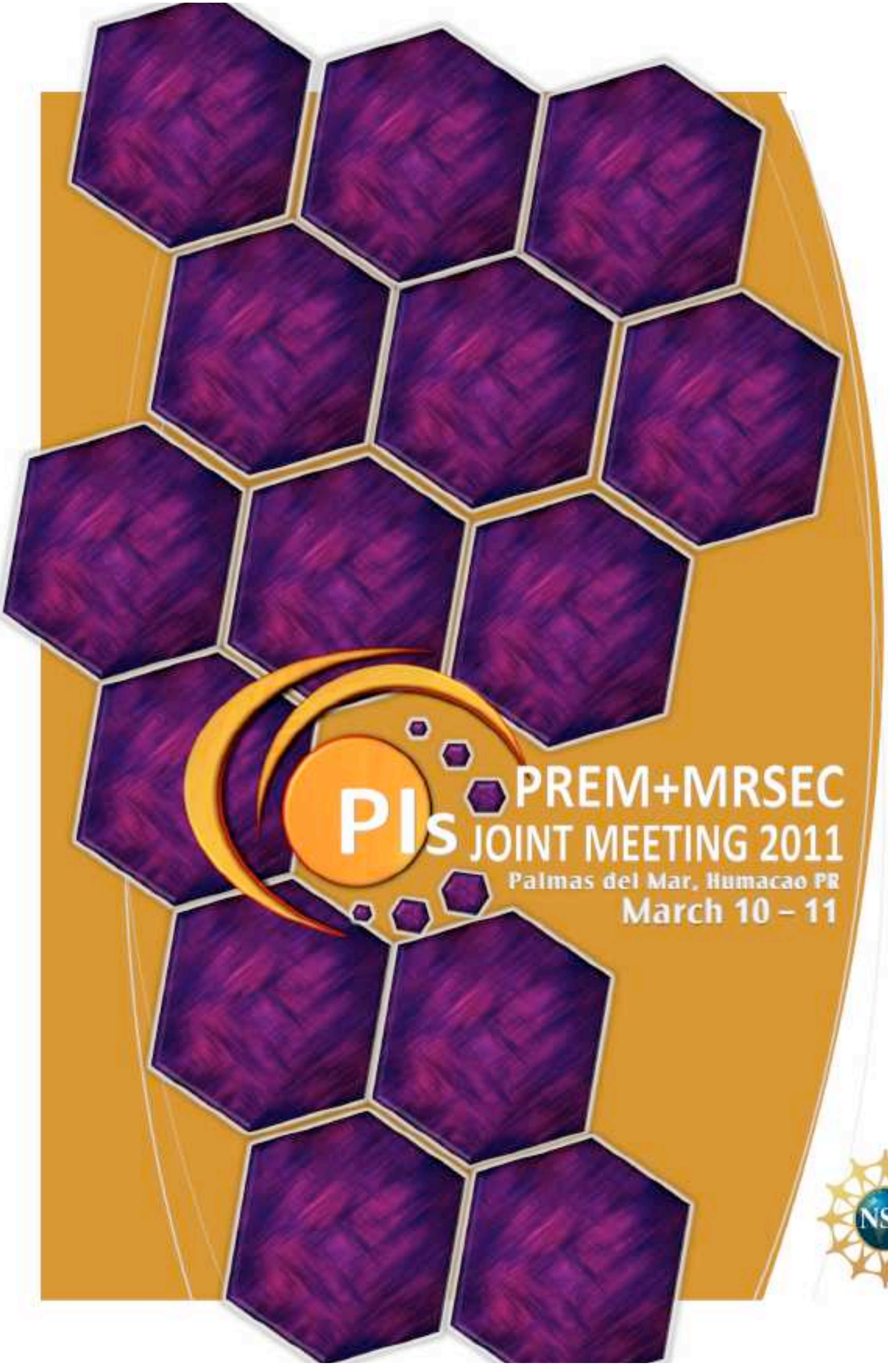


PIs PREM+MRSEC JOINT MEETING 2011

Palmas del Mar, Humacao PR
March 10 – 11

NSF

Hotel Four Points by Sheraton at Palmas del Mar
170 Candelero Drive
Humacao, Puerto Rico, 00791
Phone: 787-850-6000

Partnerships for Research and Education in Materials (PREM)
Materials Research Science and Engineering Centers (MRSEC)
Division of Materials Research
National Science Foundation

1st PREM and MRSEC PIs Joint Meeting

March 9-11, 2011

Palmas del Mar, Humacao, Puerto Rico

Table of Contents

Short Program

WEDNESDAY MARCH 9th, 2011

Swimming Pool Area	
6:00 PM	Registration Opens
7:30 PM	Welcome and Reception

THURSDAY MARCH 10th, 2011

<table>
<tr><th colspan="4">Laurel and Roble Rooms</th></tr>
<tr><td>7:30 AM</td><td colspan="3">Registration and Breakfast</td></tr>
<tr><th colspan="4">1st Session: MRSEC and PREM Joint Session</th></tr>
<tr><td>8:15 AM</td><td colspan="3">Introduction by all participants</td></tr>
<tr><td>8:30 AM</td><td colspan="3">DMR Program Director Update, Sean Jones and Tom Rieker</td></tr>
<tr><td>8:50 AM</td><td colspan="3">Ian Robertson, DMR Division Director</td></tr>
<tr><td>9:30 AM</td><td colspan="3">Creating Useful Highlights</td></tr>
<tr><td>10:15 AM</td><td colspan="3">Webmaster Updates, Irina Zaks</td></tr>
<tr><td>10:30 AM</td><td colspan="3">Break</td></tr>
<tr><th colspan="4">2nd Session: MRSEC and PREM Parallel Sessions</th></tr>
<tr><td colspan="2">PREM: Flamboyán Room</td><td colspan="2">MRSEC: Almendro Room</td></tr>
<tr><td>10:45 AM</td><td>Meeting Agenda, Paresh Ray</td><td rowspan="2">10:45 AM</td><td rowspan="2">MRSEC Directors
Close Meeting</td></tr>
<tr><td>10:50 AM</td><td>Panel: Evaluation and Assessment</td></tr>
<tr><td>11:45 AM</td><td>Break</td><td>11:45 AM</td><td>Elections</td></tr>
<tr><td rowspan="2">12:00 PM</td><td colspan="3">NSF and PREM students: Restaurant
Others: Roble Room</td></tr>
<tr><td colspan="3">Lunch</td></tr>
</table>

<table>
<tr><th colspan="4">3rd Session: MRSEC and PREM Joint Session</th></tr>
<tr><td colspan="4">Mini-Research Symposium</td></tr>
<tr><td></td><td>A: Flamboyán</td><td>B: Almendro</td><td>C: Laurel</td></tr>
<tr><td>1:00 PM</td><td>Umass</td><td>Northwestern</td><td>Princeton</td></tr>
<tr><td>1:15 PM</td><td>UTPA</td><td>Clark Atlanta</td><td>New Mexico Highlands</td></tr>
<tr><td>1:30 PM</td><td>Brandeis</td><td>Georgia Tech</td><td>Ohio State</td></tr>
<tr><td>1:45 PM</td><td>Minnesota</td><td>Maryland</td><td>Johns Hopkins</td></tr>
<tr><td>2:00 PM</td><td>Tuskegee</td><td>UTSA</td><td>Cal State Northridge</td></tr>
<tr><td>2:15 PM</td><td>Harvard</td><td>Yale</td><td>CMU</td></tr>
<tr><td>2:30 PM</td><td>Penn</td><td>NYU</td><td>Cornell</td></tr>
<tr><td>2:45 PM</td><td colspan="3">Break</td></tr>
</table>

3:15 PM	Chicago	CSM	Oklahoma/Arkansas
3:30 PM	Humacao	Norfolk State	Jackson State
3:45 PM	Washington	CalTech	Nebraska
4:00 PM	New Mexico	Mayaguez	UCSB
4:15 PM	Colorado	MIT	Brown
4:30 PM	CCNY	Howard	Xavier
4:45 PM		Wisconsin	Penn State
5:00 PM	Break		
Laurel and Roble Rooms			
5:30 PM	Student Poster Presentations		
Flamboyán and Almendro Rooms			
7:00 PM	Dinner Banquet		

FRIDAY MARCH 11th, 2011

1st Session: MRSEC and PREM Joint Session			
Laurel and Roble Rooms			
7:30 AM	Breakfast		
8:00 AM	Panel: Mentoring Advancement of Junior Faculty		
2nd Session: MRSEC and PREM Parallel Sessions			
PREM: **Laurel**		MRSEC: **Roble**	
9:00 AM	Preparing Compelling Individual Investigator Proposals	9:00-9:45 AM	MRSEC Working Groups Meet
9:15 AM	Tour of PREM Facilities at UPR-Humacao	9:45-10:15 AM	Working Groups Reports Out
		10:15-10:45 AM	Education Assessment
11:00 AM	Wrap-Up	10:45 AM	Adjourn
Flamboyán and Almendro Rooms			
11:30 AM	Lunch		
12:30 PM	Meeting Adjourned		

