

CHEMICAL AND BIOMOLECULAR ENGINEERING

E-NEWSLETTER

FALL 2009

Leadership Changes in ChBE



There were several leadership changes in Chemical and Biomolecular Engineering over the summer. After nine years of dedicated service to the Department, Prof. Jim Goodwin stepped down as Department Chair. Under his leadership the Department was reshaped in numerous areas: the undergraduate curriculum was modified to provide more flexibility, including emphasis areas of study and a biomolecular engineering track; the graduate program is now composed almost exclusively of Ph.D. students; the research expenditures per faculty rank as one of the highest in the College of Engineering and Science and the University; and the high-bay area in Earle Hall has been totally renovated to add improved space for research and the Unit Operations Laboratories. Research expenditures, peer reviewed papers published, and Ph.D. students

graduated per faculty all rank the Department in the top 20-30 graduate programs in chemical engineering in the U.S. Jim will now devote more of his time to teaching and research and continue serving as the editor of the internationally renowned scientific journal *Catalysis Communications*.



Prof. Doug Hirt was appointed as Interim Department Chair. Doug, now in his 20th year at Clemson, has been active in the teaching and research missions of the Department. Over the last decade he has been heavily involved in Clemson's NSF Center for Advanced Engineering Fibers and Films (CAEFF), having served as Research Thrust Leader, Deputy Director, and for the past 2+ years as Director where he shaped the general overhaul of CAEFF operations, including reprioritizing research focus areas to match promising opportunities for funding and collaboration, facilitating equipment purchases to create an enabling infrastructure, revamping the industry partner agreement to encourage more company members, and ensuring that CAEFF research continued to be integrated in education programs. Doug stepped down as CAEFF Director to concentrate

on his new duties. A search for the permanent Chair will begin in the near future.

Dr. Amod Ogale, Professor of Chemical and Biomolecular Engineering, was subsequently appointed as CAEFF Director after serving as Research Thrust Leader and Deputy Director. Amod was primarily responsible for industrial relations and overseeing all facilities and infrastructure in the Center, which are now housed primarily in Earle Hall. He has been on the faculty for 23 years and is known internationally for his work on novel routes for processing of structural fibers, films, and nanocomposites. Amod's current research involves rheology, microstructure, and processing of liquid ...continued...





crystalline polymers and carbon fiber precursors for ultrahigh thermal conductivity carbon fibers. For ultra-low conductivity carbon fibers, his group is developing a novel ultraviolet radiation-based stabilization process for polyacrylonitrile precursor fibers. Amod's research group has pioneered the use of real-time Raman spectroscopy for measurement of crystallinity and molecular orientation of polymeric blown films. He serves on the editorial review board of two journals and the Advisory Board of American Carbon Society, and is the International Councilor for the Electrical & Electronics Division of Society of Plastics Engineers. Together with Mark Thies, Amod is co-organizing CARBON 2010, the Annual World Conference on Carbon, to be held in Clemson July 2010.

FOCUS ON PEOPLE

Clemson Researcher Teams up Internationally with Marie Curie Fellowship



Professor Mark Thies in Athens, Greece

ChBE professor Mark Thies has received a Marie Curie Fellowship for \$142,000 to develop molecular models for advanced-carbon materials that have the potential to be used in strong, yet lightweight transportation vehicles, wind, turbines and more energy-efficient aircraft.

Mark was one of 22 international researchers to be selected for the award by the European Union. These fellowships are designed to encourage collaboration between European and internationally recognized researchers. The award has enabled Mark to work with Doros Theodorou of the National Technical University of Athens in Greece.

"The complexity of today's research problems requires not only interdisciplinary, but even international teams such as the one we are now forming," said Thies. "By combining our expertise in

The research by Mark and his graduate students at Clemson, currently funded by both the Air Force and the American Chemical Society, has focused on the synthesis of carbonaceous pitches of novel composition. Such pitches can serve as unique starting materials for high-performance carbon fibers and carbon-carbon composites.

Mark returned to Clemson in August after spending a year on sabbatical working with Dr. Theodorou in Greece.

- Feature by Susan Polowczuk (CU News Services)

Clemson Student Receives "Best Student Presentation Award" by AIChE Nuclear Engineering Division

Each year the AIChE Nuclear Engineering Division (NED) presents an award for best student presentation. This year, the winner of the 2009 NED Outstanding Student Presentation Award was our own Sarah Mena. Her talk entitled "Sulfur-Iodine Cycle: Phase Equilibrium Data for the Ternary Iodine-Water-HI and the Binary Iodine-Water Systems" was given in the Advances in Thermochemical Hydrogen Production Session at the AIChE Annual Meeting in Nashville. She received a \$500 scholarship for first prize.

