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## CCT Weekly July 17- July 23, 2011

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### LSU Associate Professor Theda Daniels-Race Researches Non-Traditional Energy

After the BP oil spill and with the economic and political demands to lessen dependence on fossil fuels, Louisiana is actively supporting research toward the development of alternative energy.

Theda Daniels-Race, associate professor of the LSU Department of Electrical and Computer Engineering and the Center for Computation & Technology, has received \$147,194 from the Louisiana Board of Regents to discover how combinations of new hybrid materials can be used in non-traditional means of energy production, transmission, and storage. Daniels-Race's proposal titled, "Nanoscale Electronic Characterization of Hybrid Electronic Materials," was funded for a three-year period.

"As the words alternative energy can be applied to a broad range of engineering technologies, in this work we will investigate the basic science behind these potential applications from a very fundamental electronic materials perspective—that is, at the molecular/nanoparticle level. In this way, we not only have the opportunity to observe new science, but we will be able to learn about, and therefore exploit, the fundamental physicochemical properties needed to engineer hybrid materials and their functions in alternative energy processes," said Daniels-Race.

A new form of hybrid electronic materials (HEMs), known as GUMBOS, or a Group of Uniform Materials Based on Organic Salts, will be investigated. GUMBOS were recently discovered by LSU Vice Chancellor Isiah M. Warner of the Office of Strategic Initiatives, Boyd Professor and Philip W. West Professor of Analytical & Environmental Chemistry. They represent a first in that they are a new nanomaterial composed of ionic liquid species in the frozen state.

"What is different about GUMBOS," said Daniels-Race "is that, unlike traditional ionic liquids which have melting points less than 100 degrees Celsius, GUMBOS can be synthesized to exist in the solid-state as nanoparticles in the 25 to 250 degrees Celsius range. As designer nanoparticles, their properties can be tailored to meet a host of applications in areas ranging from energy to biomedical functions to environmental uses. GUMBOS provide the prospect of utilizing new science with the objective of addressing fundamental alternative energy needs of efficiency, lower production costs, and materials-to-device engineering and development."

Daniels-Race will work with Warner and his group, who will provide the GUMBOS needed for the research.

"We believe that in this study of HEMs for alternative energy applications we combine the discovery of new materials with exciting engineering developments in an area of urgent national interest," said Daniels-Race. "As conventional and highly developed electronic materials, such as silicon, reach their predictable limits, and the nation's focus upon alternative means of energy production increases, this investigation stands well-poised to meet the academic and practical demands for new discoveries."

For more information on this and other research at the LSU Center for Computation & Technology, visit: <http://www.cct.lsu.edu/home>

### CCT Spotlight: Joel E. Tohline

Joel E. Tohline, CCT Director, is a native Louisianan, born in Crowley. He has lived in seven different cities across the state, so he considers all of Louisiana his hometown.

Joel's primary research focus is on numerical simulations of fluid flows that arise when the two components of a binary star system exchange matter with one another. He is also interested in many aspects of high-performance computing and scientific visualization.

"From a very young age, I was fascinated by astronomy and NASA's space program (I was in high school when Armstrong & Aldrin walked on the moon) and I enjoyed mathematics. When I realized that research in astrophysics involved applied mathematics, I began to pursue physics & astronomy as a career. I was also fortunate to have had the opportunity to learn how to write a fortran program before I entered college; the timing was good because the college I attended acquired its first computer (and IBM 1130) shortly after I arrived and I was allowed to play with it at night. Computer programming was as fun for me as mathematics, so I coupled both tools with my scientific interests in astrophysics ... and here I am," said Joel.

For fun, Joel enjoys taking road trips with his wife, their favorite destinations being national parks and Walt Disney World. His favorite gadget is his big screen, HD tv that he watches college football games on and his favorite movies, "2001 Space Odyssey," "Pulp Fiction," and "Billy Elliot."

Joel also spends his free time developing and analyzing mathematical models of astrophysical systems, especially showing the overlap between complex numerical models and simpler models that have analytic mathematical solutions.

### Pats on the back:

- Theda Daniels-Race received an award from the Board of Regents titled "Hybrid Electronic Materials for Energy/Aerospace Applications." The award is for \$30,000 for one year.
- Thanks to everyone involved in the Stop Motion Animation Summer Camp & the Petascale Programming Environments & Tools course last week!