Detailed Program

WEDNESDAY MARCH 9th, 2011

Swimming Pool Area	
6:00 PM	Registration Opens
7:30 PM	Welcome and Reception: Musical Performance by ***Los Magos de Oriente***

THURSDAY MARCH 10th, 2011

Laurel and Roble Rooms	
7:30 AM	Registration and Breakfast

Laurel and Roble Rooms	
1st Session: MRSEC and PREM Joint Session	
8:15 AM	Introduction by all participants
8:30 AM	DMR Program Director Update, Sean Jones and Tom Rieker
8:50 AM	Ian Robertson, DMR Division Director
9:30 AM	Creating Useful Highlights
10:15 AM	Webmaster Updates, Irina Zaks
10:30 AM	Break

2nd Session: MRSEC and PREM Parallel Sessions

PREM Session: **Flamboyán Room**	
10:45 AM	Meeting Agenda, Paresh Ray
10:50 AM	Panel: Evaluation and Assessment (Moderator: Idalia Ramos) *How to Be a Good Evaluation Consumer*, Cynthia Shuman, Kansas State University *MRSEC Education Evaluation Activities*, Christine Jones, University of Colorado *Best Practices in Evaluating the Humacao PREM*, Mirza Rivera, UPR Medical Sciences
11:45 AM	Break

MRSEC Session: **Almendro Room**	
10:45 AM	MRSEC Directors Closed Meeting
11:45 AM	Elections

Restaurant (NSF and Students) and **Roble Room** (Others)	
12:00 PM	Lunch

3^{rd} Session: MRSEC and PREM Joint Session

Session A: Mini-Research Symposium, Flamboyán Room

Session co-chairs:
1:00 PM Nicholas Pinto, Mehmet Saikaya; 3:15 PM Mahesh Hosur, Todd Emrick

Hours	Institution	Speaker	Title
1:00 PM	UMass	Todd Emrick	Directing Assembly of Materials into Nanoscopic Assemblies and Patterns
1:15 PM	UTPA	Karen Lozano	Science and Engineering of Polymeric and Nanoparticle-based Materials for Electronic and Structural Applications
1:30 PM	Brandeis	Bob Meyer	Chiral Self-Assembly
1:45 PM	Minnesota	Tim Lodge	Ion Gels as Gate Dielectrics in Plastic Electronics
2:00 PM	Tuskegee	Mahesh Hosur	Synthesis and Characterization of Polymeric Nanocomposites
2:15 PM	Harvard	TBA	TBA
2:30 PM	Penn	Arjun Yodh	Some "Low Energy" Particle Physics
2:45 PM	Break		
3:15 PM	Chicago	Sid Nagel	Making a Splash with PREM
3:30 PM	Humacao	Nicholas Pinto	Electrospinning Conducting Polymer and Metal Oxide Nanofibers for Devices and Sensors
3:45 PM	Washington	Mehmet Sarikaya	Molecular Biomimetics - Genetically Designed Self-Assembled Functional Materials
4:00 PM	New Mexico	Heather E. Canavan	Leadership through Collaborative Research on Biomaterials in the UNM-Harvard PREM
4:15 PM	Colorado	Noel Clark	Liquid Crystals and the Origin of Life
4:30 PM	CCNY	Jeff Morris	A few examples of dynamics of particulate and heterogeneous materials

Session B: Mini-Research Symposium, Almendro Room

Session co-chairs:
1:00 PM Nelson Cardona-Martinez, Craig Taylor; 3:15 PM Xiao-Qian Wang, Janice Reutt-Robey

Hours	Institution	Speaker	Title
1:00 PM	Northwestern	Mark Hersam	Self-Assembled Dielectrics on Graphene
1:15 PM	Clark Atlanta	Xiao-Qian Wang	Structural, Electronic, and Optical Properties of Functionalized Graphene
1:30 PM	Georgia Tech	Dennis Hess	Epitaxial Graphene for Electronic Devices
1:45 PM	Maryland	Janice Reutt-Robey	Molecular Electrostatics and Structure Evolution at Organic Semiconductor Interfaces
2:00 PM	UTSA	Dhiraj Sardar	Characterization of Rare Earth Nanomaterials and their Biological and Photonic Applications
2:15 PM	Yale	John Tully	3D Imaging and Chemical Specificity by Atomic Resolution Force Microscopy

2:30 PM	NYU	Mike Ward	Pathological Crystallization and Disease
2:45 PM	Break		
3:15 PM	CSM	Craig Taylor	Novel Materials for Use in Renewable Energy Applications
3:30 PM	Norfolk State	M. A. Noginov	Plasmonic Metamaterials: Low Loss and Gain
3:45 PM	CalTech	Sossina Haile	Electrocatalysis at the Nanoscale
4:00 PM	Mayaguez	Nelson Cardona-Martínez	Bifunctional Materials for the Catalytic Hydrogenation of Cellulose
4:15 PM	MIT	Yang Shao-Horn	Oxygen Electrocatalysis for Clean Energy Conversion and Storage
4:30 PM	Howard	T. E. Huber	Mobility and Thermopower of Surface and Bulklike Charges in Bi and Sb Nanowires
4:45 PM	Wisconsin	Juan de Pablo	TBA

Session C: Mini-Research Symposium, Laurel Room

Session co-chairs:
1:00 PM Lamartine Meda, Vin Crespi; 3:15 PM Tatiana Timofeeva, Nitin Padture

Hours	Institution	Speaker	Title
1:00 PM	Princeton	N. Phuan Ong	Topological Insulators -- a New Playground for Experimentalists
1:15 PM	New Mexico Highlands	Tatiana Timofeeva	Progress of Photonic Materials Studies
1:30 PM	Ohio State	Nitin Padture	Carbon-Based Materials for Spintronics
1:45 PM	Johns Hopkins	Oleg Tchernyshyov	Dynamics of Bloch Domain Walls in Thin Magnetic Films
2:00 PM	Cal State Northridge	Gang Lu	Quantum Simulation of Materials at Micron Scale and Beyond
2:15 PM	CMU	Greg Rohrer	Measuring and Interpreting the Structure of Grain Boundary Networks
2:30 PM	Cornell	Melissa Hines	Mastering Nanostructured Materials: Atomic Membranes and Complex Electronic Materials
2:45 PM	Break		
3:15 PM	Oklahoma/ Arkansas	Matthew Johnson	C-SPIN Activities in Quantum Structures & Narrow Band-gap Semiconductors
3:30 PM	Jackson State	Paresh Chandra Ray	Size and Shape Dependent Nonlinear Optical Properties of Nanomaterials and Its Application in Biological and Chemical Sensing
3:45 PM	Nebraska	Evgeny Tsymbal	Novel Functionalities of Ferroic Heterostructures
4:00 PM	UCSB	Ram Seshadri	Oxides as Semiconductors: Understanding ZnO and Beyond
4:15 PM	Brown	Pradeep Guduru	Why Mechanics Phenomena are Essential to Design of Battery Materials
4:30 PM	Xavier	Lamartine Meda	Nanostructured Transition-Metal Oxides as Electrodes for Lithium-Ion Batteries

4:45 PM	Penn State	Vin Crespi	Collective Behavior of Autonomous Micromotors

Laurel and Roble Rooms	
5:30 PM	Students Poster Presentation

Flamboyán and Almendro Rooms	
7:00 PM	Dinner and "Bomba Workshop" by Marién Torres López and ***Group Tambuyé***

FRIDAY MARCH 11th, 2011

1st Session: MRSEC and PREM Joint Session	
Laurel and Roble Rooms	
7:30 AM	Breakfast
8:00 AM	Panel: Mentoring Advancement of Junior Faculty (Moderator: Karen Lozano) Melissa A. Hines, Cornell University Mónica Olvera de la Cruz, Northwestern University Juan de Pablo, University of Wisconsin Cheryl Stevens, Xavier University of Louisiana Hongtao Yu, Jackson State University

2nd Session: MRSEC and PREM Parallel Sessions

PREM Sesssion: **Roble Room**	
9:00 AM	Preparing Compelling Individual Investigator Proposals
9:15 AM	Tour of PREM Facilities at UPR-Humacao
11:00 AM	Wrap-Up
MRSEC Session: **Laurel Room**	
9:00-9:45 AM	MRSEC Working Groups Meet
9:45-10:15 AM	Working Groups Reports Out
10:15-10:45 AM	Education Assessment
10:45 AM	Adjourn

