


# TAKING AIM AT THE SUSTAINABLE ENERGY CHALLENGE

A large, detailed bronze sculpture of a Native American archer is the central focus. The archer is depicted in a dynamic, forward-leaning pose, holding a bow and arrow. The sculpture is set within a grand, vaulted hall with a high, arched ceiling made of glass and metal. In the background, a large, ornate clock face is visible on the wall. The overall atmosphere is one of historical grandeur and architectural detail.

THE UNIVERSITY of TENNESSEE 

DEPARTMENT OF CHEMICAL AND BIOMOLECULAR ENGINEERING 2008 ANNUAL REPORT

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CHEMICAL AND  
BIOMOLECULAR  
ENGINEERING 2008  
ANNUAL REPORT

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WRITER & EDITOR  
Kim Cowart  
Communications Director

DESIGN &  
PRODUCTION  
Mitchell Williamson  
Graphic Designer

WRITER  
L. Ashley Susong  
Communications Assistant

CONTRIBUTING  
PHOTOGRAPHERS  
Nick Myers,  
UT Photo Services  
Rip Noel,  
Rip Noel Studios  
L. Ashley Susong

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Cover photo of the sculpture of Heracles by Antoine Bourdelle  
at the Musee d'Orsay in Paris by Dr. Brian J. Edwards

“The high costs of energy and the associated phenomenon of global warming have already caused dramatic economic and environmental issues on an unprecedented scale. The only truly long-term solution to this problem is significant and continuous investment in the fundamental science and engineering of sustainable, cost efficient and environmentally friendly technologies for energy production and utilization.”

## Department Head's Message From Dr. Bamin Khomami

It has become readily apparent during the past year that the economies of the entire planet are correlated inextricably with the availability of an abundant supply of affordable energy. The high costs of energy and the associated phenomenon of global warming have already caused dramatic economic and environmental issues on an unprecedented scale. The only truly long-term solution to this problem is significant and continuous investment in the fundamental science and engineering of sustainable, cost efficient and environmentally friendly technologies for energy production and utilization. This is a herculean task facing humanity that must be addressed in the near future with a highly focused aim on the long-term target of sustainable energy research and development, as represented symbolically by the bronze statue of Heracles that adorns the cover of this report.

Here at the University of Tennessee, our department has taken the lead on campus to address the challenges of sustainable energy production through a number of new initiatives targeting various aspects of the overall solution. The Sustainable Energy Education and Research Center (SEERC) was instituted as of January 2008 to promote international leadership in this vital field of research, as well as to educate students with regard to the technological and social aspects of sustainable and environmentally friendly energy production and utilization. This center will serve as an interdisciplinary

hub of activity for researchers and educators from many departments and international scholars, as well as foster collaborations with the nearby Oak Ridge National Laboratory.

Our department was also the leader in obtaining a large, highly competitive Integrative Graduate Education and Research Training (IGERT) grant from the National Science Foundation to train the next generation of Ph.D. scientists and engineers in the frontier areas of sustainable energy production, storage and utilization. This award is to be used to implement the STAIR Program (Sustainable Technology through Advanced Interdisciplinary Research), which focuses on both fundamental research and curriculum development under the umbrella of renewable energy sources. You can learn more about each of these programs in the article featured in this report.

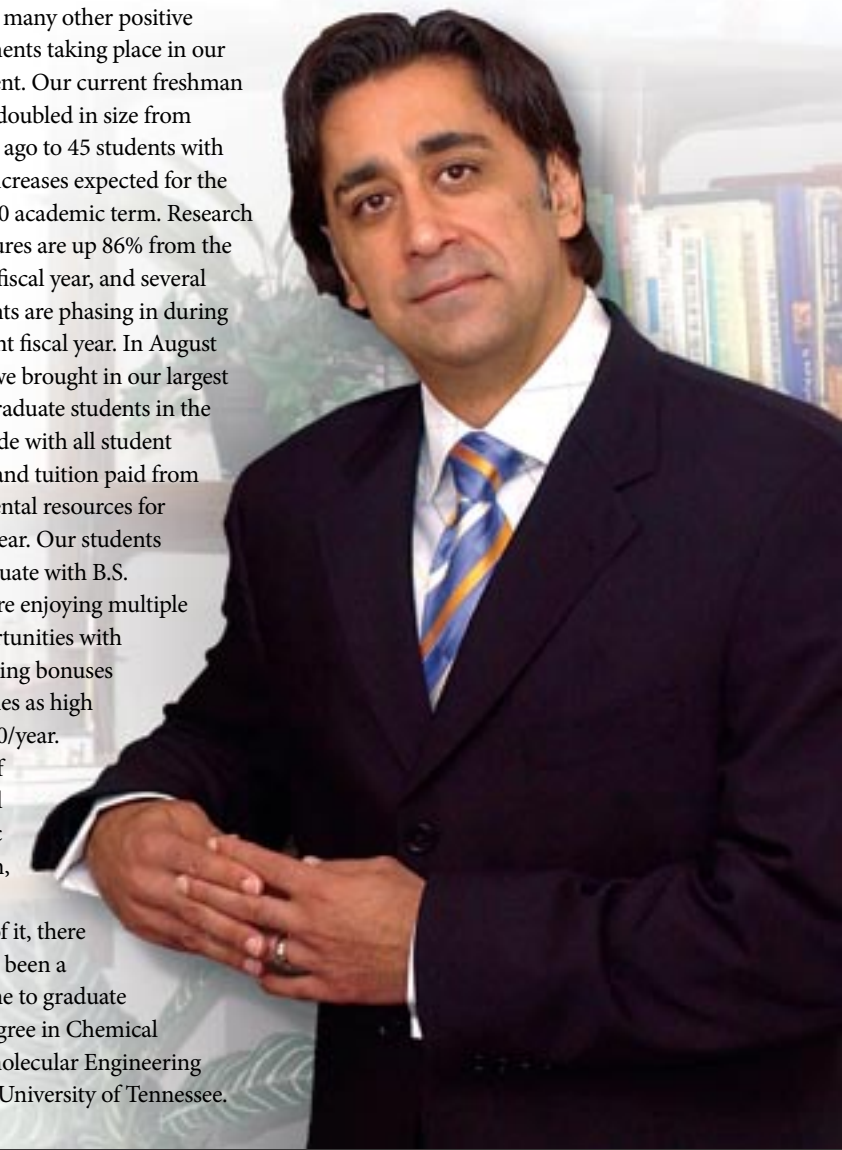
We have been very fortunate over the past two years to hire three outstanding mid-career associate professors in strategic areas of our departmental focus on sustainable energy technology. Drs. Eric Boder and Stephen Paddison were added to our faculty last year in the fields of biomolecular engineering and proton exchange fuel cell membranes. This year we complemented this expertise by attracting Dr. Ramki Kalyanaraman, whose research focuses on energetic beam processing and functional nanocomposites. An article on Ramki is

featured in this report. Current searches are ongoing to attract additional faculty members with complementary expertise to our department.

