MISSISSIPPI EPSCoR Experimental Program to Stimulate Competitive Research

JSU's Cohly travels to India

An EPSCoR international travel grant funded Dr. Hari

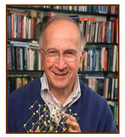
Cohly of Jackson State University (JSU) to travel to India to continue collaborations with Hindustan College of Science and Technology (HCST). This collaboration enabled the faculty to work on several projects including hydrogen gas production and to design projects for the training of individuals in rural India on visual analytics, health management, and self sufficiency in energy production using remediation technology from urine and sludge. An Memorandum of Understanding (MOU) was signed between JSU and HCST. The active collaboration is between the Department of Biotechnology in HCST and Department of Biology at JSU.

Cohly submitted a joint manuscript between faculties of Dayalbagh Educational Institute(DEI, Chaturvedi) and JSU which was presented in Spircon 2010. He initiated a new collaboration between JSU/HCST and two private companies -- one in the USA (AlfaGene Bioscience, Inc; POC Dr Asit Panja) and the other in India (Lifezone Biotech; POC Dr. Anil Mavila), both specializing in stem cells. While in India, Cohly attended a workshop on "Vocational Training and Entrepreneur Development" and presented his approach on hydrogen gas production using urine and sludge as the starting materials at Sharda University, Gr. Noida.

Fall Forum at UM features Hoffman

The second annual EPSCoR Fall Forum was held on the University of Mississippi campus. Dr. Roald Hoffman was the keynote speaker for the day long forum.

Hoffmann, an American theoretical chemist,



won the 1981 Nobel Prize in Chemistry. He currently teaches at Cornell University in Ithaca, New York.

Hoffman expressed "applied theoretical chemistry" to characterize the particular blend of computations stimulated by experiment and the construction of generalized models and frameworks for understanding — that is his contribution to chemistry. The pedagogical perspective is very strong in his work.

Hoffman is also a published poet and playwrite. A reading of Hoffman's play 'Should've" was presented on the eve of the Forum to the forum participants and the UM community. Standing room only, the play exhibited the social responsibility of scientists and artists on one level. "Should've" is also about three people trying to resist the transforming power of death. They are unable to do so, sundered as they are by the memories and a past that emerges from that death. And, eventually, the consequences shape a different bond among the three.

During the Forum, the *Lightning Talk* session was popular among the attendees. Nine researchers had five minutes to present the research that they were conducting in an effort to recruit collaboration of researchers from other institutions on their projects. During an extended lunch, researchers had adequate time to visit with their colleagues to further foster collaborations among the researchers and the various institutions.

Joe Lichtenhan, co-founder , president and Chief Executive Officer of Hybrid Plastics in Hattiesburg, MS gave a presentation on the use of Polyhedral Oligomeric Silsesquioxanes (POSS®) in health and medical products. POSS is a revolutionary new Nanotechnology based on silicon-derived building blocks. Lichtenhan showed slides illustrating how he used POSS to close a wound on his foot with no scarring. POSS nanomaterials are biocompatible, recyclable, nonflammable, and competitively priced with traditional polymer feedstocks.

Twenty-two posters were displayed by researchers illustrating a basis for developing new collaborations and strengthening existing collaborations among researchers.

Jason Hale provided an update on the EPSCoR data management plan. He discussed the data management, online survey that project members will be asked to complete in the coming weeks. He also discussed online collaboration tools.

National and State Advisory Board members attended and provided feedback to administrators and researchers on the progression of the project.

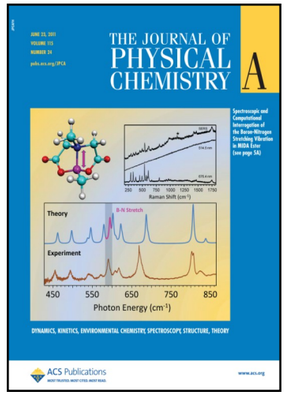
MISSISSIPPI EPSCoR

UM Captures Front Cover of Major Journal

University of Mississippi's Dr. Greg Tschumper and Dr. Nathan Hammer, with under-

graduate Nikki Reinemann, first author, share the front cover of the Journal of Physical Chemistry in the June 16, 2011 issue. Reinemann is a chemistry major and computational chemistry researcher from Batesville, MS. She is under the direction of Dr. Nathan Hammer.

The title of the article is Vibrational Spectroscopy of N-Methyliminodiacetic Acid (MIDA) - Protected Boronate Ester: Examination of the B-N Dative Bond. Authors of the article included: Reinemann, D., Wright, A., Wolfe, J., Tschumper, G., and Hammer, N.



About the cover: The B-N stretching mode in methylboronic acid MIDA ester is shown to occur in the vicinity of 600 cm^{-1} , making it one of the lowest, if not the lowest, experimentally observed.