Flamboyán and Almendro Rooms	
11:30 AM	Lunch
1:00 PM	Meeting Adjourned

List of Student Posters

Poster Number	Title	Page
P1	**Synthesis of Poly (Urea-Formaldehyde) Microcapsules for Self-Healing Polymers** Maritza Flores, Nancy Puente, Magdalena Chipara and Mircea Chipara	15
P2	**Toward the Preparation of Co-crystals of Sulfapyridine** Jamal Pratt, Janna Hutchinson and Cheryl L. Stevens	15
P3	**Development of the Nanomaterial Based SERS Optical Ruler and Its Application in Biology**, Teresa Demeritte, Dulal Senapati, Anant Kumar Singh and Paresh Ray	16
P4	**Experimental and Theoretical Study of Neutral and Charged Piperidone Derivatives,** Alexandr Fonari, Evgeniya Leonova, Michail Makarov, Michail, Irina Odinets, Marina Fonari and Mikhail Antipin	16
P5	**Biobased Surfactants for Molecular Gels and Lubricants** Nneoma Ezeude and George John	17
P6	**Host-defense Peptide-mimetic Foldamers**, Carlos J. Martes, Janice M. Almodóvar, Francisco J. Chaparro, Juan C. Nieves, Manuel Rosario, Samuel H. Gellman, Juan López, Patricia Ortiz, Sean P. Palecek and Madeline Torres	17
P7	**Uncovering the Extracellular Matrix with Thermoresponsive Microgels** Jamie Reed, Rhutesh Shah, Thomas Angelini, Dave Weitz and Heather Canavan	18
P8	**Microwave Testing of Ferromagnetic Composites**, Quincy Williams	18
P9	**DNA Damage in Human Skin Keratinocytes by Surface Functionalized Multi-walled** Carbon Nanotubes, Danielle McShan and Hongtao Yu	19
P10	**Poly(Styrene-b-Ethylene-alt-Propylene) Diblock Copolymer Phase Diagrams** Haidy E. Soto, Soo Hyung Choi and Tim Lodge	19
P11	**Structural and Electronic Properties of Fluorographene** Chantel Nicolas, Duminda K. Samarakoon, Zhifan Chen and Xiao-Qian Wang	20
P12	**Fabrication of Zinc Oxide Semi-Conducting Thin Films using AP-MOCVD for Transistor Applications** Jordan Holmes, Howard E. Katz, Jason Matthews, Bo Zhang, and Keneshia Johnson	20
P13	**Growth of Ruthenium Oxide Nanoplates**, Lamartine Meda and Geoffrey D. Stevens	21
P14	**Computational Methods for Calculating Transport Properties of DNA Base Pairs Coupled to Graphene Nano-Ribbons** Jacob Gayles, Luis Agapito, Christian Wolowiec and Nicholas Kioussis	21
P15	**From Carbon Nanotubes to Carbon Atomic Chains** Gilberto Casillas-García and Miguel José Yacamán	22
P16	**Electronic Properties of Cycloaddition-Functionalized Graphene** Kelvin Suggs, Darkeyah Reuven and Xiao-Qian Wang	22

Synthesis of Poly (Urea-Formaldehyde) Microcapsules for Self-Healing Polymers

P1

Flores, Maritza[1], Puente, Nancy[2], Chipara, Magdalena[3], Chipara, Mircea[4]

[1]Department of Chemistry, [2]Department of Electrical Engineering, [3]Department of Physics and Geology, [4]Department of Mechanical Engineering The University of Texas Pan-American, Edinburg, Texas, 78539.

Contact author: mflores@broncs.utpa.edu

Self-healing polymers are matrices embedded with a healing reagent, catalyst and polymer solution. When a crack is present on the microcapsule's shell it releases the healing agent to repair the damage. Urea-Formaldehyde microcapsules filled with dicyclopentadiene (DCPD) were synthesized using the *in situ* method. Three polymer solutions of polystyrene-block-polyisoprene-block-polystyrene were dissolved in dichlorobenzene to create rouge, microcapsules with Grubbs catalyst and simply microcapsules mixture samples later characterized by Ramam spectroscopy to test the self-healing capabilities of the polymers. Stirring rates ranging from 400 rpm to 600 rpm yielded microcapsules with diameters from 300μm to 60μm. Different stirring rates, synthesis time length, and a 10% increase in the amount of DCPD used were completed to obtain microcapsules with smaller diameters and thinner walls. Smaller microcapsules were preferred when using them in combination with the polymers solutions mentioned above. Dichlorobenzene was used as a solvent in the polymer solutions because it extended the lifetime of the microcapsules. It is expected to obtain better self-healing capabilities results when using microcapsules with smaller diameters and thinner walls. Water-soluble polymers are also being considered for self-healing properties since it was observed that the lifetime of microcapsules was elongated by keeping the capsules hydrated.

The authors gratefully acknowledge funding received from NSF under DMR grant number 0934157.

Toward the Preparation of Co-crystals of Sulfapyridine

P2

Pratt, Jamal, Hutchinson, Janna, and Stevens, Cheryl L.

Xavier University of Louisiana, New Orleans, LA 70125.

Contact author: cklein@xula.edu

Polymorphism (the ability of a substance to exist in more than one distinct crystalline form) is an important consideration for characterizing the properties of drug candidates. In addition, co-crystals provide additional options for new possible solid forms in pharmaceutical applications. Sulfapyridine, a compound that is known to have antibacterial activity, was previously determined to have five different polymorphic forms depending on the crystal growth conditions. However, crystallographic results of solvates or cocrystals have not yet been reported. In an effort to investigate the polymorphism and possibility of preparing cocrystals of sulfapyridine, we have crystallized sulfapyridine dioxane solvate, sulfapyridine tetrahydrofuran solvate, and sulfapyridine piperidinium solvate and determined the x-ray crystal structures at 170 K. The unit cell packing diagrams show solvent channels in the THF and dioxane structures and large solvent pockets in the piperidine structure. These channels and pockets should be large enough to accommodate a co-crystal. In the sulfapyridine dioxane solvate structure and the sulfapyridine THF solvate structure, there are disordered solvent molecules and no stacking of aromatic rings. This is in contrast to the unit cell packing found in the x-ray crystal structures of sulfapyridine and sulfapyridine piperidinium solvate at 170 K which shows stacking of aromatic rings between adjacent molecules. The structures are stabilized by a hydrogen bond network involving both sulfapyridine and solvent molecules except in the case of dioxane which does not participate in the hydrogen bonding.

Support of this research from the NSF-PREM (DMR-0934111), NIH-RISE (2R25GM060926), and NIH-RCMI (1G12RR026260) programs is gratefully acknowledged.

P3

Development of the Nanomaterial Based SERS Optical Ruler and Its Application in Biology

Teresa Demeritte, Dulal Senapati, Anant Kumar Singh, and Paresh Chandra Ray

Department of Chemistry, Jackson State University, Jackson, MS, 39217.

Contact author: paresh.c.ray@jsums.edu

Optical-based distance measurements are essential for tracking bio-molecular conformational changes, drug discovery and it have been used in a wide range of applications in analytical biochemistry. Here we will discuss our development on gold nanomaterial based long range optical ruler for probing bio-molecular dynamics and to detect trace amount of toxic metals and pathogens from environmental samples.

P4

Experimental and theoretical study of neutral and charged piperidone derivatives

Fonari, Alexandr [1], Leonova, Evgeniya [1,2], Makarov, Michail[2], Odinets, Irina[2], Fonari, Marina[1,3] and Antipin, Mikhail[1,3]

[1]New Mexico Highlands University, Las Vegas, NM 87701; [2]A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences,Vavilova str. 28, Moscow, Russia; [3]Institute of Applied Physics Academy of Sciences of Moldova, Academy str., 5 MD2028,Chisinau, Moldova.

Contact author: alexandr.fonari@gmail.com

Symmetric 3,5-bis(arylidene)piperid-4-ones (APs) attract a particular interest due to their remarkable physical properties as well as bioactivity. The unique pharmacological properties of APs have been explained by the presence of the conjugated 1,5-diaryl-3-oxo-1,4-pentadienyl (dienone) pharmacophore moiety, which can selectivity interact with cell thiols, without touching of hydroxyl and amino groups, which are present in DNA and RNA, thereby the genotoxic side effects may be excluded. In addition, symmetric D- π-A -π-D compounds a good candidates for non-linear optical organic materials with two-photon absorption and fluorescence properties as well as for the structural units for photo-crosslinkable, and coordination polymers. The combination of their bioactivity and physical properties suggests that such materials have potential as the agents for the localized treatment of cancers via photodynamic therapy.

Here we report the synthesis, spectroscopic, X-ray investigation, and DFT characterization for (3E,5E)-3,5-bis(benzylidene)-4-oxopiperidiniumtetrafluorborate [C19H18NO][BF4] (**1**), (3E,5E)-3,5-bis[4-(dimethyl ammonio) benzylidene]-4-oxopiperidinium hexafluoro(μ-hydroxo)diborate tetrafluorborate monohydrate [C23H30N3O][B2F3OH]2[BF4] H2O (**2**), and (3E,5E)-3,5 bis[4(diethylammonio) benzylidene]-4-oxopiperidinium tris(tetrafluorborate) monohydrate [CHNO][BF] HO (**3**) obtained via the aldol-crotonic condensation in the presence of boron trifluoride etherate.

As revealed by quantum chemical calculations, donation of an electron pair in the system by terminal dimethyl-amino donor groups increases static hyperpolarizability fivefold, comparing to the protonated donor groups, which lack the lone electron pairs.

Acknowledgements: This work was supported by the NSF-DMR grant 0934212. The authors are grateful for this support.

Biobased Surfactants for Molecular Gels and Lubricants

P5

Ezeude, Nneoma[1], John, George[2]

The City College of New York- CCNY CUNY, Department of Chemistry, Partnership for
Research and Education in Materials, New York, NY, 10031.

