



UM Comp Chem group secures NSF MRI grant

Congratulations to the University of Mississippi's Computational Chemistry researchers for being awarded a \$300,000 Major Research Instrumentation (MRI) grant from the National Science Foundation. The project, entitled "MRI: Acquisition of a GPU Cluster for Computational Science in Mississippi," is under the direction of Gregory Tschumper, Brian Hopkins, and Robert Doerksen. It will result in a major hardware upgrade at the Mississippi Center for Supercomputing Research (MCSR).

The MCSR provides free accounts for the research and instructional use of students and faculty at all of Mississippi's public universities.

MARK YOUR CALENDARS!

Mississippi EPSCoR Annual State Meeting

March 4-5, 2014

Mississippi State University

Leszczynski: Recognized in Ukraine

Dr. Jerzy Leszczynski once again visited the National University of Kiev in Ukraine in June. In an earlier trip, Leszczynski, Director of Jackson State University's Interdisciplinary Center for Nanotoxicity, visited with the president at Taras Shevchenko National University (TSNU) of Kyiv.

Noted scientists were greeted by the president of the University, member of Ukrainian Academy of Sciences, Dr. Leonid Hubersky. During the meeting, Hubersky thanked Leszczynski for the work he carries out in order to strengthen cooperation between the two universities.

The president emphasized that the Memorandum, signed in 2011 with JSU, has been successfully implemented and he expressed hope that this is only the beginning of further long-term, fruitful collaborations. Leszczynski assured the president that the collaboration will be expanded — "We are interested in new ideas in research and education, we are pleased to cooperate and provide all possible support from our side."

Leszczynski presented to the university a series of books (10 volumes) that he has edited on recent advances in computational chemistry with some being written in collaboration with Ukrainian authors.

During the meeting the double-degree programs, exchange of teachers and students, joint seminars, conferences etc. were discussed.

Hubersky (l, below) presented to Leszczynski an Award of the Academic Council of the University, the most distinguished TSNU recognition.



Dass receives NSF CAREER award

Dr. Amal Dass, assistant professor in the Department of Chemistry and Biochemistry at the University of Mississippi received a 2013 Faculty Early CAREER award from the National Science Foundation. The CAREER Award is titled: "CAREER: Monodisperse Metal Alloy Nanoparticles."

Dass is a member of the MS EPSCoR Computational Chemistry focus group. His research interests include gold nanoparticles, nanomaterials, analytical chemistry, and

mass spectrometry. He credits his work with the EPSCoR project as being instrumental in collecting the preliminary data that made the CAREER Award possible.

Nanoscience is a new area of science that has generated excitement worldwide. Nanomaterials are being developed to address some of the world's biggest challenges, including: clean, affordable energy; stronger, lighter, more durable materials; medical devices and drugs to detect and treat diseases; sensors to detect harmful chemi-

cal or biological agents; lighting that uses a fraction of the energy; low-cost filters to provide clean drinking water. We work on molecular gold nanoparticles (<2nm) that have precise number of gold atoms and ligands. Commercialization of nanomaterials and design of nanoengineered products will require: understanding of the fundamental properties; controlled synthetic and processing conditions.

The Dass research group works on synthesis and characterization of these molecular gold nanoparticles.

MSU awarded NIH COBRE

MSU's College of Veterinary Medicine has secured a \$10M Centers of Biomedical Research Excellence (COBRE) grant from the National Institutes of Health that will further research focusing on diseases that affect animal and human health. The unique nature of the grant establishes a mentoring program for a core group of researchers.

In addition to principal investigator Stephen Pruett, the head of MSU-CVM's basic sciences department, MSU researchers in this group include Janet Donaldson, associate professor in biological sciences; Keun Seok Seo, assistant professor in CVM's basic sciences and EPSCoR funded faculty, Mariola Edelman, assistant research professor with the Institute of Genomics, Biocomputing and Biotechnology; Bindu Nanduri, assistant professor in CVM's basic sciences, and Henry Wan, a CVM associate professor.

Over the course of the five-year grant, the researchers will work on projects that promote a greater understanding of animal and human health.

EPSCoR helps sponsor BEST Robotics

Nineteen middle and high schools from across the state competed in the Boosting Engineering, Science and Technology Robotics Competition (BEST).

Students are given limited

A \$650,000 grant to the University of Mississippi, allowed three high school students to conduct summer research on the UM campus. Their research was part of a summer research program made possible by the National Science Foundation grant.

Assistant professor of Chemistry and Biochemistry, Dr. Amal Dass, proposed the grant in July 2012 after a trial run of a mentoring program. One portion of the grant's funding allowed elite high school students to assist in research while graduate students mentored and worked closely with the high school students.

The program accepted three high school students: Grace Brososky, 17, of Georgia, David Bryde, 17, of Mississippi, and Jake Thrasher, 17, of Alabama.

"I'd really like to make a practical difference in the world," Brososky said. "Last year I became really interested in the Google science fair." Brososky's project in the fair was recognized as a finalist in multiple mediums.