There are many other positive developments taking place in our department. Our current freshman class has doubled in size from two years ago to 45 students with further increases expected for the 2009-2010 academic term. Research expenditures are up 86% from the previous fiscal year, and several large grants are phasing in during the present fiscal year. In August of 2008, we brought in our largest class of graduate students in the past decade with all student stipends and tuition paid from departmental resources for the first year. Our students who graduate with B.S. degrees are enjoying multiple job opportunities with large signing bonuses and salaries as high as \$80,000/year. In spite of the global economic downturn, or maybe because of it, there has never been a better time to graduate with a degree in Chemical and Biomolecular Engineering from the University of Tennessee.

### Bamin Khomami

Armour T. Granger and Alvin & Sally Beaman  
Distinguished Professor and Head of  
Chemical and Biomolecular Engineering





One of the greatest challenges facing the 21<sup>st</sup> century is finding a solution for sustainable energy. Due to the confluence of a number of critical factors, the need to address this energy challenge has never been greater. The time to act is upon us, and the University of Tennessee is poised to meet the challenge head-on.

Because the energy outlook is highly uncertain, a multi-faceted approach examining technology and policy options must begin now. The Sustainable Energy Education and Research Center (SEERC) and the Sustainable Technology through Advanced Interdisciplinary Research (STAIR) Program are UT's response to the global energy challenge. Helmed by Dr. Bamin Khomami, SEERC aims to establish UT as a global hub for activities related to sustainable energy education, basic research and innovation by creating a world-renowned research center. The STAIR Program, under the direction of Dr. David Keffer, is a National Science Foundation (NSF) funded arm of the Integrative Graduate Education and Research Traineeship (IGERT) Program that endeavors to generate the next generation of highly skilled scientists, engineers and educators who will become creative agents for change.

These two initiatives complement each other; students in the STAIR

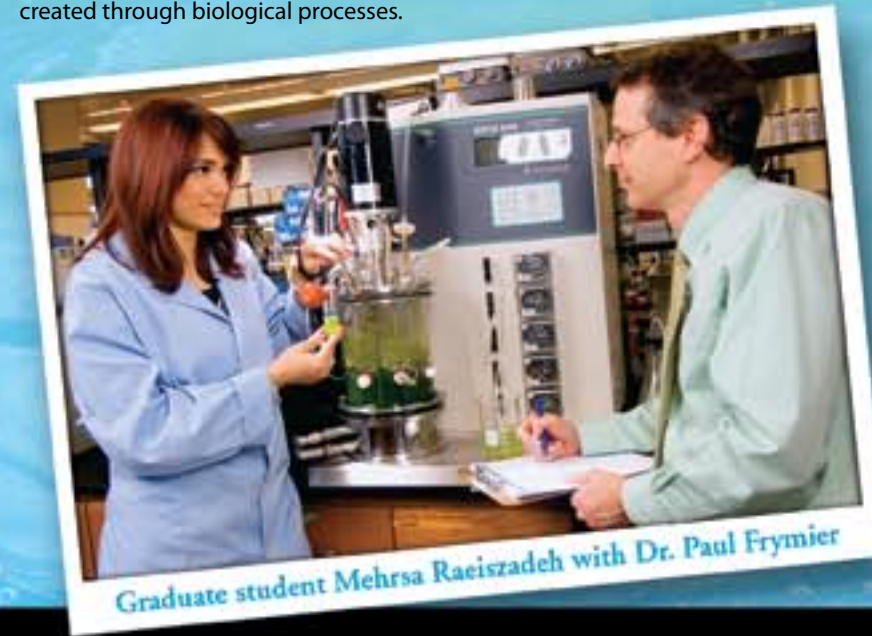
Program also perform research with the SEERC. Both programs place an emphasis on the necessity of an interdisciplinary approach to solving the energy crisis and departments from the College of Arts and Sciences as well as several disciplines across the College of Engineering are involved with both SEERC and STAIR.

Even the foci of these programs overlap. SEERC identified its three main research thrusts as bio fuels, fuel cells and advanced materials for energy applications. The latter category includes hydrogen storage through metal porphyrin frameworks and decorated carbon fullerenes; inorganic and organic photovoltaic materials and photocatalysts; and hybrid photovoltaic materials created through biological processes.

The STAIR Program places emphasis on biological production of hydrogen; discovery of nanoporous materials for hydrogen storage; and identifying structure/property relationships in hydrogen-based fuel cells.

Dr. Paul Frymier, associate professor in the Department of Chemical and Biomolecular Engineering (CBE), is working with Professor Barry Bruce on a project to measure the rates of electron transport in the photosynthetic complexes in cyanobacteria—otherwise known as the common blue-green algae.

"We use these photosystems to make hydrogen and are interested in improving the rate of hydrogen production," Frymier said.



Graduate student Mehrsa Raeeszadeh with Dr. Paul Frymier

"Knowing the rates of electron transport will tell us if this is a limiting step in the process of generating hydrogen and, more importantly, where we can best apply our effort to improve these rates."

Because cyanobacteria live in nearly every conceivable environment – from fish tanks to bare rock, soil to animal fur – a reliable means by which to produce sustainable energy from such an abundant source would be a triumph, not only for the researchers in the SEERC, but also for the entire human race.

Michelle Minton, a graduate student in the Department of Materials Science and Engineering (MSE) and IGERT fellow, participates in the STAIR Program and is developing a porphyrin framework to safely house hydrogen fuel. She works with Drs. Claudia Rawn in the MSE Department and Dr. David Keffer, associate professor in the CBE department. The cyanobacteria-based fuel that could possibly be developed in the SEERC could be housed in one of Minton's porphyrin chambers.

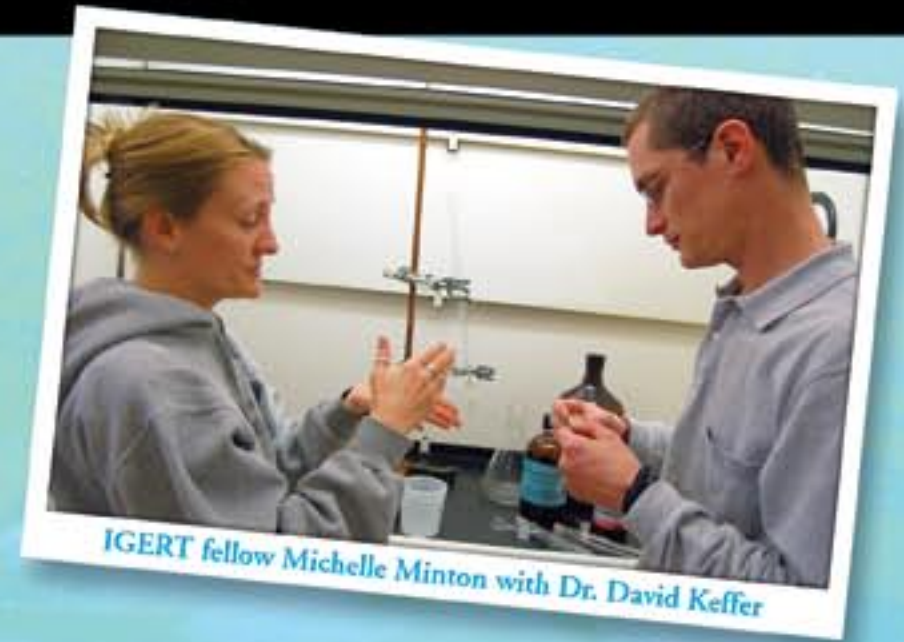
Part of the funding for Frymier's research in the SEERC is dependent upon the STAIR Program. He constructed a state-of-the-art instrument for making measurements of electron transport using laser flash photolysis. Frymier secured grants

from the Tennessee State Board of Architectural and Engineering Examiners (TSBAEE) and the NSF to help fund the research.