Contact author: nezeude00@ccny.cuny.edu

Bioinspired molecular design and materials. Our research focuses on the interdisciplinary frontier of organic materials. We integrate the knowledge and techniques in organic chemistry, materials science, supramolecular chemistry, green chemistry, and nanotechnology to design new biofunctional materials for the exploration in molecular assemblies, development of soft nanomaterials and biomimetics, and other fundamental problems. Molecular self-assembly leading to nanostructured morphologies and materials; for example, lipid nanotubes, helical nanofibers, vesicles, liquid crystals and low molecular weight gelators from synthetic/biobased amphiphiles, which could be of use in drug/gene delivery and health care applications .

Acknowledgements: Supported by NSF PREM Grant# DMR-0934206.

Host-defense peptide-mimetic foldamers

P6

Martes, Carlos J.[1,2], Almodóvar, Janice M.[1], Chaparro, Francisco J.[2,3], Nieves, Juan C.[1], Rosario, Manuel[3],
Gellman, Samuel H.[4], Lopez, Juan[3], Ortiz, Patricia[2], Palecek, Sean P.5, Torres, Madeline[2]

[1]Industrial Biotechnology Program, [2]Department of Chemical Engineering, [3]Department of Chemistry,
University of Puerto Rico-Mayaguez, Mayaguez, PR, 00681, [4]Department of Chemistry, [5]Department of
Chemical Engineering, University of Wisconsin-Madison, Madison, Wisconsin. 53701.

Contact author: carlos.martes@upr.edu

Beta-peptides are short nanorods made from artificial amino acids (beta-amino acids) that are designed to mimic host defense peptides (HDPs). Some of these synthetic peptides have shown similar, if not higher, antimicrobial effectiveness than other commercially available drugs. Antimicrobial beta-peptides also possess some advantages over naturally occurring HDP, such as greater conformational stability, resistance to proteases and activity at physiological salt concentrations. Key structural features that determine their antimicrobial activity have been identified and characterized to certain extent. However, the mechanism of action of these beta-peptides is not completely understood. In addition, the most potent beta-peptides are also highly hemolytic. Thus, a combination of expertise in synthetic organic chemistry, biochemistry, microbial physiology, molecular biology, and computational modeling is necessary to enhance the antimicrobial properties of beta-peptides, elucidate their mechanism of action and develop their biomedical applications. Here, we showcase several approaches and preliminary data, underway, to address underlying questions regarding the development and characterization of host-defense peptide mimetic foldamers and polymers. Among the most prominent projects are: the identification of genes in yeast important in the mechanism of action of beta-peptides using a genetic approach, the characterization of beta-peptide secondary structures via RAMAN spectroscopy, and the assessment of beta-peptide toxicity to epithelial cells.

Acknowledgements: Andrew Greenberg, UW REU Program-Nanotechnology, UWNSEC-MREC, NSF.

P7 Uncovering the Extracellular Matrix with Thermoresponsive Microgels

Reed, Jamie[1], Shah, Rhutesh[2], Angelini, Thomas[2], Weitz, Dave[2], Canavan, Heather[1]

[1]Center for Biomedical Engineering, Chemical & Nuclear Engineering, University of New Mexico, Albuquerque, NM 87131-0001; [2]School of Engineering an Applied Sciences, Harvard University, Boston, MA 02138.

Contact author: canavan@unm.edu

The extracellular matrix, or ECM, remains a hidden biological interface between a cell and a substrate. One method for examining proteins, such as those in the ECM, is flow cytometry (FC), which is a fast, high throughput method of quantification. Since FC is a solution technique, it is necessary to dissociate the cells from the surface. Traditional cell harvesting methods, such as enzymatic digestion and physical scraping, damage the ECM proteins as well as the cell morphology. Recently it has been shown that a thermoresponsive polymer, poly(*N*-isopropyl acrylamide) or pNIPAM, can be used to harvest a sheet of cells without damaging the integrity of the ECM. Above its lower critical solution temperature (LCST), this polymer is relatively hydrophobic, and mammalian cells grown on pNIPAM-grafted surfaces act in a similar fashion as those grown on typical tissue culture polystyrene (TCPS): they proliferate into a confluent sheet. Below the LCST (i.e., room temperature) the polymer physically changes, becoming more hydrophilic and swelling. Furthermore, when the temperature of the cell culture is dropped below the LCST of the polymer, the cells will detach as an intact cell sheet. These intact cell sheets, however, are not ideal for investigation in a flow cytometer, which requires individual cells for quantification. In this work, we developed a novel method for single cell detachment using pNIPAM microgels on the order of 20-200 micrometers. After fabrication, these gels were examined to ensure pNIPAM's characteristic thermoresponse was maintained, followed by cell culture on the gels. From these results, we conclude that these microgels have the capability of giving us access to this buried biological interface.

Acknowledgements: Steven Candelaria, Kirsten Cicotte, Elizabeth Dirk, Vanessa Eriacho, Laura Pawlikowski, Connie Wilkings. This work is supported by NSF-PREM program grant #DMR-0611616, 3M Corporation and the UNM CBME. JR was supported by NSF GRFP.

P8 Microwave testing of Ferromagnetic composites

Williams, Quincy

Norfolk State University, Norfolk, VA 23504.

Contact author: q.l.williams13807@spartans.nsu.edu

For theory purposes and applications, it is important to know the relations that constrain both microwave permeability and bandwidth of electromagnetic absorbers. Conventional mixing rules cannot give accurate estimates of constitutive properties when polymers contain inclusions with high static permeability; therefore these limits need to be determined experimentally. Two polymer composites of Moly-Permalloy and polystyrene were fabricated in house both with approximately 8% concentration of Moly-Permalloy. Sample 1 was formed under 1.5 T magnetic field, producing a composite with magnetic inclusions oriented predominately in the direction of magnetic field, while sample 2 was formed with magnetic inclusions randomly dispersed. Microwave ferromagnetic resonance (FMR) testing demonstrated the real permeability varied from ~ 0.6 to 1.4 in the dependence of the magnetic field. The random sample showed a broad absorption line while in the oriented composite the FMR was narrower, with its position depending on the orientation of the sample with respect to the direction of the magnetic field.

Acknowledgements: Supported by NSF PREM.

DNA Damage in Human Skin Keratinocytes by Surface Functionalized Multi-walled Carbon Nanotubes

P9

McShan, Danielle and Yu, Hongtao

Department of Chemistry and Biochemistry, Jackson State University, Jackson, MS, 39217.

Carboxylate-functionalized multi-walled carbon nanotubes (MWCNTs) are more water soluble and are promising for biological and biomedical applications. However, there have been concerns on their ability to cause cellular and DNA structural damages. In this report, we explore the toxicity and phototoxicity of four MWCNTs in a human skin keratinocyte cell line (HaCaT). The four MWCNTs, non-purified (NP), purified (P), half-functionalized (HF), and fully functionalized (FF), were prepared by High Pressure Carbon Monoxide method. Cells in cultured media were exposed to 20 μg/mL of MWCNTs, with or without simulated sunlight irradiation. The cell viability was determined by the standard MTT assay. DNA damage was determined by standard Comet assay (alkaline) for direct DNA cleavage and by formamidopyrimidine DNA glycosylase (FPG) Comet assay that leads to cleavage of DNA sites with modified purines, thus amplifies the detection for oxidative DNA damage. It turns out that all four MWCNTs are not cytotoxic toward the skin cells, with or without light irradiation. While all the four MWCNTs exhibit very little direct DNA damage tested in the alkaline Comet assay, they cause significant oxidative DNA damage in the FPG Comet assay. The amount of oxidative damage does not depend on light irradiation or the type of MWCNTs, but depends on the incubation time. These suggest that the oxidative DNA damage can be repaired under these conditions within 8 hours of incubation. Although these MWCNTs only cause oxidative DNA damage that can be easily repaired, the safety of their use warrants further investigation.

Poly(Styrene-b-Ethylene-alt-Propylene) Diblock Copolymer Phase Diagrams

P10

Soto, Haidy E.[1], Hyung Choi, Soo[2] and Lodge, Tim[3]

[1]Department of Mechanical Engineering, [2]Department Chemistry, [3]Department Chemistry
University of Texas-Pan American, Edinburg, TX 78539, University of Minnesota, Minneapolis, MN 55455.

Contact author: haidyenid@hotmail.com

Micelles were observed when dissolving the diblock copolymer Poly(styrene-b-ethylene-alt-propylene), SEP, in Squalane. These micelles self-arrange into aBody Centered Cubic (BCC) lattice given proper temperature conditions. This arrangement is an ordered state: material behaves in an elastic manner. When increasing solution temperature, the micelles disassemble into a disordered formation exhibiting viscous behavior. The temperature at which micelles form and move freely within the solvent is the critical micelle temperature (CMT). The temperature at which micelles form and arrange themselves into a BCC formation is the order-disorder transition temperature (ODTT). Dynamic light scattering and rheology testing were used to determine the CMT and ODTT respectively for SEP with molecular weights of (17-73) and (26-66). Using data collected from different polymer-to-solvent concentrations, a phase diagram was created.