Sarah is an M.S. student working under the guidance of Prof. Mark Thies. Congratulations Sarah!!!





FOCUS ON EDUCATION

ChBE Students Take Unit Ops Lab in Vienna

For the past eight years, a growing number of our undergraduates have been taking the senior-level unit operations lab in Vienna, Austria. Our connection with the Vienna Summer Program came about through the College of Engineering and Science's membership in the Global E3 Engineering Education Consortium. The UO lab program



was originally started in 2001 by the University of Wisconsin and Technische Universität Wien (TU Vienna), both members of Global E3, to develop a summer UO lab that provided an international experience for U.S. ChE students. In 2002 TU Vienna invited other U.S. schools to participate, and we took steps to have the program approved as a substitute for our Clemson UO lab (ChE 407), and began recruiting students. We ended up with 10 students that first year, and Clemson has been a co-partner with Wisconsin on the U.S. side ever since. In subsequent years we have had 2 (2003), 7 (2004), 4 (2005), 5 (2006), 6 (2007), 9 (2008), and 9 (2009) student participants.

The program is an outstanding opportunity for our students. TU Vienna is recognized as a top European ChE program, Vienna is a great, central location in Europe for gaining valuable international experience, and the program "off-loads" the demanding senior lab from their fall senior schedule. We have assessed the lab as being of very high quality academically and providing an academically rigorous laboratory experience with excellent lab facilities and meeting our expectations for high emphasis on developing communication skills. From the very first year, the feedback from our students has been overwhelmingly positive in all respects. Finally, it is worth noting that the Vienna Summer School has become one of the larger and more consistently well subscribed international programs offered to its students by the College of Engineering and Science, as well as being the major opportunity for chemical engineering students to gain an invaluable edge in the job market by having an international experience on their resume.

~Feature by Professor Emeritus Steve Melsheimer





Clemson flexes some computational muscle

Good news for students and researchers in ChBE

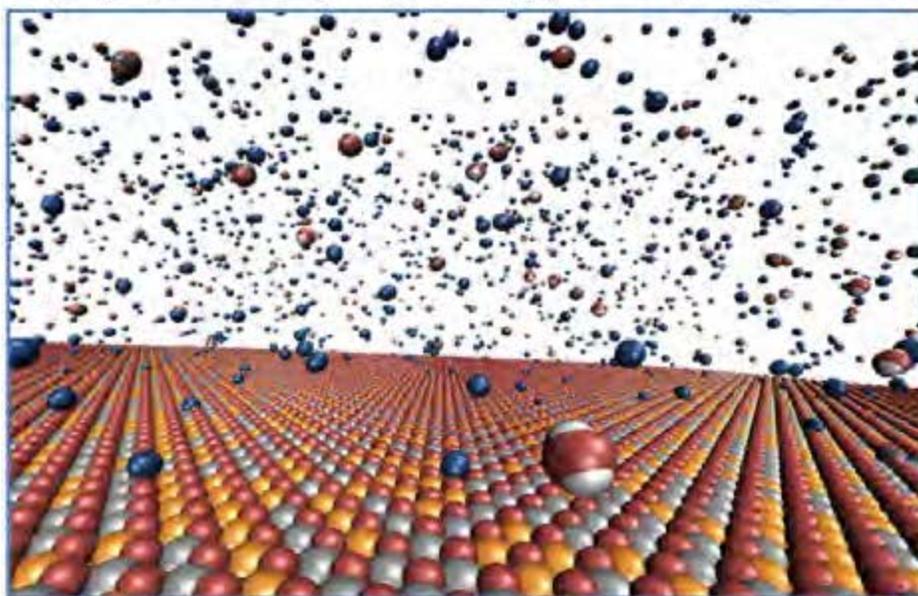
by Jay McAiley, Ph.D.
Postdoctoral Fellow
jmcail@clermson.edu

Our alumni may already be aware of the buzz that's been going around regarding Clemson computing. In recent years, under the direction of Vice Provost and Chief Information Officer Jim Bottum, Clemson computing facilities have undergone some pretty vast improvements. Following the arrival of Bottum in 2006, the newly restructured Clemson Computing and Information Technology (CCIT) division has beefed up its operations on all fronts. Improvements range from Clemson's new blazing fast network infrastructure to our state-of-the-art classroom technology and campus computer labs. Additionally, CCIT now meets many of the College of Engineering and Science's special computing needs, which were previously only supported internally within our College.