"Previously, we have only had qualitative evidence and data from a much less reliable system," said Frymier. "Our new machine should enable us to make decisions based on more quantitative information, which is when engineers are in their comfort zone. We look forward to our first paper incorporating these new data."

Funding for the SEERC-related work comes not only from the NSF and TSBAEE grants but also from the IGERT grant. Over the next five years, \$4 million will be devoted to helping UT faculty, Oak Ridge National Laboratory staff and many undergraduate and graduate students find a sustainable solution to the energy crisis. The creation of the STAIR Program will help recruit Ph.D. students to ensure a future generation of sustainable energy engineers.

The STAIR Program develops an integrated graduate curriculum at UT that is available to any graduate student in the participating departments who is interested in sustainable energy. By supporting a group of Ph.D. students, the STAIR Program also builds the long-term foundation for research success in



IGERT fellow Michelle Minton with Dr. David Keffer

sustainable energy at UT through the support of interdisciplinary collaborations.

"SEERC and STAIR bring a broader view of energy and sustainability to UT," Frymier commented. "They look at a broad array of technologies to not only deal with the long term solution but also with bridging technologies to get us to the future as sustainably as possible."

"As an engineer, I was trained to strive for the best solution, and usually the best solution is arrived at when many potential solutions are pursued," Frymier continued. "Fossil fuels were the 'one size fits all' solution to energy for many years, but the energy future

may not look the same; there may be many different solutions."

From America's reliance on foreign oil to the lack of resources in developing countries, there has never been a more pressing time to become involved with the race to replace our dependency on fossil fuels with truly sustainable energy. The Sustainable Energy Education and Research Center and the NSF-sponsored Sustainable Technology through Advanced Interdisciplinary Research Program are two ways the University of Tennessee College of Engineering is working to help solve this global problem.

Dr. Ramki Kalyanaraman is ready to demonstrate the power of two.

The new joint associate professor in the Department of Chemical and Biomolecular Engineering (CBE) and the Department of Materials Science and Engineering (MSE) is excited about the opportunity to increase multi-disciplinary research projects in both academic units.

"I would like to make this joint position a paradigm for future hires by being highly successful as a scientist and educator. Specifically, I want to clearly demonstrate through research and the training of our next generation of engineers and scientists that combining fundamentals from these two fields can provide novel materials solutions," Ramki said.

Ramki grew up in India, where his mother was an educator and his father was a pilot. He was intrigued by the technical aspects of his father's job, and his mother, a voracious reader, made sure that Ramki and his brother had access to all types of books at a very young age. Ramki particularly remembers Jules Verne's science fiction classic *20,000 Leagues Under the Sea* as a book that initiated his interest in understanding how things work.

Ramki received his M.Sc. and M.Tech from the Indian Institute of Technology in Kharagpur and Kanpur,

respectively. He was awarded his Ph.D. in Materials Science and Engineering in 1998 from North Carolina State University. He was previously an assistant professor at Washington University in St. Louis, Mo.

Ramki commented, "The long-term success in solving these problems will require close interactions between the development of new materials and cost-effective processing. I believe that a strong interaction between MSE

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**"I have a very friendly and open style of interacting with students, and my teaching method is to create an environment in which all students feel excited, responsible and, most importantly, engaged in classroom activities"**

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Ramki became interested in joining the University of Tennessee-Knoxville faculty after learning about UT's renewed emphasis on materials science and sustainable energy.

"The leadership of the CBE department, with support from the UT administration, has clearly indicated that the department is being positioned to lead in cutting-edge research for future energy needs,"

and CBE is essential for this success. Since my background in materials science and my interest in renewable energy coincides with this work, I am very excited to be a part of this initiative."

Advances in materials will require input from all forms of knowledge, Ramki added, and inter-disciplinary research is the best pathway.

Currently, he is focused on the science of pattern formation and self-organization for the creation of nanoscale materials. He hopes to take his conclusions and apply them toward new materials for energy harvesting, information processing and sensing.

In addition to his research efforts, Ramki also enjoys his teaching responsibilities.

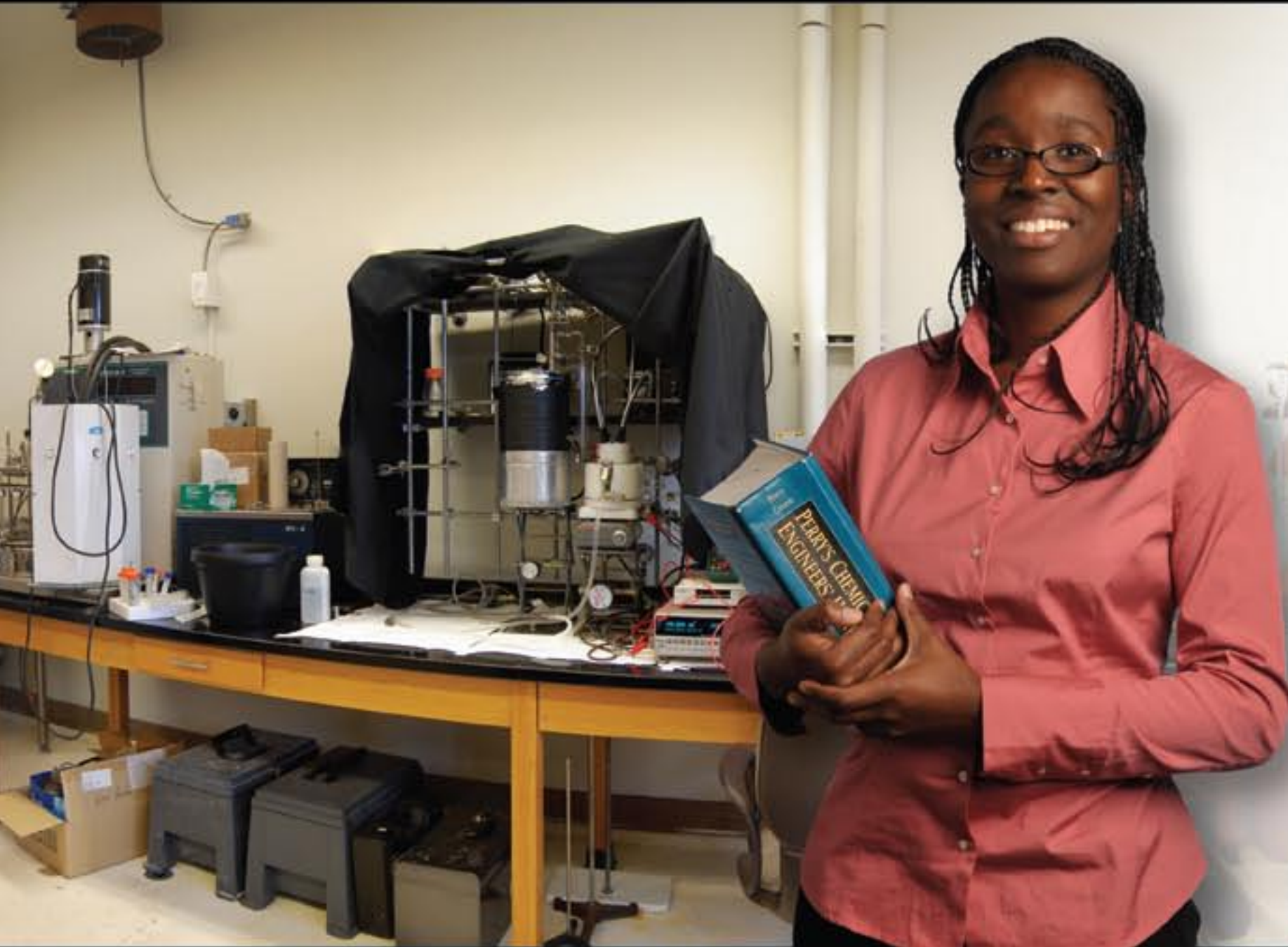
"I have a very friendly and open style of interacting with students, and my teaching method is to create an environment in which all students feel excited, responsible and, most importantly, engaged in classroom activities," he said.