The authors gratefully acknowledge funding received from NSF under DMR grant number 0934157.

P11 Structural and Electronic Properties of Fluorographene

Nicolas, Chantel[1], Samarakoon Duminda K. [1], Chen, Zhifan[2] and Wang, Xiao-Qian[2]

Department of Chemistry[1] and Department of Physics[2], Clark Atlanta University, Atlanta, Georgia 30314.

Contact author: xwang@cau.edu

We have investigated the structural and electronic characteristics offluorinated graphene based on first-principles density-functional calculations. A detailed analysis of the energy order for stoichiometric fluorographene membranes indicatesthat there exists prominent chair and stirrup conformations, which correlateswith the experimentally observed in-plane lattice expansion contrary to a contraction in graphane. The optical response of fluorographene is investigated using *GW*-Bethe Salpeter equation approach. Our results are in good conformity with the experimental observed optical gap and reveal predominant charge-transfer excitations arising from strong electron-hole interactions. The appearance of bounded excitons in the ultraviolet region can result in an excitonic Bose-Einstein condensate in fluorographene.

Acknowledgements: National Science Foundation (Grant No. DMR-0934142).

P12 Fabrication of Zinc Oxide Semi-Conducting Thin Films using AP-MOCVD for Transistor Applications

Holmes, Jordan[1], Katz, Howard E.[2], Mathews, Jason[3], Zhang, Bo[2], and Johnson, Keneshia[3]

[1]Prince George's Community College, Largo, MD, [2]Department of Materials Science and Engineering,
Johns Hopkins University, Baltimore MD 21218 ,[3] Department of Chemistry, Howard University,
Washington, DC 20059.

Zinc oxide is a well-known semi-conducting material with useful electronic capabilities. It has high electron mobility, a wide direct band gap and exceptional transparency. Because of these attributes zinc oxide can be used to make high-quality thin-film transistors. Zinc oxide films were grown on p type silicon (conducting layer) /silicon dioxide (Insulating layer) substrates by Atmospheric Pressure Metal Oxide Chemical Vapor Deposition (AP-MOCVD) from a organo-metallic precursor which volatilizes at low temperature. The films were annealed to reduce carbon impurities and the behavior of transistors fabricated from the films was measured. Process optimization is on-going.

Growth of Ruthenium Oxide Nanoplates

P13

Meda, Lamartine and Stevens, D. Geoffrey

Department of Chemistry, Xavier University of Louisiana, Drexel Drive, New Orleans, LA, 70125.

Contact athor: Lmeda@xula.edu

By carefully manipulating and controlling the growth conditions, ruthenium oxide (RuO2) two-dimensional (2-D) nanostructure were self-assembled into a stack of plates on indium tin oxide coated glass substrate. The nanoplates were grown in a horizontal hot-wall metalorganic chemical vapor deposition (MOCVD) from ruthenocene. Each nanoplate has a thickness of approximately 60 nm and the average area is 1000 x 300 nm2. Each stack of nanoplates is approximately 1.2 mm in height. A continuous layer of RuO2 thin film, which may serve as the growth template, is observed on the bottom of the nanoplate stacks. Field-emission scanning electron microscopy reveals that each stack of nanoplates was grown vertically aligned on the substrate and exhibited elongated shape. Structural properties which were examined by X-ray diffraction show that the nanoplates are polycrystalline.

Acknowledgements:

This research was supported by NSF (DMR-0934111) through PREM.

Computational Methods for Calculating Transport Properties of DNA Base Pairs Coupledto Graphene Nano-Ribbons

P14

Gayles, Jacob, Agapito, Luis , Wolowiec, Christian and Kioussis, Nicholas

Department of Physics and Astronomy, CSU Northridge, Northridge, California 91330.

Contact author: jdgayles16@gmail.com

We utilize computational methods based on Density Functional Theory (DFT) and the Non-Equilibrium Green's Function (NEGF) formalism to solve the Schrödinger equation for DNA base pairs coupled to metallic graphene nano-ribbons. Our purpose is to analyze electron transport properties to differentiate between the heterocyclic DNA base pairs. We are conducting this research to develop a protocol for sequencing individual base pairs with a transverse electric field as DNA double-strand translocates between two graphene nano-ribbons. Our results show that not only is each base pair differentiable for applied transverse biases, but also it is possible to distinguish bipolar biases within each base pair. Graphene is a good choice for the electrodes because of the large currents we see. The use of electric fields will increase the present rate at which strands can be sequenced while increasing the accuracy of the measurements.

P15

From Carbon Nanotubes to Carbon Atomic Chains

Casillas-García, Gilberto and Yacamán, José Miguel

Physics and Astronomy Department, University of Texas at San Antonio, One UTSA circle,
San Antonio, TX, 78249.

Contact author: gilbertocasillas@gmail.com

Carbyne is a linear allotrope of carbon. It is formed by a linear arrangement of carbon atoms with sp-hybridization. Due to its unique geometry, it is expected to have many interesting properties as carbon nanotubes and graphene. We present a reliable and reproducible experiment to obtain these carbon atomic chains using few-layer-graphene (FLG) sheets and a High Resolution Transmission Electron Microscope (HRTEM, Jeol JEM-2010F at 200 KV). First the FLG sheets were synthesized from worm-like exfoliated graphite and then drop-casted on a lacey-carbon copper grid. Once in the TEM, two holes are opened near each other in a FLG sheet by focusing the electron beam into a small spot. Due to the radiation, the carbon atoms rearrange themselves between the two holes and form carbon fibers (i.e., a multiwall carbon nanotube (MWCNT)). The beam is concentrated on the carbon fibers in order excite the atoms and induce a tension until MWCNT is formed. As the radiation continues the MWCNT breaks down until there is only a single wall carbon nanotube (SWCNT). Then, when the SWCNT breaks, an atomic carbon chain is formed, lasts for several seconds under the radiation and finally breaks. This demonstrates the stability of this carbon structure. During the experiment carbon chains inside the outmost carbon nanotubes were observed several times which implies that these chains are formed many times during the same experiment. The linear atomic chains are clearly visible under the microscope despite it was operated at 200 KV.

Acknowledgements: This research was supported by the NSF-PREM Grant No. DMR-0934218.

P16

Electronic Properties of Cycloaddition-Functionalized Graphene

Suggs, Kelvin, Reuven, Darkeyah and Wang, Xiao-Qian

Department of Physics and Center for Functional Nanoscale Materials Clark
Atlanta University, Atlanta, Georgia 30314.

Contact author: kelvlorenz@yahoo.com

We have studied the electronic characteristics of covalently functionalized graphene by nitrene chemistry using first-principles density functional calculations. The perfluorophenylazide functionalization leads to a band-gap opening in graphene and transition from a semimetallic to a semiconducting state. The [2 + 1] cycloaddition-induced gap is shown to be attributed to the modification of the π conjugation that depends on the concentration of aziridine adducts. The implications of tailoring the band structure of functionalized graphene for future graphene-based device applications are discussed.

Acknowledgements: This work was supported by the National Science Foundation DMR-0934142.

Mechanical and Thermal Characteriztionof XD-Grade Carbon Nanotube/Epon 862 processed by Dual Phase Dispersion Technique

P17

Okoro, Chinedu[1], Hossain, Mohammad[2], Hosur, Mahesh, Jeelani, Shaik and Rangari, Vijaya

Tuskegee University, Center for Advanced Materials, TCAM, Tuskegee, AL 36088.

Contact author: cokoro2764@tuskegee.edu

Carbon nanotubes have expanded the generation of multifunctional, high-performance engineering composites. For nanocomposite materials, proper dispersion of carbon nanotubes is essential in attaining optimal results. In this research, a dual-phase dispersion method is studied combining a high intensity ultrasonic liquid processorwith a three roll milling technique. Xd-grade carbon nanotubes (xd-CNTs) were infused into Epon 862 epoxy and then mixed with epicure curing agent W using a high-speed mechanical agitator. To reduce the chance of voids the mixture was preheated and placed in a vacuum oven to remove trapped air and reaction volatiles. Mechanical and thermal analysis was performed to assess improvements when combining these two dispersion methods. Flexural and dynamic mechanical analysis (DMA) were performed on neat, 0.015wt%, and 0.15wt% xd-CNT/epoxy plaques to identify the loading effect on the mechanical properties of the composite material. Flexural tests were performed using Zwick Roell 2.5. Flexural results indicate homogeneity with improvements in mechanical properties of up to 15% in strength as well as modulus enhancement of up to 25%, respectively.

Interfacial adhesion and dispersion is improved with viscosity reduction and utilizing the secondary mixing method. Scanning electron microscopy (SEM) were performed using Joel 2001 at 5 and 10kV. Micrographs depict the fracture morphology of the tested specimens indicating proper dispersion of the xd-CNTs by fracture propagation and cleavage plane displacement. Dynamic mechanical analysis (DMA) were performed using TA Instrument Q800. DMA studies revealed an increase in storage modulus in the nanophased specimens as CNT loading increased. Thermal analysis was performed using thermo-gravimetric analysis (TGA), differential scanning calorimetry (DSC) and thermo-mechanical analysis (TMA). TGA results revealed minimal reduction in decomposition temperature despite the increase of xd-CNTs. DSC results indicate enthalpy changes with the increase in xd-CNTs present. However, glass transition temperatures vary slightly. Lastly TMA results indicate a steady reduction in the coefficient of thermal expansion as xd-CNTs increase mainly attributed to enhanced CNT dispersion and distribution causing reduced polymer chain movement.