JSU's Comp Chem host SSCCMS

For the past 10 years, Jackson State University's Department of Chemistry has hosted the Southern School on Computational Chemistry and Materials Science (SSCC&MS). There was no difference this year as JSU hosted the 2011 SSCC&MS conference that was supported and co-organized by the Mississippi EPSCoR Computational Chemistry group. The conference included four National Science Foundation (NSF) supported summer institutes: CREST, REU/ RET and PREM Programs. At total of 25 students from the four programs gave approximately 15 minute oral presentations the second day of the SSCC&MS conference to both fulfill their summer institute research requirements and to officially serve as speakers of the conference.

The SSCC&MS also featured 12 renowned speakers to open conference activities including Jorge M. Seminario, Texas A&M University; Perla Balbuena, Texas A&M University; Jiande Gu, Chinese Academy of Sciences; Frances Hill, US Army Engineer Research and Development Center; Tiffani Holmes, Fort Valley State University; Tomasz Puzyn, University of Gdansk; U.S. Rai, Banaras Hindu University; B. Ramu Ramachandran, Louisiana Tech University; Dulal Senapati, Jackson State University; Andrzej Sygula, Mississippi State University; Szczepan Roszak, Wroclaw University of Technology; and He Wang, Tulane University.

More than 40 posters were presented during the poster session and 12 talks were given by invited speakers. A significant number of the poster presentations were given by high school, undergraduate, and graduate students. For the poster competition, six individual received prizes for their posters. Graduate student Toyketa Horne and undergraduate Jean Negou shared 1st place honors, graduate student Sadia Afrin Khan was awarded 2nd place, graduate student Ivana Malvacio took 3rd place, while undergraduate Christen Robinson and high school student Nabhan Karim both received Honorable Mention.

Some 50 participants represented six countries during the conference: China, Poland, Argentina, Puerto Rico, Ukraine, and Russia.

Plans are underway for JSU to host the 20th Current Trends in Computational Chemistry (CCTCC) conference, October 27-29, 2011. The two and a half day conference series will discuss applications and the latest developments of computational chemical techniques for calculating various chemical systems.

The conference will cover both *ab initio* and semi-empirical models, as well as *ab initio* molecular dynamics methods. Researchers from various research laboratories and scientists from academia are the targeted attendees. Twenty-six distinguished speakers (including two Nobel Laureates) have accepted speaking invitations and ~200 poster presentations will be made with a total attendance expected of ~ 200-250 participants.

The conferences provides a venue for rapid communication of new developments in the field among researchers. The CCTCC series has a long and successful history of bringing together researchers from various disciplines and providing a forum for discussions and interactions.

University of Mississippi undergraduate students visited with experts at the University of Reading in London as part of the EPSCoR International Exchange Program. Under the direction of Dr. Nathan Hammer, students visited with Dr. Marcio Siqueira, hip pressure Raman expert at UR. Pictured with Dr. Siqueira is (l-r) Annie McClellan, Nikki Reinemann, and Lynn Joe.

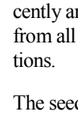
2011 Seed Grant Recipients

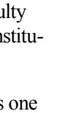
The 2011 EPSCoR Seed Grant recipients were selected recently and included faculty from all four research institutions.

The seed grants serve as one component of the larger project — to fund promising new, collaborative research projects. Six seed grant recipients were chosen by the NSF EPSCoR Steering Committee after careful evaluation of the proposals submitted. "The selection process was very difficult because we had so many outstanding proposals," stated Dr. Susan Bridges, Science Coordinator for Mississippi EPSCoR. "Our goal is to build expertise and collaboration at Mississippi universities in computational modeling of biological and biochemical systems."

The 2011 recipients are:

Jian Chen (USM) - Storytelling Bubbles: Integrating Symbolic Representation, Data Ink Manipulation, and Metaphorial Interface for Fluid Time-Varying Biology Data Analysis.





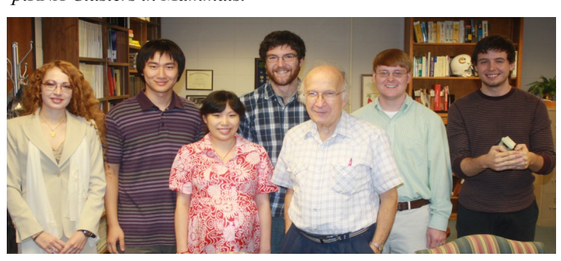
Federico Hoffman, Andy Perkins *(MSU) - Evolution of piRNA Genes and piRNA Clusters in Mammals.*

Seongbong Jo, Robert Doerksen (UM) - *Computational Modeling-Aided Design, Synthesis and Evaluation of Redox-Sensitive Polymer Nanoparticles for Cancer Targeted Drug Delivery.*