Ramki and his wife, Veena, who also has a Ph.D. in engineering, are enjoying their new life in Knoxville with their son, Rohan, who is a year old.

Ramki hopes he won't remain the only joint faculty member between the two departments for much longer.

"I would love to see more joint faculty hires in the future," he said. "We also need to look at more joint graduate research in the next few years. Natural phenomena do not distinguish between different disciplines, so why should our man-made endeavors be any different?"





Ifeyinwa Iwuchukwu—Ifey, as she is known around campus—began her journey to the University of Tennessee's Ph.D. program in chemical and biomolecular engineering a long way from The Hill—six thousand miles, in fact: Ifey hails from Nigeria.

Ifey obtained her undergraduate degree in chemical engineering from Enugu State University of Science and Technology in Enugu, Nigeria. She was the only student who received First Class Honors in her graduating class and decided to continue her education in America.

Ifey found the University of Tennessee through the Internet, and she received her master's degree in chemical engineering from UT's Space Institute in Tullahoma, Tenn. Ifey then came to UTK to obtain her Ph.D. in chemical and biomolecular engineering under the direction of Dr. Paul Frymier.

"Ifey is a conscientious student and is very deliberate in the laboratory, which is necessary for experimental work," Frymier said. "She spent a lot of time at Oak Ridge National Laboratory this past summer and drove back and forth many times a week, often having to go late at night to check her equipment."

She is involved in the American Institute of Chemical Engineers (AIChE), the National Society of Black Engineers (NSBE), Society of Women Engineers

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**"I am trying to solve the world's energy crisis. I hope to re-engineer the components of photosynthesis in cyanobacteria as a possible solution to sustainable fuels production. I can do this in small spaces, on the lab scale for right now, but it can later be optimized on the global scale. It's very exciting work."**

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(SWE) and ORNL. She worked with a team of other students in Fall 2008's AIChE's ChemE Car competition under the direction of Frymier. Ifey is also involved with Frymier's research at the Sustainable Energy Education and Research Center (SEERC).

"I am trying to solve the world's energy crisis," she said. "I hope to re-engineer the components of photosynthesis in cyanobacteria as a possible solution to sustainable fuels production. I can do this in small spaces, on the lab scale for right now, but it can later be optimized on the global scale. It's very exciting work."

"Her experimental apparatus is custom built, and she was in charge of the construction and assembly of it from the ground up," said Frymier. "It allows her to conduct most of her work on campus. This was a priority for us because she is not only a student but also a mother of two young children. She is able to continue to make progress with her research and maintain a family as well."

Ifey has been married to her husband Ernest for six years. While at UTSI, she gave birth to her first child, a daughter named Oge who is now four years old. It was during her teaching assistantship in the Engineering Fundamentals

Division that she gave birth to her baby boy, a one-year-old called Ife.

"I should have named them Master's and Doctorate," she joked.

"It is very rewarding to see her make progress in her academic and professional development," Frymier said. "She has high aspirations and is interested in running her own research program in a faculty appointment. She will be a fantastic representative of our program in whatever role she assumes when she graduates."



When Rebecca Empting visited the University of Tennessee with her older sister, Erin, who was interested in studying architecture, several advisors swayed them both to enroll in the College of Engineering. Erin graduated with a degree in civil engineering, and Rebecca isn't far behind. She plans to graduate in May 2009 with a degree in chemical and biomolecular engineering before heading to medical school.

"I learned of the combination of chemistry and math with physics in chemical engineering," Empting said. "It seemed a perfect fit for me because of my aptitude for physics and math and my interest in chemistry, and it would leave many doors open for me after graduation."

Originally from Germantown, Tenn., Empting graduated from Houston High School. Before moving into the dorms at UT, she had never lived anywhere besides her childhood home.

"The University of Tennessee is the perfect school for me. Not only did I receive several scholarships, I am relatively close to my hometown," Empting said. "Sports were also a big factor for me. I love cheering on the Volunteer men's and women's basketball team and the football team."

When she's not cheering on the Vols, Empting is highly involved with

College of Engineering activities. She is the vice-president of the American Institute of Chemical Engineers (AIChE) for the 2008-2009 year. She spent two years conducting research under Dr. David Keffer, and the Fall 2008 semester saw her recruiting for the Sustainable Technology through Advanced Interdisciplinary Research (STAIR) graduate program, which is directly involved with the Sustainable Energy Education and Research Center (SEERC). On her free morning once a week, she travels to Baptist West Hospital to shadow a physician to gain medical experience from an alumnus of the biomedical engineering program at UT.

She also completed a summer internship at Dow Chemical Company in Midland, Mich.

"I gained experience in the workforce and learned a lot more of what chemical engineering is all about. That experience was invaluable to my education," she said.

"My favorite engineering memory is traveling to Philadelphia to the National AIChE Conference to show off all the hard work that several other students and I put into the Chem-E Car," Empting said. The Chem-E Car challenge is an annual competition between universities to create a chemically powered vehicle.

"Although we placed 11<sup>th</sup>, I really enjoyed the time I put into it as well as the trip itself."

She has received several scholarships including the HOPE Scholarship, the Volunteer Scholarship, the Dow Chemical Company Outstanding Junior Scholarship and the Herbert and Lillian Duggan Engineering Scholarship.

"I have thoroughly enjoyed my time in the department and the College of Engineering," Empting said. "I have worked very hard, and it has all been worth it."