Acknowledgement: PREM Grant # DMR-0611612, T-CAM staff and students.

P18

Engineering of Hybrid Organic-Inorganic Solar Cells

Goodwin, Earl[2], Dávila-Santana, Melissa[1], Kim, David[2], Reifsnyder, Danielle[2], Vedrine-Pauléus, Josee[1], Murray, Chris B.[2] and Kagan, Cherie R.[2]

[1]Department of Physics and Electronics, University of Puerto Rico at Humacao, Humacao, PR, 00791.
[2]Departments of Electrical and Systems Engineering/Materials Science and Engineering, and Chemistry, University of Pennsylvania, (PREM/LRSM), Philadelphia, PA, 19104.

Contact author: kagan@seas.upenn.edu

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 (phenyl-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.

P19

Synthesis of 3DOm Particles for Applications in Energy Conversion

Flores, Melinda[1], Zambrano, Steve[2] and Han, Aijie[3]

[1]Department of Biology, [2]Department of Mechanical Engineering, [3]Department of Chemistry, University of Texas-Pan American, 1201 W. University Dr., Edinburg, Texas 78539.

Contact author: mflores1@broncs.utpa.edu

Nanoporous materials science is a growing area of research with a wide range of potential applications. The structures of three-dimensionally ordered mesoporous materials (3DOm) with controlled porosity on various length scales grant such variability in application. The basic synthetic methodology of 3DOm employs infiltration, polymerization, vacuum drying, centrifugation, and carbonization. Poly(methyl methacrylate) (PMMA) colloidal crystal templates are used in combination with phenol-formaldehyde or resorcinol-formaldehyde precursor solutions to synthesize 3DOm particles. The programmed carbonization of the sample is carried out to remove the PMMA templates spheres, leaving behind interconnected hollow spheres. Their pore sizes, surface areas, pore volumes, and skeletal geometries are easily tailored by controlling the synthesis conditions. These 3DOm materials have many potential applications such as catalysts, sensors, and energy. This study focuses on the prospective function of 3DOm materials for uses in energy conversion.

The authors gratefully acknowledge funding received from NSF under DMR grant number 0934157.

Multifunctional Nanoporous Materials Sustainable Catalysis

P20

Reyes-Luyanda, Damian[1], Flores-Cruz, Josseant[1], Morales-Pérez, Pedro J.[1], Encarnación-Gómez, Luis G.[1],Cao, Shuo[1], Garcia-Ricard, Omar[1], Santiago-Rodriguez, Yohaselly[1], Hernández-Maldonado, Arturo[1], Curet-Arana, Maria C.[1], Shi, Fengyuan[2], Voyles, Paul M.[2], Pagan-Torres, Yomaira[3], Dumesic, James A.[3], and Cardona-Martínez, Nelson[1].

[1]Department of Chemical Engineering, University of Puerto Rico -Mayagüez, Mayagüez, PR, 00681;
[2]Department of Materials Science and Engineering, University of Wisconsin Madison, WI 53706;
[3]Department of Chemical and Biological Engineering, University of Wisconsin Madison, WI 53706.

Contact author: damian.reyes@upr.edu

We will describe our efforts to rationally combine surface functionality and pore structure to design novel materials for the sustainable conversion of biomass resources into renewable fuels and chemicals and for removal of bulk CO2.Supported Ru catalysts were prepared by evaporative deposition on various ordered mesoporous silicas (SBA-15) with different functionalities and characterized using nitrogen adsorption, X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDAX) and Scanning Transmission Electron Microscopy (STEM). The catalytic performance of these materials was compared to Ru/C or Pd/C and the corresponding supports. For ruthenium supported on arenesulfonic acid-functionalized mesoporous silica (Ru/SBA-15S) the activity and selectivity of the bifunctional catalysts as a function of functionality loading, reaction time and temperature were studied by monitoring the cellulose conversion and production of sugars and sugar alcohols in a high-pressure batch reactor. Sorbitol is the main product obtained by the hydrolysis of cellulose to glucose followed by the corresponding reduction. Secondary products include sugars, ethylene glycol and glycerol. The activity of mesoporous silica catalysts increases with an increase in sample acidity and the addition of Ru allows control of the selectivity towards sugar alcohols. Ru/SBA-15S displays the best catalytic performance. Ru/SBA-15S is not hydrothermally stable, losing a significant fraction of its surface area, crystallinity, and acidity after prolonged exposure to water at 483K. However, even after 72h under these conditions the catalyst retains some of its acidity and the activity is still higher than fresh unfunctionalized Ru/SBA-15 and Ru supported on amorphous silica. Initial efforts to improve the hydrothermal stability of our catalytic materials will also be presented. Silylated Ru/SBA-15 is more hydrothermally stable than SBA-15 and its catalytic performance is comparable to that of a commercial Pd/C catalyst. We are currently developing alkaline earth metal based nanoporous coordination polymers for CO2 capture. Ongoing work includes the assembly of the pillared-layer coordination polymer by hydrothermal synthesis using a bidentate pyridine pillar ligand with amide functionality. Finally we are developing expertise in the use of periodic density functional theory calculations to help design improved catalytic metal sites.

Acknowledgements: This work was supported by the National Science Foundation (DMR-0934115 and in part by HRD-0833112). One of the authors (DRL) was supported in part through funding from a PRLSAMP Bridge to the Doctorate Scholarship (HRD-0601843). The authors wish to express their gratitude to the undergraduate students Ronald Carrasquillo-Flores and Carmen P. Márquez-Miranda for their help in obtaining some of the results presented here.

P21

Direct Observation of Nd3+ in Cubic Nd3+:Sc2O3 Nanocrystals

Dennis, Robert C., Casillas, Gilberto, Yacamán, Miguel and Sardar, Dhiraj K.

The University of Texas at San Antonio Department of Physics and Astronomy, San Antonio, TX 78249.

Contact author: Dhiraj.Sardar@utsa.edu

We report the direct observation of Nd3+ doped uniformly in cubic (Ia-3) Nd3+:Sc2O3 nanocrystals using a second generation abberation corrected scanning transmission electron microscope (STEM) with high angle annular dark field imaging (HAADF). Clustering and dopant nucleation is minimized using an homogeneous thermal decomposition synthesis of precursor Nd3+:Sc(OH)3. These results are briefly related to the spectroscopic characterization of Nd3+ in Nd3+:Sc2O3 nanocrystals (e.g. energy transfer between neighboring pairs of dopants and site selection of dopant atoms). The direct imaging of dopants at sub-atomic resolutions allows for a detailed understanding of doping profiles, spectroscopic phenomena, and crystalline host formation.

Acknowledgements: This work was sponsered by the National Science Foundation Partnerships for Research and Education in Materials (PREM) DMR grant number 0934218 in collaboration with the Northwestern University Materials Research Science and Engineering Center.

P22

Synthesis and Characterization of Zn bis β-difunctional Complexes for the fabrication of ZnO_2 via Metal Organic Chemical Vapor Deposition for Applications in Microelectronics.

Johnson, Keneshia, Bo, Zhang, Katz, Howard and Matthews, Jason S.

Department of Chemistry, Howard University, 525 College Street N.W., Washington DC, 20059.

A series of Zn *bis* β-difunctional complexes were synthesized and evaluated for use as precursors for MOCVD of ZnO thin films. The free ligands were prepared via the reaction of N, N-diethylacetoacetamide and 2, 4-pentanedione with the appropriate amine. The single source precursors were synthesized via the reaction the free ligands with diethylzinc. The isolated products were characterized using FT-IR, ^{1}H-NMR, ^{13}C-NMR, GC-MS and MALDI. The volatility and thermal stability of the precursors were assessed using TGA. Thin films of ZnO were grown on a SiO_2 substrate utilizing a horizontal hot-walled CVD reactor. The thin films were characterized using SEM and XPS and employed in the fabrication of a transistor.

Electrospun undoped and Sb-doped tin oxide nanofibers: From charge transport to device and sensor applications

P23

Carrasquillo, Katherine V.[1], Reyna Maritza[1], Ramos Idalia[1], Pinto, Nicholas J.[1], Santiago Jorge J.[2], Agarwal, Ritesh[3].

[1]Department of Physics and Electronics, UPR-Humacao, Humacao, PR 00791; [2]Department of Electrical Engineering, UPENN, Philadelphia, PA 19104; [3]Department of Materials Science and Engineering., UPENN, Philadelphia, PA 19104.