Todd Mlsna (MSU), Yixin Chen, Dawn Wilkins (UM) – *The Development of Analytical Equipment and Software For Identification of Biomarkers of Respiratory Diseases.*

Keisha Walters (MSU), Charles McCormick (USM) – *In Vitro Inhalation and Deposition of Polymer-Stabilized Gold Nanoparticles for Validation of Computer Simulated Particulate Distributions in the Lung.*

Dongmao Zhang (MSU), Jerzy Leszczynski (JSU) – *Deciphering the Drastic pH Dependence of the Surface Enhanced Raman Spectrum of Thiobarbituric Acid on Gold Nanoparticle: A Combined Computational and Experimental Investigation.*



UM research students under the direction of Dr. Keith Hollis visited with Nobel Prize winner, Roald Hoffman. (L-R) Billy Forrest, Xiaofei Zhang, Bei Cao, Aron Huckaba, Hoffmann, Wesley Clark, and Matt Dukes.

Research Ring Approved by Governor

Dr. Felix Okojie (r), chair of the Mississippi Research Consortium (MRC), stands with Gov. Haley Barbour during the recently announced agreement with AT&T that will provide the MRC with 20 times the broadband capacity that is currently available. Mississippi's research universities and other state research centers will be able to communicate much more efficiently, thanks to expanded broadband technology said Barbour. The Mississippi Research Network, will link the eight entities in what Barbour called a "research ring" and give them the capacity to move more data quickly. Okojie commented that "having more broadband capacity will give institutions an advantage in competing for grant money, and he anticipates a significant return on Mississippi's investment. We envision the research enterprise growing significantly as a result of this capacity." Mississippi will rent the fiber optic technology to provide the service from AT&T for eight years at a cost of $16 million. Barbour said renting the equipment instead of purchasing it makes it easier for the state to update the technology, if necessary, at the end of eight years.

Dr. Glake Hill, Jackson State University, is one of three EPSCoR researchers that have collaborated with the MSU LeaderState program and the Jackson Public School Junior ROTC program. Dr. Hill along with Dr. Robert Hester, UMMC, and Dr. David Magers, MC are providing STEM outreach to JROTC students at each of the Jackson Public High Schools during the fall semester.

JSU's Fly publishes in International Journal

A journal paper on "Implementation of the Binary Coding Scheme and the Tree Traversal Algorithms to Test for Ancestor-Descendant Relationships in K-ary Trees," was published by Pervis Fly (first author), Natarajan Meghanathan, and Raphael E. Isopkehi in the September, 2011 issue of the International Journal of Research and Reviews in Applied Sciences. The research was conducted by Fly, as an undergraduate computer science senior and student researcher in the Center for Bioinformatics and Computational Biology. Supported through EPSCoR funding, Fly was mentored by Meghanathan (top) and Isokpehi (bottom), who are faculty researchers in the MS-EPSCoR program.

In earlier research, Meghanathan had proposed a binary coding scheme and an O(1) time algorithm to determine the ancestor-descendant relationships between any two nodes in a tree. The approach proposed by Meghanathan assigns a unique binary code to each node in the tree. The value of the binary code for a node is the concatenation of the code for its parent node (referred to as prefix) and the unique binary representation of the immediate children of the parent node (referred to as suffix). For any two node I and J, if the binary code of node I forms the prefix of the code of node J, then node I is the ancestor for node J; otherwise not.

In this research, Fly implemented the binary coding scheme and the algorithm for k-ary trees, a tree in which any leaf node has up to k children, as well as compared the performance of the coding scheme/algorithm with the classical post-order, pre-order and in-order traversal techniques for the k-ary trees. Researchers observe the binary coding scheme and the algorithm to be very efficient in determining ancestor-descendant relationships for k-ary trees. For example, the time taken to test for ancestor-descendant relationships between any two nodes (averaged over 1000 potential pairs of nodes) in a 5-ary tree increased only from 3.6 ms to 82.4 ms as the number of nodes in the trees was increased from 500 to 50,000. On the other hand, the time incurred with the tree-traversal algorithms increased from 12.5 ms to 59,000 ms; the three traversal techniques incurred almost the same time.

Fly graduated with a BS degree in Computer Science from JSU during Spring, 2011 and he is currently pursuing a Ph.D in Biomedical Sciences at the University of Michigan.

Meghanathan and Isokpehi are associate professors in the Departments of Computer Science and Biology at JSU.

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University of Mississippi's Computational Chemistry researchers, Nathan Hammer, Gregory Tschumper, Randy Wadkins, and Robert Doerksen, directed the third annual Ole Miss Physical Chemistry Summer Research Program at UM. Thirty physical chemistry students met over the summer for organized lectures, mini-courses, and social activities.