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Mike Stone (B.S./ChE '63) is a strong believer in the power of continuing education, and he is proving it by funding scholarships for students in the Department of Chemical and Biomolecular Engineering (CBE).

Stone grew up in Union City, Tenn., in the western part of the state. He had twin cousins who attended Georgia Tech and were studying to be chemical engineers. The two were also enrolled in the cooperative engineering program at Tech, and Stone was fascinated with their stories about engineering projects. He decided to attend UT-Knoxville, since it was an in-state school and more affordable.

Stone recalls several of his former professors as very capable, intelligent teachers. He had particular regard for his faculty advisor, Dr. Don Bogue, and also for Dr. John Prados, a longtime chemical engineering professor who has been with the university since the 1950s.

The best part of his engineering education, however, was the co-op experience.

"Co-op was almost like a vacation to me," Stone commented. "I worked at Monsanto Chemical Company's elemental phosphorus plant in Columbia, Tenn., first in the engineering department, then in production and the research and development laboratory. I got lots of

good experience, and the co-op salary helped to pay my way through the university."

After graduation, Stone joined Allied Chemical in Hopewell, Va., where he was a Production Unit Supervisor in the nylon molding polymers unit. He went on to work for Copolymer Rubber and Chemical in Baton Rouge, La., where he held positions in process engineering and project management, and Kaiser Aluminum and Chemical Corporation in Oakland, Calif., where he was employed in corporate engineering, corporate development, business management, sales and marketing and strategic planning. Stone spent the last eight years of his career with G.S. Roofing Products Company in Dallas, Texas, where he served as vice-president and was responsible for corporate development, project engineering, research and development, transportation and distribution, safety, quality control and environmental issues.

Stone completed a business correspondence course six years after his graduation from UT, and he thought that the additional business and leadership skills helped him advance in his career.

"I think the business courses marked a turning point in my career," he remarked. "If someone is an above-average engineer, eventually he or she

will be given new responsibilities that go beyond engineering. Having that extra business knowledge is a big plus."

Stone recently funded four scholarships in the CBE department, each worth \$12,500, in honor of Dr. John W. Prados. The students must be majoring in chemical engineering with a minor in business and also must be enrolled in the cooperative engineering program. If there are more than four candidates available for the scholarships, the selection will be based on financial need. Stone also plans to work with the Office of Professional Practice, which oversees the co-op program, to offer students

graduating from the program a \$400 grant to purchase books related to business, financial analysis and leadership training.

"I hope that eventually the recipients of these scholarships will also be inspired to help others," Stone said. The importance of continuing education is a message that Stone would like to convey to all University of Tennessee College of Engineering graduates.

Stone retired in 1998 and moved to Lake Tahoe, Nev., where he enjoys skiing, hiking and the beautiful scenery. Stone has two sons and two granddaughters.



Mike Stone with four of his student scholarship winners. From left to right; Mark May, Amanda Mathews, Dr. John W. Prados, Angel Vogel, John M. Stone, Associate Dean for Academic and Student Affairs Masood Parang and Patrick Bowland.

The CBE department hosted two College of Engineering Distinguished Lecture Series presentations during 2007-2008.



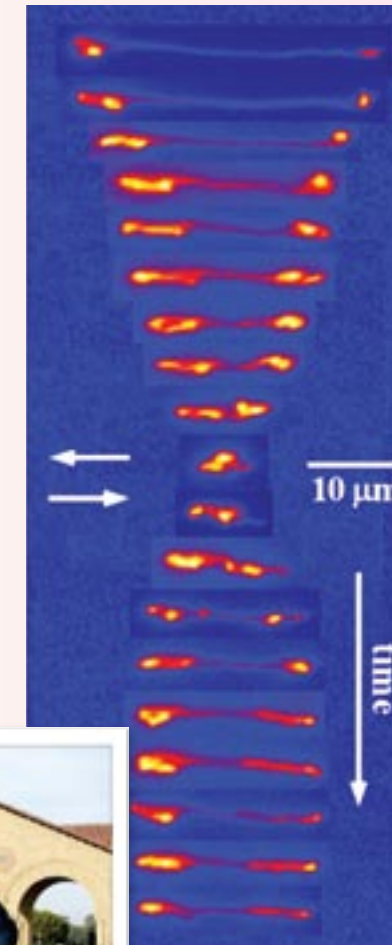
Dr. Eric Shaqfeh, Professor of Chemical and Mechanical Engineering at Stanford University in Stanford, Calif.,

gave a presentation titled *Progress and Prospects in Understanding Single Molecule Polymer Dynamics* on October 29, 2007 in the Walters Life Sciences Building.

Shaqfeh, who holds a dual appointment as a professor of mechanical engineering and associate chair of chemical engineering at Stanford, reviewed the state of research for single molecule DNA dynamics studies in bulk flows including extensional, shear and mixed flows.



Dr. Eric Shaqfeh and his research group at Stanford

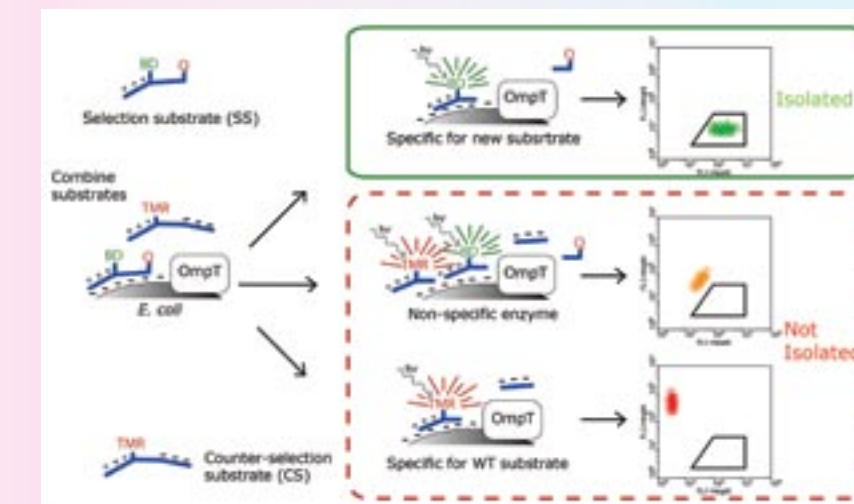


Picture of a single molecule DNA tumbling in a shear.

Dr. George Georgiou, Professor of Chemical and Biomolecular Engineering at the University of Texas-Austin (UTA) presented *New Strategies for the Discovery of Therapeutic Antibodies and Enzymes* on March 12, 2008, in the Science and Engineering Research Facility (SERF) on the UT campus.

Georgiou, who is a member of the Institute for Cell and Molecular Biology at UTA, discussed his research group's long-term interest in the engineering of proteins for pharmaceutical and biotechnology applications.

**Both Dr. Shaqfeh and Dr. Georgiou are members of the CBE department's Board of Advisors.**



Two-color flow cytometric assay used for the isolation of OmpT variants with altered specificities.