Contact author: katherine.carrasquillo@upr.edu

Tin oxide (SnO2) nanostructures are of considerable scientific interest as new ways are being sought to use them in sensors and electronic devices. This material possesses two vital characteristics that make them technologically attractive viz. it is optically transparent and semiconducting. Undoped tin oxide is a non-stoichiometric semiconducting material (oxygen vacancies turns it n-type) with a large band gap (~ 3.6 eV) at room temperature and hence can be used in transparent conducting electrodes for organic light emitting diodes and solar cells. Using a simple electrospinning technique, we have fabricated nanofibers of undoped and Sb-doped SnO2. The n-type semiconducting properties of undoped SnO2 nanofibers have been exploited to fabricate field effect transistors that operate in the enhancement and depletion modes. By crossing these nanofibers with a p-doped polymer nanofibers, we have shown that the heterojunction results in a p-n diode that is tunable via exposure a UV light source. The band gap of the Sb-doped SnO2 nanofibers, calculated from the UV-Vis spectra is approximately 4.4e.V. The conductivity measurements show an increment in the conductivity of the doped fibers as compared with the undoped ones. Sb-doped nanofibers were electrically characterized as a function of temperature for different doping ratios of (7.8%, 13% and 15%) in an effort to look more closely at the insulator-metal transition.

Acknowledgements: This research was sponsored by the PENN-UPRH PREM grant (NSF-DMR-0934195).

Liquid Viscous Metamaterial with Tunable Anisotropy

P24

Mayy, Mohammad

Norfolk University, Norfolk, VA 23504.

Contact author: m.mayy@spartans.nsu.edu

We demonstrate a liquid viscous metamaterial consisting of gold nanorods coated with organic molecular coronas, which anisotropy can be controlled by an applied mechanical sheer force.

Acknowledgements: Supported by NSF PREM.

P25 Lattice Boltzmann Simulations of Drop Impact on Heterogeneous Surfaces

Connington, Kevin[1], Lee, Taehun[2], Koplik, Joel[3] and Morris, Jeffrey[4]

The City College of New York - CCNY CUNY, Benjamin Levich Institute for Physico-Chemical Hydrodynamics[1,3,4], Partnership for Research and Education in Materials New York, NY, 10031.

Contact author: kevin.connington@gmail.com

The dynamics of drop impact on heterogeneous substrates is important to understand from a materials research-application perspective. The phenomenon occurs in many situations, from ink-jet printing to fuel injection processes. Since drop impact is a physically complicated process, difficult to understand through experiments and theory alone, it is important to develop methods to study such a process numerically. The impact process poses many computational difficulties as well. Some of these difficulties include the tracking of a liquid-gas interface that undergoes extreme deformation in a short time period, accurately including the effects of surface tension, and realistically resolving the dynamic liquid-gas-solid contact line. Due to its kinetic nature, the Lattice Boltzmann Method(LBM) can incorporate mesoscopic physics into its formulation to resolve these difficulties, which otherwise pose significant problems for traditional continuum solvers. In our simulations, the interface is captured, instead of tracked, by keeping account of an order parameter in the fluid as in the phase field method. A diffuse interface method is utilized to resolve the complex physics that occurs at the interface. Here we report preliminary results describing situations such as inclined drop impact on a homogeneous substrate, normal impact on a substrate of heterogeneous wettability, and normal impact on a superhydrophobic surface.

Acknowledgements: Supported by NSF PREM Grant # DMR-0934206.

P26 VMD plug-in for the study of fluid-surface interaction

Medina Cuadrado, Mirgery[1] , Cortés Martínez,Carlos[1] , Martínez, Frances[1], Sotero Esteva, José O.[1] and Moore, Preston[2]

[1]Department of Mathematics, University of Puerto Rico at Humacao, Humacao, PR 00791, [2]Department of Chemistry, University of the Sciences in Philadelphia, Philadelphia, PA, 19104.

Contact author: mirgery.medina@upr.edu

Macroscopic models that describe surface tension describe a surface of a liquid as a two-dimensional region. Molecular Dynamics (MD) simulations describe fluids as a set of points in space. Therefore there is no obvious way to describe the surface of a film or droplet. Moreover, recent results have shown the existence of an inter phase between the liquid and gas phases in a fluid film, making the problem of detecting such a surface more difficult. We have already corroborated the phenomenon in an Argon liquid nano-droplet MD simulation.

The *Model building, Simulation and Data Analysis Script* (MoSDAS) is a tool with graphical user interface developed by the computational science research group at the UPR-Humacao. This application has been improved in order to experiment with ways of measuring surface tension at the nano scale. As a result, the process of the building configuration files required by MD Simulations was simplified. MoSDAS is being written using Python, the Tkinter library and runs as a plug-in to the widely used *Visual Molecular Dymamics* (VMD) software. In particular, MoSDAS has been improved with new options to create and manipulate fluid droplets and molecular structures that serve as solid surfaces in order to generate a hybrid structure as an entire new system. The software produces the configuration files required to run the simulation.

Acknowledgements: PENN-UPRH PREM (NSF No. DMR-0934195).

Structured Material Obtained by Surfactant and Microemulsion Templating **P27**

Carroll, Nick J.[1] and Petsev, Dimiter, N.[1]

[1]Department of Chemical and Nuclear Engineering and Center for Biomedical Engineering, University of New Mexico, Albuquerque, New Mexico 87131.

Contact author: Dimiter@unm.edu

Herein we present methods for synthesizing monodisperse mesoporous silica particles and silica particles with bimodal porosity by templating with surfactant micelle and microemulsion phases. The fabrication of monodisperse mesoporous silica particles is based on the formation of well-defined equally sized emulsion droplets using a microfluidic approach. The droplets contain the silica precursor/surfactant solution and are suspended in hexadecane as the continuous oil phase. The solvent is then expelled from the droplets, leading to concentration and micellization of the surfactant. At the same time, the silica solidifies around the surfactant structures, forming equally sized mesoporous particles. We show that hierarchically bimodal porous structures can be obtained by templating silica microparticles with a specially designed surfactant micelle/microemulsion mixture. Oil, water, and surfactant liquid mixtures exhibit very complex phase behavior. Depending on the conditions, such mixtures give rise to highly organized structures. A proper selection of the type and concentration of surfactants determines the structuring at the nanoscale level. Tuning the phase state by adjusting the surfactant composition and concentration allows for the controlled design of a system where microemulsion droplets coexist with smaller surfactant micellar structures. The microemulsion droplet and micellar dimensions determine the two types of pore sizes.

This work was supported by NSF (PREM/DMR 0611616).

Colloidal Liquid Crystal Gels: Synthesis and Characterization **P28**

Diestra-Cruz, Heberth[1], De La Cruz, Edwin[2], Rinaldi, Carlos[1] and Acevedo ,Aldo[1]

[1]Chemical Engineering Department, University of Puerto Rico-Mayagüez, Mayagüez, PR 00681;
[2]Chemistry Department, University of Puerto Rico-Mayagüez, Mayagüez, PR, 00681.

Contact author: aldo.acevedo@upr.eduxs

Liquid crystalline materials are known to exhibit a rich range of physical and chemical properties in natural and biological systems. Inspired by the functional versatility evident in biological systems, in recent years, an increasing number of studies have sought to capitalize on the ability of liquid crystals to change properties in response to external stimuli to design active materials. Nevertheless, the fluid nature of the liquid crystal limits their applicability. Our proposed work seeks to overcome that limitation by designing, synthesizing, and characterizing solid-like colloidal liquid crystal (CLC) gels with tunable optical, mechanical, and magnetic properties. In this presentation, we report on the advances of our team on the synthesis and characterization of colloidal magnetic particles, as well as the evaluation of CLC gels with model particles.

Acknowledgements: This work is supported by Wisconsin-Puerto Rico Partnership for Research and Education in Materials, with funds from NSF.

P29

Ab Initio Calculation of Copper Dimer Excited States

Sams, Courtney and Eloranta, Jussi

California State University at Northridge, Northridge, CA 91330-8268.

Contact author: jmeloranta@gmail.com

The ground and several excited states of copper dimer (X, A, B and C) were calculated by the coupled clusters equation-of-motion method. A qualitative agreement with gas phase spectroscopic observables, such as the electronic origins, harmonic and anharmonic vibrational frequencies and radiative lifetimes, were obtained. For the B and C states the calculations verify the experimentally generated potential energy curves for these states and further identify the weakly allowed A state to originate from the spin-orbit mixture of the B and A states. It was found that the present level of accuracy could only be reached when scalar relativistic corrections (Douglas-Kroll; DK) were included along with the DK compatible triple zeta level basis set. Finally, the interaction between the copper dimer and atomic helium was calculated to elucidate the possible solvation structure of the dimer in superfluid helium. It was found that while Cu atoms are heliophobic, Cu2 dimers are heliophilic and should remain inside helium droplets.

Acknowledgements: NSF-PREM Program.

P30

Synthesis and Rheological Characterization of Non-Spherical Micro and Nanostructures

Baah, David[1], Vickers, Dwayne[2], Jones, Wanda[3], Archer, Lynden[3] and Floyd Smith,Tamara[1]

[1]Tuskegee University, Tuskegee, AL, 36088., [2]Northeastern University, Boston, MA, 02115, [3]Cornell University, Ithaca, NY, 14850.

