



Computational Center for Molecular Structures and Interactions

Jackson State University, Department of Chemistry
STUDENT HIGHLIGHTS

Graduate and Undergraduate Summer Internships and Research

Special points of interest:

- Jackson State University awards two Doctorate Degrees. (photos only)
- Graduate and Undergraduate students reflect on their summer research opportunities.
- 12th Annual CCTCC Conference
- CCMSI 2003 Summer Institute Winners and overview

This summer three students participated in summer internship opportunities. Ms. Angela Fortner, an undergraduate student, was offered an internship opportunity at the California Institute of Technology located in Pasadena, California with Dr. C. Patrick Collier. Ms. Fortner's summer research focused on creating a viable system for studying protein translocation of fluorophore-labeled oligonucleotides by using a technique called fluorescence resonance energy transfer. The Ph.D. graduate students, Ms. Tomekia Simeon and Ms. Teri Robinson

The Summer Institute hosted students from all over the world. There was a total of twenty-three partici-

also received appointments for summer graduate opportunities. Ms. Simeon, a graduate of Tougaloo College, was employed with the Wright-Patterson Air Force Base in Ohio, where her mentor was Dr. J.P. Blaudeau. Her research focused on the study of platinum containing oligomers and polymers. This research is important because polymeric materials have a vast potential for exciting new applications due to their interesting optical and nonlinear optical properties. Ms. Teri Robinson, a graduate of Jackson State University, received an appointment to work at the NASA-Ames Research Center in Mountain View, California where her mentor was Dr. Galina Chaban. Her research focused on studying the reaction paths of proton transfer in adenine.

Jackson State University



Dr. Glake Hill, Jr.
Department of Chemis-



Dr. Gareth Forde
Dept. of Environmental Sci-

CCMSI News

12th Annual CCTCC Conference

* * * * *

The 12th Annual Current Trends in Computational Chemistry Conference will be held on October 31, 2003-November 1, 2003 at the Hilton in Jackson.



Teri Robinson
Jackson, MS, USA
Graduate



Tomekia Simeon
Jackson, MS, USA
Graduate



Angela Fortner
Jackson, MS, USA
Undergraduate

on the relative energetics and geometry change upon adenine's complexation with water.

CCMSI Summer Institute Highlights

CCMSI Summer Institute Highlights

This year, Jackson State University and the Chemistry Department hosted visiting faculty and students from various schools and universities. The students and faculty were from Fayetteville State University, Tennessee State, University of Zululand of South Africa, Southern University in Baton Rouge, LA, Universidad Metropolitana, Texas Southern University, Albany State University, Tougaloo College, Fort Valley State University, Hampton University, Mississippi State University,

Norfolk State University, Charles University at Prague, Wroclaw University of Technology, and Dnepropetrovsk National University of Ukraine. These summer's participants came from many parts of the world to partake in educational research in the area of Computational Chemistry for the duration of eight weeks. Dr. Andrzej Sadlej, from Nicolaus Copernicus University in Torun, Poland, was the head professor that gave daily lectures. Dr. Andrzej Sokalski, from Wroclaw University of Tech-

nology in Wroclaw, Poland, was also a Summer Institute professor. The institutes main focus is the development of efficient computational technologies and applications of modern methods of computational chemistry, investigations of molecular structures, properties, and interactions. Nightly lectures were given by Anna Kaczmarek, of Torun, Poland, and Robert Zalesny, from Wroclaw, Poland. After morning lectures, each participant met with their mentor and discussed their research topic, of which they had to present at the closing ceremony held in Orange Beach, Alabama.

2003 CCMSI Summer Participant Winners

All of the summer participants applied and were recommended by a professor or instructor from their home institutions to be apart of such a wonderful summer experience. The morning and evening lectures consisted of topics of Mathematical objectives, theoretical models, and other computational chemistry topics. Each student worked diligently in preparing an oral presentation of his or her own research topic. After demonstrating their topics at the

Closing Ceremony, the students were reviewed and evaluated by professors and mentors. Each student did a superior job in presenting their work, however, only the top three students were delegated as winners. The winners were awarded certificates and an opportunity to go to Prague, Czech Republic, Europe to present their work. The First Place winner, Daniel Grant, of Albany State University, researched on the topic, *Interactions between Hy-*

drated Barium and Methylated Guanine-Cytosine Watson-Crick DNA Base Pair. His mentor was Gareth Forde. There were two Second Place recipients. In Second Place, Christina Washington, of Fort Valley State University, researched on the topic, *Aromatic Interactions.* Lastly, in Second Place, Jason Ford-Green, from Florida A & M University, research topic was *Insight into weak SiO₂ surface interactions.* Dr. Glake Hill, Jr. was both Christina and Jason's mentor.

CCMSI Summer HONORABLE Mention

After awarding the top three winners, there were several of other presentations that deserved recognition. **Honorable Mention Certificates** were given out to five summer participants. Arnaldo M. Porrata, of the Universidad of Metropolitan in Pruetto Rico, gave a presentation on *Conformational Study of Cyclopentadecane.* His mentors were graduate students, Dalephine Cain-Davis and Judge Brown. Carolyn Cummings, of Tennessee State University, gave

a presentation on *Proton Transfers.* Her mentor was Dr. Glake Hill, Jr. Anu Bamgbelu, of Norfolk State University, presented on the topic of *The Comparative Study of Excitation Energies of Conjugated Polymer Material.* Her mentor was graduate student, Jaroslaw Szymczak. Marcus Harris, of Dillard University, gave a presentation on *A DFT Study of the Water-Assisted.* His mentor was graduate student, Reeshemah Allen. Lastly, Pornpun Rattanankin, of Mississippi State University, presented

Ab Initio Study of the Rotation Around the C=C Bond in Push-Pull Systems. Her mentor was Dr. Yezgeniy Podolyan.



Winners



Daniel J. Grant
Albany State University
1st Place Winner



Christina Washington
Fort Valley State University
2nd Place Winner



Jason Ford-Green
Florida A & M University
2nd Place Winner