**Paul Bienkowski**

**Professor**  
Ph.D., Purdue University

**Research areas:**  
Thermodynamics; environmental biotechnology



**Eric Boder**

**Career Development Associate Professor**  
Ph.D., University of Illinois-Urbana

**Research areas:**  
Molecular biotechnology and bioengineering; protein engineering



**Duane Bruns**

**Associate Professor**  
Ph.D., University of Houston

**Research areas:**  
Process dynamics; control and automation



**Robert Counce**

**Professor**  
Ph.D., University of Tennessee

**Research areas:**  
Green engineering; process design; separations



**David Keffer**

**Associate Professor**  
Ph.D., University of Minnesota

**Research areas:**  
Molecular modeling; confined fluids; separations; sustainable energy



**Bamin Khomami**

**Granger and Beamon Distinguished Professor and Head**  
Ph.D., University of Illinois-Urbana

**Research areas:**  
Transport properties of complex fluids; sustainable energy; multi-scale modeling and simulation



**Charles Moore**

**Professor Emeritus**  
Ph.D., Louisiana State

**Research areas:**  
Areas of distillation design; operation and control



**Stephen Paddison**

**Associate Professor**  
Ph.D., University of Calgary

**Research areas:**  
Computational materials science as applied to fuel cell electrolytes and electrocatalysts



**Shengting Cui**

**Research Associate Professor**  
Ph.D., University of Virginia

**Research areas:**  
General molecular modeling of materials properties and fluid phenomena



**Brian Edwards**

**Professor and Associate Head**  
Ph.D., University of Delaware

**Research areas:**  
Thermodynamics; fluid mechanics; molecular modeling



**Paul Frymier**

**Associate Professor**  
Ph.D., University of Virginia

**Research areas:**  
Engineering and optimization of photosynthetic routes to biohydrogen



**Ramakrishnan Kalyanaraman**

**Associate Professor**  
Ph.D., North Carolina State University

**Research areas:**  
Thin films; phase transformation; energetic beam processing; functional nanocomposites



**Simioan Petrovan**

**Research Associate Professor**  
Ph.D., Technical University Iasi, Romania

**Research areas:**  
Characterization (rheological in particular) and processing of polymers



**John Prados**

**University Professor Emeritus**  
Ph.D., University of Tennessee

**Research areas:**  
Engineering education with special emphasis on active, collaborative learning and teamwork



**Tse-Wei Wang**

**Associate Professor**  
Ph.D., Massachusetts Institute of Technology

**Research areas:**  
Bioinformatics; organization and search in large databases; data mining

## CBE Board of Advisors

The Department of Chemical and Biomolecular Engineering's Board of Advisors consists of a distinguished group of academics, business professionals and industrial leaders from noted universities and international corporations.

The purpose of the board of advisors is to ensure that the department is focused on its mission of education, research and service to the university and technical communities. The board meets once a year to examine and evaluate CBE's undergraduate and graduate curricula and to advise the department head and faculty with regard to these issues.

The board provides insight as to the activities of peer departments at other universities and offers information about the requirements of relevant industries. The board also acts as a liaison between the department and the dean's office and university administration, providing a candid assessment of the department's strengths and weaknesses, as well as communicating the department's directions, goals and resource requirements.

*Current members of the CBE Board of Advisors are:*



**Mr. Victor H. Agreda** Director of the Chemical Development Division at Eastman Chemical Company in Kingsport, Tenn. Agreda is a member of Tau Beta Pi and the American Institute of Chemical Engineers (AIChE) and is the Chair of the Eastman Acetyl Technology Council.



**Dr. Robert Armstrong** Deputy Director of the Massachusetts Institute of Technology (MIT) Energy Initiative/Chevron at MIT in Cambridge, Mass. Armstrong is past president of the Society of Rheology and has served as Head of the Chemical Engineering Department at MIT. Armstrong has received numerous awards for his research and teaching contributions, including the Warren K. Lewis and the Professional Progress Award of the American Institute of Chemical Engineers and the Bingham Medal of the Society of Rheology.



**Dr. George Georgiou** is the Joan and Keys Curry/Cullen Trust Endowed Chair and a professor in the Department of Chemical Engineering at the University of Texas-Austin. Georgiou is the recipient of the Marvin J. Johnson Award in Microbial and Biochemical Technology from the American Chemical Society and also received the Professional Progress Award for Outstanding Progress in Chemical Engineering from the American Institute of Chemical Engineers. He also received the University Cooperative Society's Research Excellence Award for Best Paper at UT-Austin and the E. Bergman Award from the US-Israel Science Foundation.



**Mr. James B. Porter Jr.** is the former Chief Engineer and Vice-President of Engineering Operations at the DuPont Corporation, headquartered in Wilmington, Del. Porter, a University of Tennessee graduate, is a member of the Construction Industry Institute, the Engineer and Construction Contracting Associates and serves on the Board of Directors of AIChE. He is currently retired.



**Dr. Eric Shaqfeh** is Professor of Chemical and Mechanical Engineering at Stanford University in Stanford, Calif. Shaqfeh is a Fellow of the American Physical Society and also received the American Society of Engineering Education (ASEE) Research Award, National Science Foundation Presidential Young Investigator Award, the American Physical Society Francois Frenkiel Award and the David and Lucile Packard Fellow in Science and Engineering.



**Mr. Bruce Combs** is the Global Site Logistics Director, Base Plastics, for the Dow Chemical Corporation in Freeport, Texas. Combs, a University of Tennessee chemical engineering graduate, is the past president of the Society of Professional Engineers (SPE), South Texas section.

## CBE Awards and Recognitions

The Department of Chemical and Biomolecular Engineering and the local chapter of the American Institute of Chemical Engineers (AIChE) held the annual Awards Dinner on Monday, April 14, 2008. The following individuals were recognized at the event:

### Faculty & Staff Awards

Outstanding Staff Member  
**Frank Holiway**

Outstanding Advisor Award  
**Dr. Paul Frymier**

Outstanding Teacher Award  
**Dr. Paul Frymier**

Tom and Ruth Clark  
Chemical Engineering Excellence  
Award in Teaching  
**Dr. Paul Frymier**

### Student Awards

Dow Outstanding Junior  
**Michael Spain**

Kenneth M. Elliott  
Outstanding Senior Award  
**Bradley Harris**

Jim and Sandra McKinley Outstanding  
Graduate Student Award  
**Ifeyinwa Iwuchukwu**

Most Exceptional Student Award  
**Jared Johnson**

American Chemical Society  
Outstanding Senior Award  
**Robyn Chaplin**

Alpha Chi Sigma Albert Cooper Award  
**Kristen Dobrodziej**

### AIChE Awards

AIChE Service Award  
**Jared Johnson**

AIChE Outstanding  
Student Award  
**Michael Spain**

AIChE Outstanding  
Baccalaureate Award  
**Jared Johnson**

### College-wide Awards & Recognitions

Dennis and Connie Dennihan  
Scholarships for  
Outstanding Performance  
**Mark May and Matthew Clark**

Eastman Outstanding Scholar Award  
**Shelley Parker**

Several CBE faculty and students were also recognized at the **College Honors Banquet** on April 8, 2008:

Allen & Hoshall Award  
**Dr. David Keffer**

Charles Edward Ferris Award  
**Dr. Robert "Pete" Counce**

COE Teaching Fellow Award  
**Dr. Tse Wei Wang**

COE 2008 Research Fellow  
**Dr. David Keffer**



## Journal Articles and Book Chapters Published

For the Period of July 1, 2007 to June 30, 2008

1. A molecular dynamics study of the stress-optical behavior of a linear short-chain polyethylene melt under shear, C. Baig, B.J. Edwards and D.J. Keffer, *Rheo. Acta*, 46, 1171-1186 (2007).
2. Using multiple-mode models for fitting and predicting the rheological properties of polymeric melts. Part II. Single and double step-strain flows, B. Jiang, P.A. Kamerkar, D.J. Keffer and B.J. Edwards, *J. Appl. Polym. Sci.*, 105, 2884-2892 (2007).
3. Energetic and entropic elasticity of nonisothermal flowing polymers: experiment, theory and simulation, T.C. Ionescu, B.J. Edwards, D.J. Keffer and V.G. Mavrantzas, *J. Rheol.*, 52, 105-140 (2008).
4. A multiscale modeling demonstration based on the pair correlation function, C.Y. Gao, D.M. Nicholson, D.J. Keffer and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, 152, 140-147 (2008).
5. An examination of droplet deformation and break-up between concentrically rotating cylinders, M. Dressler and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, 152, 86-100 (2008).
6. A generalized Hamiltonian-based algorithm for rigorous equilibrium molecular dynamics simulation in the canonical ensemble, D.J. Keffer, C. Baig, P. Adhangale and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, 152, 129-130 (2008).
7. Rheological and entanglement characteristics of linear chain polyethylene liquids in planar couette and planar elongational flows, J.M. Kim, D.J. Keffer, M. Kröger and B.J. Edwards, *J. Non-Newtonian Fluid Mech.*, 152, 168-183 (2008).
8. Visualization of conformational changes of linear short-chain polyethylenes under shear and elongational flows, J. M. Kim, B. J. Edwards and D. J. Keffer, *J. Mol. Graph. Model.*, 26, 1046-1056 (2008).
9. Atomistic simulation of energetic and entropic elasticity in short-chain polyethylenes, T.C. Ionescu, V.G. Mavrantzas, D.J. Keffer and B.J. Edwards, *J. Rheol.*, 52, 567-589 (2008).
10. A quantum mechanical study of the decomposition of  $CF_3OCF_3$  and  $CF_3CF_2OCF_2CF_3$  in the presence of  $AlF_3$ , B. Jiang, D.J. Keffer and B.J. Edwards, *J. Phys. Chem. A*, 112, 2604-2609 (2008).
11. Comparison of perfluoropolyethers and n-alkanes under shear via nonequilibrium molecular dynamics simulation, B. Jiang, J.M. Kim, D.J. Keffer and B.J. Edwards, *Mol. Sim.*, 34, 231-242 (2008).
12. Atomistic simulation of energetic and entropic elasticity in short-chain polyethylenes, T.C. Ionescu, V.G. Mavrantzas, D.J. Keffer and B.J. Edwards, *Virt. J. Biol. Phys. Res.*, 15, 6 (2008).
13. Comparison of rheological properties of perfluoropolyethers through simulation and experiment, B. Jiang, N.J. Crawford, D.J. Keffer, B.J. Edwards and J.J. Adcock, *Mol. Sim.*, 33, 881-888 (2007).
14. Molecular dynamics study of structure and transport of water and hydronium ions at the membrane/vapor interface of nafion, M. Esai Selvan, J. Liu, D.J. Keffer, S. Cui, B.J. Edwards and W.V. Steele, *J. Phys. Chem. C*, 112, 1985-1993 (2008).
15. Molecular-level modeling of the structure and wetting of electrode/electrolyte interfaces in hydrogen fuel cells, J. Liu, M. Esai Selvan, S. Cui, B.J. Edwards, D.J. Keffer and W.V. Steele, *J. Phys. Chem. C*, 112, 1975-1984 (2008).
16. A decade of yeast surface display technology: Where are we now?, L.R. Pepper, Y.K. Cho, E.T. Boder and E.V. Shusta, *Comb. Chem. High Throughput Screen.*, 11, 127-34 (2008).
17. Rheology of 1-butyl-3-methylimidazolium chloride cellulose solutions. I. Shear rheology, R.J. Sammons, J.R. Collier, T. G. Rials and S. Petrovan, *J. Appl. Polym. Sci.*, 110, 1175 (2008).
18. Elongational rheology of polymer/clay dispersions: determination of orientational extent in elongational flow processes, E.A. Stefanescu, S. Petrovan, W.H. Daly and I.I. Negulescu, *Macromol. Mat. Eng.*, 293, 303-309 (2008).
19. Effect of bacterial chemotaxis on biodegradation in a porous medium, C.J. O'Lenick, P.R. Bienkowski, P.D. Frymier and R.N. Weinstein, *Bioremed. J.*, 12, 131-144, (2008).
20. A reagentless enzymatic amperometric biosensor using vertically aligned carbon nanofibers (VACNF), M.L. Weeks, T. Rahman, P.D. Frymier, S.K. Islam and T.E. McKnight, *Sensors & Actuators: B. Chemical*, 133, 53-59 (2008).
21. A proud legacy of quality assurance in the preparation of technical professionals: *ABET's 75th anniversary retrospective*, J.W. Prados, ABET, Inc., Baltimore, MD (2007).
22. Effect of low concentration salt on organic contact angle in ionic surfactant solutions: insight from theory and experiment, S.A. Morton, III, D.J. Keffer and R.M. Counce, *Sep. Sci. Tech.*, 43, 310-330 (2008).
23. University partnerships with industry and government, R.M. Counce, L.C. Markel, P.R. Bienkowski, S.P. Singh, J.D. Randolph, R.T. Jubin, B.E. Lewis, B.E. Murphree, R.A. Reimer, R.A. Heckrotte and B. Alderson, *Internat. J. Eng. Edu.*, 24, 480-487 (2008).
24. Self-similar shear-thickening behavior in CTAB/NaSal surfactant solutions, M. Vasudevan, A. Shen, B. Khomami and R. Sureshkumar, *J. Rheol.*, 52, 527-550 (2008).
25. Flow-induced chain scission in dilute polymer solutions: algorithm development and results for scission dynamics in elongational flow, H. Sim, B. Khomami and R. Sureshkumar, *J. Rheol.*, 51, 1223-1251 (2007).
26. A computationally efficient approach for hi-fidelity fine graining from bead-spring models to bead-rod models, V. Venkataramani, R. Sureshkumar and B. Khomami, *J. Non-Newtonian Fluid Mech.*, 149, 20-27 (2008).
27. Molecular modeling of proton transport in the short-side-chain perfluorosulfonic acid ionomers, I.R. Hristov, S.J. Paddison and R. Paul, *J. Phys. Chem. B*, 128, 2937-2949 (2008).