Those of us engaged in research pursuits especially enjoy access to Clemson's new high-performance supercomputer named Palmetto—the likes of which are unsurpassed by all but a few academic sites in the country. Boasting 120 trillion bytes (120 TByte) of data storage and 6,176 processor cores, Palmetto has an overall performance of 46 trillion floating-point operations per second (46 TFLOPS). From a Clemson historical perspective, that's at least 50 million times faster than the IBM System/360 model that crunched numbers in the basement of the P & A building while my dad was a ChE freshman (rat cap and all) in 1965. At that time, the S/360 was absolutely cutting-edge. Today, Clemson not only continues its tradition of keeping up with computer technology, but is pushing forward as a leader among high-performance computing sites worldwide.



A row of servers in Clemson's Palmetto cluster. This supercomputer ranks #9 among academic sites in the U.S., and is #89 among all sites in the entire world. (For rankings, see TOP500.org)



Simulation of car exhaust gas adsorption on a metal oxide catalyst support, using the Palmetto supercomputer cluster.

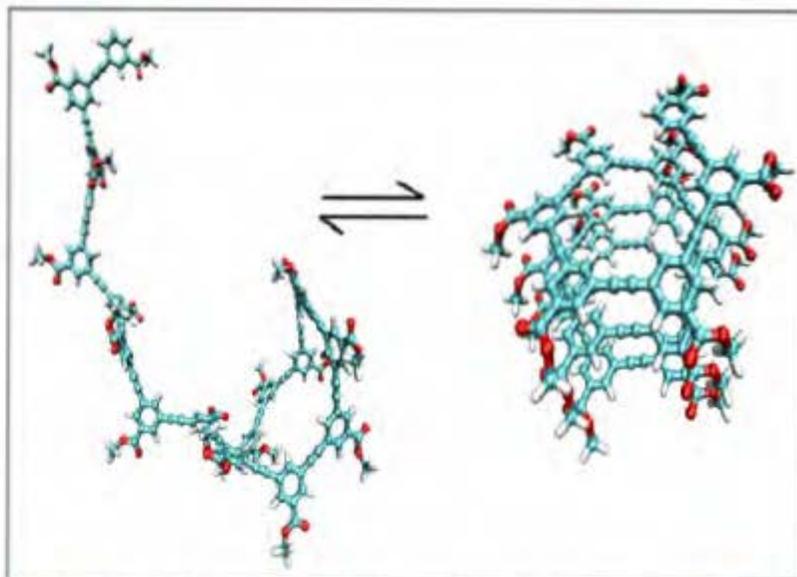
In the ChBE department, high-performance computer simulation plays an important role in both curriculum and research. Our undergraduate students are trained extensively to use industry-leading process simulation software such as Aspen Plus®, while our research groups are utilizing a number of simulation techniques—ranging from macroscopic flow solvers to meso-scale simulations, classical molecular modeling, and quantum mechanics solvers. The applications of such techniques are quite varied, ranging from chemical and materials processing to drug design.

...continued...



Currently, notable computational research in ChBE includes the Center for Atomic-Level Catalyst Design (CALCD), in which Associate Professor David Bruce serves as coordinator of simulation efforts. This Department of Energy-funded research center aims to improve the cost effectiveness of biofuel production, by examining the activity of new catalytic materials through molecular simulation. Additionally, Dr. Bruce advises several graduate students on their computational research, including PhD candidate Ha Nguyen's investigation of secondary structure in novel synthetic polymers, and my recent dissertation work on developing molecular models to study polylactic acid (PLA). Ha's work, funded by the National Science Foundation, utilizes

molecular dynamics (MD) simulation to predict the performance of helical polymers as catalyst supports. In my own dissertation research, I examined PLA—a biodegradable plastic derived from corn—using quantum mechanics solvers and MD simulation. My work was supported by the Center for Advanced Engineering Fibers and Films (CAEFF), and the resulting model will be used to predict protein-surface interactions in biological devices containing PLA films or fibers, among other applications. Other ongoing efforts in our department include Professor Mark Thies' recent work on simulating phase equilibria in advanced carbon materials, which he will continue under his recently awarded Marie Curie Fellowship. Dr. Thies' simulations will aid in developing high-performance engineering composites. All of the efforts discussed here benefit heavily from the support and infrastructure offered by CCIT.



Results from PhD candidate Ha Nguyen's simulation of a partially folded polyphenylene ethynylene (PPE) molecule (left-hand side); helical folded state shown at right.

Support Chemical and Biomolecular Engineering at Clemson University!

Please consider giving an end-of-year monetary gift to support the Department.

[Click Here](#) to make a gift.

IMPORTANT! After you complete personal contact information, you will be asked to designate where you want your gift applied. To support the department, simply scroll to the "Other" category at the bottom of the list and type ChBE in the space provided.

Or you may mail a check (made payable to the Clemson University Foundation) to:

Dr. Douglas Hirt
 Department of Chemical and Biomolecular Engineering
 Clemson University
 Box 340909
 Clemson, SC 29634-0909

Thanks in advance for your support!