Contact author: tamara.floyd@tuskegee .edu

Particles in the micro- and nanometer size range are some of the most commonly encountered forms of materials in nature. Such monodisperse spherical or nonspherical suspensions and their assemblies have specific applications in opto-electronics, photonics, catalysis, drug delivery, and field responsive rheological fluids. Particularly, particles' size, shape, and monodispersity are important factors affecting the shear induced flow characteristics of suspensions. However, the synthesis of such highly monodispersed particles with tunable functionalities has been a great challenge. In this study, we report the hydrothermal synthesis of high yielding mono-dispersed Co3O4 nanocubes and its shear induced rheological characteristics. At low volume fractions (~0-0.006), suspensions of Co3O4 in PEG400 is observed to be shear thinning. However, at volume fractions in the range of 0.36-0.62, the onset of shear thickening is observed and it decreases with increasing volume fractions. In order to extend the syntheses to other shapes and materials of interest, we employed the use of microfluidics technology. The method is dependent on the use of a UV-curable prepolymer, with an appropriate photo-initiator. A photo mask patterned with pores defining the shape of the particles is used to block UV light while the pores allow the passage of light thereby cross linking the liquid prepolymer in the light path.The prepolymer solution is passed through a microfluidic device fabricated by bonding poly(dimethylsiloxane) (PDMS) molds to a glass slide. An optical microscope is used to focus the UV light to synthesize polymeric particles. Micron-sized organic particles of various two dimensional extruded shapes are synthesized with this method using poly(ethylene glycol diacrylate) (PEG-DA) as the precursor. A preliminary rheological behavior of 0.01wt% cubic composite particles (1% SiO2 + PEG-DA) in PEG400 was observed to be slightly shear thinning. However, we anticipate a pronounced onset of shear thickening with an increase in the volume fraction.

Synthesis of [1,5-13C] 1,5 (Phenylsulfinyl) Toluene Using Diels-Alder Chemistry P31

Martinez, Rodolfo, Timofeeva, Tatiana and Rael, Gregory

New Mexico Highlands Universty, Rio Rancho, NM 87124-6613.

Contact Author: grael2@live.nmhu.edu, tvtimofeeva@nmhu.edu

The use of stable isotopes in organic synthesis has many advantages. [1,5-13C] 1,5 (Phenylsulfinyl) toluene can be synthesized with very simple 13C labled precursors. My research involves the synthesis of [2-13C]-((1*E*,3*E*)-1-ethoxy-4-(phenylsulfinyl)buta-1,3-dien-2-yl)(phenyl)sulfane which is tri substituted diene, and [1-13C](*Z*)-(prop-1-enylsulfinyl)benzene a substituted alkene to be used as a dienophile for a Diels-Alder reaction. With the specific centers of both diene and dienophile the projected six-carbon ring will direct us to our desired product. The use of 13C will allow me to easily track and identify the formation of the ring and help us predict the stereochemistry. With the final product in place further synthesis will involve Suzuki coupling. [1,5-13C] 1,5 (Phenylsulfinyl) toluene, brominating the methyl groups and substituting with methyl phenyl sulfoxide, which help us in the formation of a pyrene system labeled at the 1,3,6,8 positions.

Acknowledgements: NSF, STCPREM, New Mexico Highlands Universty, Georgia Insititute of Technology.

Taller Tambuyé

Taller Tambuyé (*Tambuyé Workshop*), Inc. was founded in 2003 to promote research, education and performance of Afro-Puerto Rican musical genres: Bomba and Plena.

Marién Torres López is a choreographer, director and founder of *Tambuyé*. She has been the principal dancer in various musical groups including *Bombazo de Puerto Rico* from Centro de Investigación Cultural Raíces Eternas (CICRE), *Plenibom,* Taller Folklórico *Yubá-Iré*, *Caribe soberao*, *Los parranderos de Loíza*, *Caribeando*, *Seis de bomba*, *Tambores calientes* y *Terraplén.* As a drum player, she has performed in *Nandi*, the first female Bomba group and *Vamos andando*, a group that fuses Bomba with peruvian instruments. Torres was an invited speaker at the Bomba Research Conference (Chicago 2007) and Bomplenazo (New York 2008), and was nominated for the most outstanding dancer award for Segundo Ruiz Belvis Cultural Center (Chicago 2009).

She is also a professor at the Inter-American University of Puerto Rico, Metropolitan Campus, where she teaches Dance and History of Puerto Rican Music.

Organizing Committee

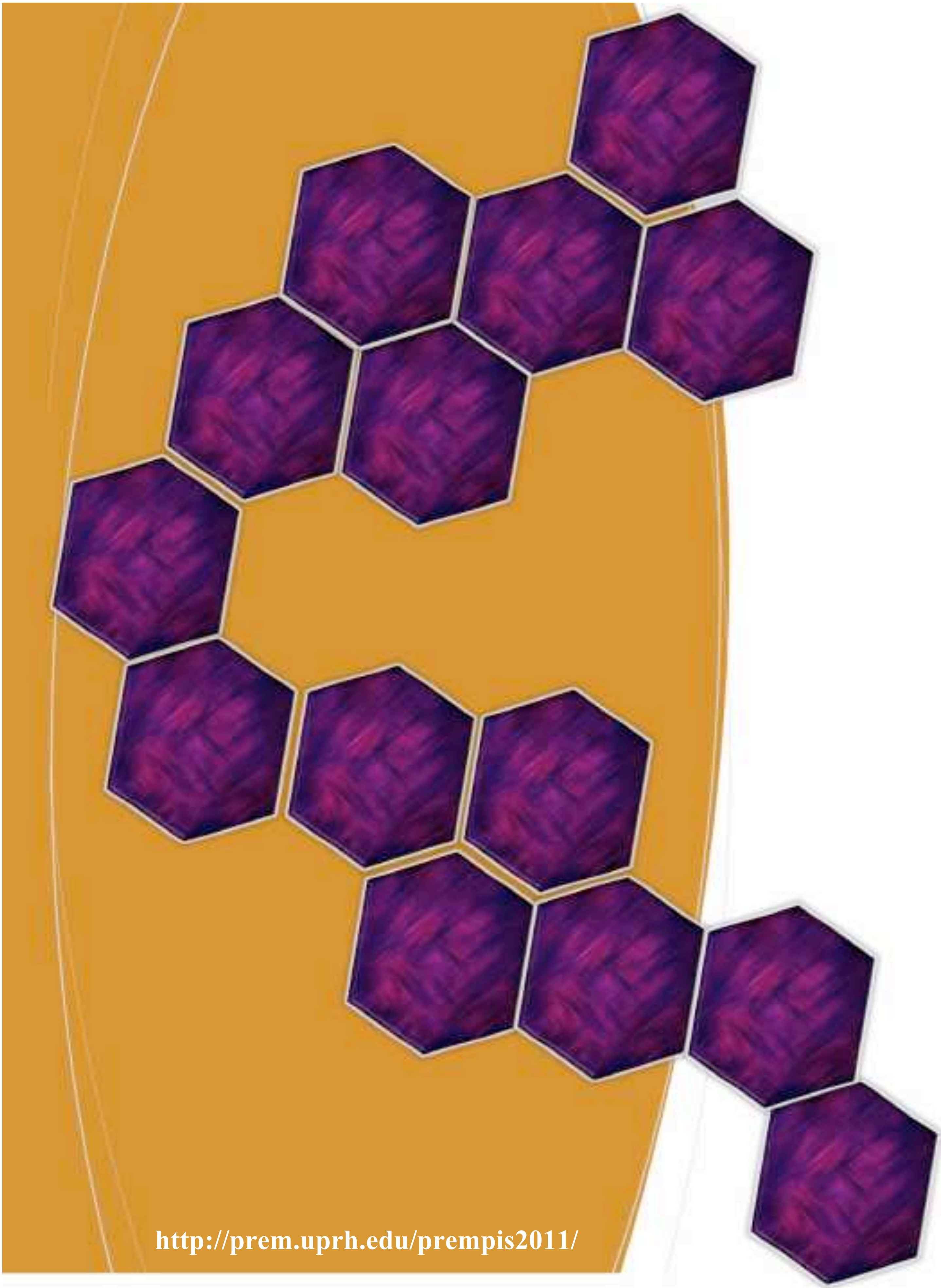
Paresh Ray, PREM Jackson State University
Karen Lozano, PREM University of Texas – Pan American
Lamartine Meda, PREM Xavier University of Lousiana
Idalia Ramos, PREM University of Puerto Rico – Humacao
Tim Lodge, MRSEC University of Minessota

NSF Program Directors

Sean L. Jones
Thomas P. Rieker

Local Organizing Committee

Idalia Ramos, PREM PI, Dept. Physics and Electronics
Nicholas Pinto, Dept. Physics and Electronics
José Sotero, Dept. Mathematics
Josee Vedrine, Dept. Physics and Electronics
Pablo Negrón, Dept. Mathematics
Gilda Jiménez, Petra Mercado High School
Ramón Rivera, PREM Outreach Coordinator
Lynette Rivera, PREM Administrative Coordinator
Anamaris Meléndez, PREM Laboratory Technician
John Morales, PREM Laboratory Technician
PREM-Humacao Students



http://prem.uprh.edu/prempis2011/