### CCT in the news:

**Seats available in summer course on many-core processors**

Source: [NCSA](#)

### Please Note:

- LSU CCT will host two onsite computational science courses being offered by the Virtual School of Computational Science and Engineering. The second course is "Proven Algorithmic Techniques for Many-core Processors" (August 15-19). Graduate students, post-docs and professionals from academia, government and industry can gain the skills they need to leverage the power of cutting-edge

computational resources at these courses, which are being offered for a \$100 per-course fee. Each course is one week long. For more information, visit <http://www.vscse.org/>.

- CCT is sponsoring a 1-day workshop on CUDA programming. This workshop should be of interest to anyone interested in developing programs to run on GPGPUs. It will be offered on July 28th from 9am - 5pm in 338 Johnston. If you are interested, please register on the HPC Training page at: <http://www.hpc.lsu.edu/training/index.php>. Schedule and a registration link are near the bottom of the page.
- The 2011 HPC User Satisfaction Survey is open for comment until August 31st. Anyone who uses high performance computing resources at LSU or LONI is invited to take a few minutes to complete the survey: [http://www.hpc.lsu.edu/survey/public/survey.php?name=hpc\\_at\\_lsu\\_user\\_2011](http://www.hpc.lsu.edu/survey/public/survey.php?name=hpc_at_lsu_user_2011). Please help us understand your needs and future requirements.
- The LSU Center for Computation & Technology will host for the first time the LSU iOS Application Boot Camp August 1-12 (10 day camp; not including weekends) on the LSU Campus. This new educational experience offers LSU undergraduates the opportunity to gain knowledge while enhancing their entrepreneurial spirit. Participants will work in groups to create their own operating App and have it loaded on their personal device by end of camp. Registration fee is \$300. For more info and to register, visit <http://www.cct.lsu.edu/iosbootcamp>.
- Applications for the SC11 Student Volunteer Program are open and close on August 12, 2011. Undergraduate and graduate students are encouraged to apply as volunteers to help with the administration of the conference. In exchange for volunteering, they will receive complimentary conference registration, housing, and most meals. In addition, limited support will be provided for transportation expenses (such as airfare) for international students and students from groups that traditionally have been underrepresented in HPC. For more information visit <http://sc11.supercomputing.org/?pg=studvol.html> or email [student-vols@info.supercomputing.org](mailto:student-vols@info.supercomputing.org).
- Prior approval is required for Special Meal Requests. Employees who make meal purchases without prior approvals may find that they must cover the cost of any monies spent for an unapproved event out of pocket, especially now that state funds are under a spending freeze. Please contact Susie McGlone ([susie@cct.lsu.edu](mailto:susie@cct.lsu.edu)) prior to any special meal with visitor(s) to file the appropriate request for approval. Prior approval could take up to two weeks, so please plan accordingly.
- Please remember to send your news concerning grants, awards, conferences, or other pertinent information to CCT Event Coordinator Jennifer Fontenot at [jennifer@cct.lsu.edu](mailto:jennifer@cct.lsu.edu)
- Follow CCT with social media to access photos and see news, events or updated information. These pages are public; you do not need an account to view the information.
  - o [Facebook group](#) : LSU Center for Computation & Technology
  - o [Twitter](#) : LSUCCT
  - o [YouTube channel](#) : LSUCCT

#### Upcoming events:

**May 30- July 29:** [NSF Research Experience for Undergraduates](#)  
**July 18-22:** [Alice in Computation Land Summer Camp](#)  
**July 23- 27:** [Workshop of Density Functional Theory](#)  
**July 31- Aug 6:** [Computational Thinking from a Parallel Perspective](#)  
**August 1- 12:** [iOS Boot Camp for LSU Undergraduates](#)  
**August 9-11:** [SIGGRAPH](#) (Booth #841), Vancouver, Canada  
**August 15-19:** [Proven Algorithmic Techniques for Many-core Processors](#)

#### Upcoming Grant Deadlines:

**Note:** Please check the [CCT deadline Web site](#), since it is updated daily.

[Faculty Early Career Development \(CAREER\) Program](#)

July 23, 2011 10:00 am

At Least \$ 400,000.00 available

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