Thrasher plans to study biochemical engineering in med-

materials to make a robot that can perform tasks. "So if they mess up, if they cut their plywood incorrectly, that's it," BEST Competition Hub Director Eric Heiselt said. "They've got to figure something else out using the materials they are given to work with so they are pretty much

icine and his goal is to assist in the fight against cancer.

"When I was younger, I had two friends diagnosed with cancer around the same time," Thrasher said. "We visited them often and seeing everyone suffering made me want to help them." Thrasher isn't intimidated by the laboratory environment.

"It's right up my alley; it's what I want to do." Thrasher said. "I want to be challenged."

Bryde said that being at Ole Miss this past summer gave him a sense of responsibility.

"I gave a tour to Grace and I took care of business with a few colleges," Bryde said. "I didn't really care about physics, but I noticed as I got further into school I had a desire to go into theoretical physics. I even developed a few favorite physicists."

Bryde said Nikola Tesla is perhaps his favorite physicist and even celebrates Nikola Tesla Day. He went further to say his experience at Ole Miss was utterly fun and extremely educational.

"I learned tons of processes, what the machines did and even how to read some of the

starting from scratch." Students put in a lot of hours preparing for this competition but it helps to prepare them for the real world and many of the students go on to study engineering in college, explained East Rankin Academy Physics teacher Angela Trigg.

graphs," Bryde said.

The trio of high schoolers worked almost exclusively in the lab during their week at UM. Students were housed in UM's Residential College to provide the college-life atmosphere.

Brososky, Bryde and Thrasher all intend to try their chances with major Boston universities, specifically the Massachusetts Institute of Technology (MIT) and Harvard University. But they are also considering other alternatives.

Chemistry professor Amal Dass said the summer program isn't like a typical summer camp. Rather, he said the high school students made legitimate contributions.

"They were active participants in research," Dass said. "If they could get their name on published research, that would give them a great advantage later in their careers."

Dass maintains the importance of real hands-on contributions in the lab as well as outside of it.

Dass believes the summer program barely scraped the surface of what could be coming. He plans to have four students come each year with one student from an underrepresented school district each year.

This fall the grant is being utilized to bring laboratory activities to North Panola High School students in Batesville, MS.

Year 5 PUI and Seed grants awarded

The EPSCoR Year 5 Private and Undergraduate Institutions (PUI) Seed Grants and the EPSCoR Seed Grants have been awarded. Below are the recipients:

Seed Grants:

PI: Shanti Bhushan (MSU)

Focus Area: Comp BioSim

Title: Laminar/Transition/Turbulent Flow Simulations of Aortic Thromboembolism in Feline Hypertrophic Cardiomyopathy

PI: Jared Delcamp (UM)

Co-PI: Greg Tschumper (UM)

Computational Chemistry

Title: Development of NIR Dyes with Novel Heterocyclic

Structures for Dye Sensitized Solar Cells: A Combined Experimental, Computational Approach

PI: Tim McLean (USM)

Comp Biology/Comp Chem

Title: An Initial Investigation to Detect and Characterize microRNAs in a Harmful Alga, *Karenia brevis*

PI: Tibor Pechan (MSU)

Co-PI: Steve Gwaltney (MSU)

Title: Quantum mechanics modeling of metabolites fragmentation in ion trap mass spectrometers

PI: Dongmao Zhang (MSU)

Computational Chemistry

Title: Understanding Mercapto-benzimidazole (MBI) Adsorption, Desorption, and Reaction on Silver Nanoparticles (AgNPs) in Water

PI: Shahid Karim (USM)

Co-PI: Steven Adamson (USM)

Computational Biology

Title: Elucidating the molecular gene networks which facilitate Japanese Beetle food digestion and insecticide resistance

PI: Svein Saebo (MSU)

Computational Chemistry

Title: Computational Studies of SO1455-POSS, a promising blood-clotting agent manufactured by Hybrid Plastics Inc.

PI: Natalia Garcia-Reyero Vinas (MSU)

Co-PI: Bindu Nanduri (MSU), Amal Dass (UM)

Comp Bio/Comp Chem

Title: A study design to determine the biological impacts of thiolated gold nanoparticles using a model species, the zebrafish

PUI Grants Awarded

PI: Pradip Biswas (Tougaloo)

Title: Studying oxidative hydrogen transfer and electronic rearrangements in DNA using DFT-based QM/MM dynamics

PI: Bidisha Sengupta (Tougaloo)

Title: Natural and synthetic flavonoids as stabilizers of quadruplex and i-motif structures in DNA-conjugated metal nanomaterials

PI: David Magers (Mississippi College)

Co-PIs: Julia Saloni (Co-Lin), Shelley Smith (Co-Lin)

Title: Computational Studies of Chemically and Biologically Relevant Molecular Systems.

UM's Engineering host MAESC

The University of Mississippi's School of Engineering hosted the 2013 Mid-South Annual Engineering and Sciences Conference (MAESC). The theme of the conference was "Academia-Industry Partnership."

