

NSF CREST  
 Computational Center for Molecular Structure and Interactions  
 Jackson State University, Department of  
 Chemistry

## JSU Hosts the 12th Annual Conference on Current Trends in Computational Chemistry

### Special Points of Interests

- Jackson State University hosts the 12th CCTCC Conference.
- Reflections on guest speakers
- Conference Participant WINNERS
- 12th Conference group photograph
- Upcoming events

For the twelfth year, Jackson State University, along with the National Science Foundation, the U.S. Army Engineer Research Development Center, Army High Performance Computing Research Center, and Parallel Quantum Solutions, assembled at the illustrious Hilton Hotel of Jackson for the 12th Annual Conference on *Current Trends in Computational Chemistry*. The Conference was held on October 31-November 1, 2003. Over 189 participants from various states and countries attended this conference. The scientific program of the 12<sup>th</sup> CCTCC blended together the development and broad applications of computational methods.

Three poster sessions consisting of over 133 presentations gave examples of research topics reflecting current computational chemistry methods. The poster presentations allowed informal interactions among all of the participants, including professors and scientists. This year there were 10 headed by 13 invited speakers including Dr. Ernest Davidson, from the University of Washington, Dr. Donald E. Thompson, the Divisional Director of Human Resource Development at the National Science Foundation, and Dr. Isabella Karle, this year's Nobel lecture speaker.



Dr. Ernest Davidson  
 University of Washing-

## 12th CCTCC Conference Speakers

On Friday morning, Dr. Ernest Davidson, from the University of Washington, spoke on the topic "*Radicals and Molecular Magnets*." Dr. Davidson currently serves as a professor of Chemistry at the University of Washington. On June 13, 2003, Dr. Davidson also served as recipient of the National Medal of Science presented by President George W. Bush. This national honor recognizes Dr. Davidson as having made significant and lasting contributions to the research and "persona of "Science".



Dr. Donald E. Thompson  
 National Science Founda-

The banquet talk was given by Dr. Donald E. Thompson. Dr. Thompson has spent twenty-five

years in higher education as a professor of education and urban planning. Dr. Thompson's motivational talk was directed to the students and future chemists of the 21st century. He encouraged and challenged his listeners in three ways:

- To think globally about science by focusing on the science realm outside of their own university or educational institution.
- To continue to engage in relationships with scientists who could serve as their mentors.
- To **not** think "outside" of the box, but to create one's own "box" by experiencing the world of science.

On Saturday evening, Dr. Isabella Karle, a recipient of numerous awards including the National Medal of Science, gave a talk on the topic "*Women in Science and Technology*". She shared a "fast tour" of several women

throughout the centuries that were influential in science and engineering. Some of the women discussed were Marie Meudrac, Mary Engle Pennington, and Hedy Lamarr. These women participated in history at a time when their presence was sparse in science and engineering. Dr. Karle also expressed the need to remember women such as Dr. Rosalind Franklin who Dr. Karle referred to as "the forgotten women of the Nobel Prize".



Dr. Isabella Karle  
 Naval Research

Tamara Taylor  
 Editor-in-Chief

Teri Robinson  
 Contributing Writer

### CCMSI SEMINAR SCHEDULE Fall 2003

09/05/03	Reeshemah Allen
09/26/03	Julia Saloni
10/03/03	Dalephine Davis
10/10/03	Olexandr Isayev
10/17/03	Dr. Manoj Shukla
10/24/03	Dr. Bakhtiyor Rasuliev
11/07/03	Dr. Blake Hill
11/14/03	Dr. David Magers
11/21/03	Teri Robinson
12/05/03	Dr. Jiande Gu

12<sup>th</sup> CCTCC Student Winners

On Saturday evening, students received certificates and awards for their outstanding research accomplishments. Among them were Teri Robinson and Jaroslaw Szymczak, both of Jackson State University; Lonnie Crosby, University of Memphis; Pornpun Rattananakin, Mississippi State University; and Danielle Hudson, Tuskegee University.

First place winner Teri Robinson presented on the topic "*Theoretical Study of Dihydrogen Bonded Complexes*

*[X<sub>3</sub>CH...HLi; X=H,F,Cl]*". Jaroslaw Szymczak, second place recipient, presented work on the "*Molecular Structures and Nature of Interactions in OCH<sup>+</sup>(Ne)<sub>n</sub>(n=1-17) Complexes*".

The third place awarded Rattananakin, Hudson and Crosby. Rattananakin, a second year graduate student, presented on the topic "*Ab Initio Study of the Rotation around the C=C Bond in Push-Pull Systems*".

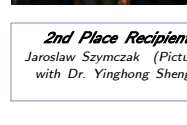
The sole undergraduate award recipient, Danielle

Hudson, gave an impressive poster presentation on "*Molecular Modeling of Helium Diffusion in Isometric Poly imides*" and Lonnie Crosby, from the University of Memphis, presented on the topic "*Study of Amorphous Silicon Dioxide Clusters for Use in an Additive Polarizability Model*".

All winners deemed their 12th CCTCC experience "exciting and enlightening"



**1st Place Recipient**  
Teri Robinson (Pictured with Drs. Abdul Mohamed and Jerzy Leszczynski)



**2nd Place Recipient**  
Jaroslaw Szymczak (Pictured with Dr. Yinghong Sheng)



**3rd Place Recipient**  
Lonnie Crosby (Pictured with Drs. Peter Pulay and Jerzy)



**3rd Place Recipient**  
Danielle Hudson (Pictured with Dr. Jerzy Leszczynski)



Group Photo

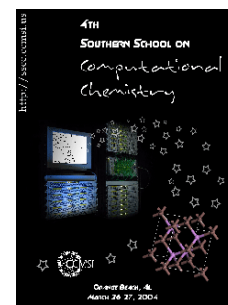


Group Photo

## Upcoming Events

4<sup>th</sup> Southern School on Computational Chemistry

You are invited to participate in the 4<sup>th</sup> Southern School on Computational Chemistry, organized together by the members of the NSF-EPSCOR Computational Chemistry Cluster, NSF-CREST Computational Center for Molecular Structures and Interactions, and the Army High Performance Computing Research Center. This conference will be held on March 26-27, 2004, in Orange Beach, Alabama. For more information, visit our website at [SSCC@ccmsi.us](mailto:SSCC@ccmsi.us).



## Summer Research Program 2004

The Computational Center for Molecular Structure and Interactions (CCMSI) summer institute will be held at Jackson State University from June through August 2004. This program is open to all graduate and undergraduate students interested in Computational Chemistry. The institute will also offer summer appointments to 2-3 faculty members. The objective of the Institute is to teach quantum and computational chemistry as well as general research skills. The format consists of formal lectures, group/team sessions and one-on-one mentoring.

For more information, contact Ms. Tracyle Lewis (Program Coordinator) at (601) 979-7824 or [tslewis@ccmsi.us](mailto:tslewis@ccmsi.us) or Tamara Taylor (Recruitment Coordinator) at (601) 540-1846 or [Tamara@ccmsi.us](mailto:Tamara@ccmsi.us).