MAESC serves as a forum to bring together scientists, engineers and professionals from southern states to present and discuss the latest research and development in science, technology, and engineering. The past 15 meetings drew significant participation from mid-south research institutions and industries in forms of research presentations and display booths.



This year's MAESC aim was to bridge the gap between recent advances in research and fast growing industrial needs and challenges. MAESC 2013 was dedicated to accelerate the nuance research and technology transfer to improve the mid-south competitiveness in the area of science, technology, and engineering.

This forum provided a wealth of practical information for innovators, researchers, and practitioners to develop new products, processes, and technologies. An industry-academic panel discussed the following topics: How to identify research in mid-south universities essential for eco-

nomics development of southern states to become more competitive in the global market; How to bridge the knowledge gap between industry and academia; and How to identify needs of future graduates to be well prepared not only for today's needs, but also for tomorrow's challenges.

Vasquez presents research at ACS

Erick Vasquez, a post doctoral student working with Dr. Keisha Walters in the Department of Chemical Engineering at Mississippi State University, was selected to present his work "Stimuli-responsive biphasic-polymer Janus magnetic nanoparticles

prepared via electrostatic interactions and surface-confined ATRP" at the 2013 Excellence in Polymer Graduate Research Symposium. The symposium was held in conjunction with the 245th American Chemical Society National Meeting.

Liljegren/Hammer host CC students

Dr. Sarah Liljegren, an assistant professor of Biology, and Dr. Nathan Hammer, an assistant professor in Chemistry and Biochemistry, hosted students from Northwest Mississippi Community College (NWMCC) this past summer. Partial funding from EPSCoR allowed these students to participate in a summer research experience.



NWMCC sophomore Megan Christy, worked alongside Liljegren in her lab. Liljegren says she thinks "the highlight of her experience was the opportunity to do some scanning electron microscopy of an Arabidopsis flower mutant during several road trips my lab made to the University of Memphis."

Christy presented a talk about her research to her peers at NWMCC that was arranged by her professor/advisor

at NWMCC, Patricia Miller. Her title was "EPSCoR Community College Research Experience" and her audience was a general biology class for majors (BIO 1133) of about 30 people.

"Megan made a huge contribution to my lab's research this summer and will be a co-author on an

upcoming paper we are currently writing. She worked with us the entire summer," Liljegren explained.



In Hammer's lab, NWMCC sophomore Philip Correrro, set up an experiment to study the infrared spectra of gas phase biological building

blocks.

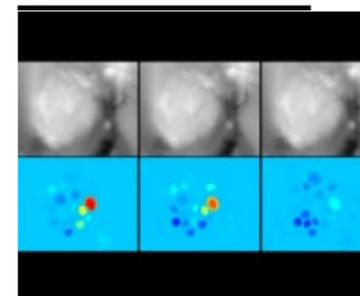
A biology (pre-med) major, Correrro is not only a stellar student at NWMCC, but is also a highly sought-after athlete.

While Christy commuted, Correrro stayed in UM's residential housing to experience a college environment for himself.

EPSCoR funding supports Wolf

Victoria Wolf, an Agricultural and Biomedical Engineering student from Mississippi State University, is working in the lab of Dr. Robert Hester at the University of Mississippi Medical Center. Wolf is supported by EPSCoR and is conducting her research towards her Master degree. She began working with Hester in January, 2013 and will graduate in May, 2014.

She recently presented a poster at the 2013 Biomedical Engineering Society meeting in Seattle, Washington in September. Her presentation was titled "Modeling the Cardiovascular and Endocrinologic Adaptations of Pregnancy."



HumMod Browser work recognized at symposium

A paper, titled "HumMod Browser: An Exploratory Visualization Tool for the Analysis of Whole-Body Physiology Simulation Data," was presented by Keqin Wu, Jian Chen, William Pruett, and Robert Hester at the 3rd IEEE Symposium on Biological Data Visualization in Atlanta, GA. The paper received "Best Paper: Honorable Mention."

HumMod Browser is a multi-scale exploratory visualization tool that allows physiologists to explore human physiology simulation data with more than 6000 attributes. Presented was a tag cloud technique to reveal the significance of time-varying attributes and then

study how a chain of tag clouds can form an exploratory visualization that assist multiple dataset comparison and query. One purpose is to reduce the high cognitive workload of understanding complex interactions within the

large attribute space. The HumMod Browser produced can give physiologists flexible control over the visualization displayed for quick understanding of complicated simulation results. The visualization is constructed through the metaphorical bubble interface to allow dynamic view controls and the data relationships and context information unfold as physiologists querying groups of connected bubbles within the hierarchical or causal relationships.

HumMod Browser contributes to the interaction design and provides multi-scale coordinated interactive exploration for a new type of physiological modeling data. Two case studies have been reported with real datasets containing more than 6000 physiology attributes, which provide supportive evidence on the usefulness of HumMod Browser in supporting effective large-attribute-space exploration.