## New Grants, Contracts and Patents

For the Period of July 1, 2007 to June 30, 2008

1. Scholarships for Engineering Students from Underrepresented Groups in the East Tennessee Region, B.J. Edwards, D. Jackson, J. Wu, D.J. Keffer and W. Odom, National Science Foundation, \$600,000, 08/15/2007 – 07/31/2011.
2. From nanoscale simulation to process engineering: Building a network for understanding polymer dynamics, B.J. Edwards, B. Khomami, D.J. Keffer, J.D. Schieber and E. Shaqfeh, National Science Foundation, \$189,959, 11/15/2007 – 10/31/2009.
3. Metal-porphyrin frameworks: A novel class of metal-organic frameworks, D.J. Keffer, B.J. Edwards, S. Agnihotri and C. Rawn, Sustainable Energy Education and Research Center, University of Tennessee-Knoxville, \$25,000, 08/01/2007 – 12/31/2007.
4. EXP-LA: Collaborative Research: Exploiting geometry and chemistry at the nanoscale to selectively preconcentrate explosive molecules, D.J. Keffer and B.J. Edwards, National Science Foundation, \$265,819, 10/01/2007 – 09/30/2009.
5. Convective and mass transfer models of the dynamics of reactive systems in C-tray polyester finishing reactors, D.J. Keffer, B.J. Edwards, B. Khomami and S. Petrovan, Eastman Chemical Co., \$120,000, 01/01/2008 – 12/31/2010.
6. Controlling the dynamics of cell adhesion using engineered integrin I-domain, E.T. Boder and D. Hammer, National Institute of Health, \$962,143, 09/01/2007 – 08/31/2012.
7. In-vitro biosynthetic production of hydrogen, P.D. Frymier and B. Bruce, UTK Scholarly and Research Incentive Funds, \$25,000, 07/01/2007 – 06/30/2008.
8. SEERC: BioH2, P.D. Frymier and B. Bruce, UTK Science Alliance, \$35,000, 07/01/2007 – 06/30/2008.
9. Laser flash photolysis for increasing biohydrogen production: probing molecular interactions to fuel our future, P.D. Frymier, TN Board of Architectural and Engineering Examiners, \$40,365, 01/01/2008 – 12/31/2008.
10. Development of acetic acid removal technology for the UREX+ Process, R.M. Counce and J.S. Watson, U.S. Department of Energy, \$108,874, 03/13/2008 – 03/12/2009.
11. Understanding pressure drop-flow rate relationships in inertialess viscoelastic flows: effects of flow instability and stress-conformation, B. Khomami, National Science Foundation, \$191,073, 05/01/2008 - 04/31/2011.
12. Atomistic simulation of interfacial metal ion exchange, B. Khomami, University of Tennessee and Oak Ridge National Laboratory, \$45,240, 01/01/2008 - 12/31/2008.
13. Hybrid photovoltaic materials and devices, B. Khomami, M. Dadmun, J. Mays and B. Bruce, University of Tennessee Science Alliance & Sustainable Energy Education and Research Center, \$155,000, 07/01/2007 - 06/30/2009.
14. Design of CVD reactors: a multiscale modeling approach, B. Khomami, MEMC Corporation, \$45,000, 09/01/2007 - 08/31/2008.
15. A computational and experimental investigation into the transport of protons near the electrolyte/water, electrolyte/catalyst and electrolyte/nanoparticle interfaces, Department of Energy, D.J. Keffer and S.J. Paddison, \$759,946, 06/01/2008 - 05/31/2012.
16. Membranes and MEA's for dry, hot operating conditions, Department of Energy and 3M Company, S.J. Paddison, \$538,999, 11/01/2007 – 10/31/2011.
17. Multi-scale modeling of proton transport, water distribution and methanol permeability in PEMs, Army Research Office, S.J. Paddison, \$249,631, 05/01/2008 – 04/30/2010.
18. Metal-porphyrin-frameworks: a novel class of metal-organic-frameworks (MOFs), D.J. Keffer and C. Rawn, The University of Tennessee Science Alliance, \$25,000, 07/01/2007 – 12/31/2007

## Conference and Invited (\*) Presentations

For the Period of July 1, 2007 to June 30, 2008

- 1.\* QC issues in recombinant protein expression in yeast, BioProcess R&D Academic Speaker Program, Merck Research Labs, Rahway, N.J., October 30, 2007.
- 2.\* Protein engineering applications in viral fusion, cell adhesion and sequence-specific immobilization. Department of Biochemistry, Cellular, and Molecular Biology, University of Tennessee, Knoxville, Tenn., September 19, 2007.
3. Engineering  $\alpha$ L I domain to modulate adhesive behavior using yeast display. L.R. Pepper, D.A. Hammer and E.T. Boder. BMES Annual Meeting, Los Angeles, Calif., September, 2007.

## Conference and Invited (\*) Presentations

- 4.\*** Applying nonequilibrium thermodynamics principles to NEMD simulations, B.J. Edwards, Department of Materials Science, ETH-Zurich, Switzerland, June 13, 2008.
- 5.\*** Applying nonequilibrium thermodynamics principles to NEMD simulations, B.J. Edwards, European Community Marie Curie Lectures: Nanostructured Materials and Modeling and Simulation, Patras, Greece, June 18-27, 2008.
- 6.\*** A computational investigation of proton transport through the electrode/electrolyte interface of proton exchange membrane fuel cell systems, D.J. Keffer, M. Esai Selvan, J. Liu, S. Cui, B.J. Edwards and W.V. Steele, Southeast Regional Meeting of the American Chemical Society (SERMACS), Greenville, S.C., October 24-27, 2007.
- 7.\*** Effect of relaxation on plastic flows and temperature rises of a Zr-based bulk-metallic glass, P.K. Liaw, W.H. Jiang, F.X. Liu, H. Choo, B.J. Edwards and B. Khomami, 2007 MRS Fall Meeting, Boston, Mass., November 26-30, 2007.
- 8.\*** Single-chain dynamics and nonisothermal rheology of linear polyethylene liquids under shear, J.M. Kim, B.J. Edwards and D.J. Keffer, North American Thermal Analysis Society 36<sup>th</sup> Annual Conference, Atlanta, Ga., August 18-20, 2008.
- 9.** Molecular-level modeling of the structure and wetting of electrode/electrolyte interfaces in hydrogen fuel cells, J. Liu, M. Esai Selvan, S. Cui, B.J. Edwards, D.J. Keffer and W.V. Steele, 15<sup>th</sup> Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, Tenn., October 21-25, 2007.
- 10.** Reactive molecular dynamics applied to proton transport in fuel cells, M. Esai Selvan, J. Liu, D.J. Keffer, B.J. Edwards, S. Cui and W.V. Steele, 15<sup>th</sup> Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, Tenn., October 21-25, 2007.
- 11.** Correlation-based coarse-graining approach to multiscale materials modeling, C.Y. Gao, P.K. Nukala, B. Jiang, D.M. Nicholson, D.J. Keffer and B.J., Edwards, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 12.** Molecular-level modeling of the structure and wetting of electrode/electrolyte interfaces in hydrogen fuel cells, J. Liu, M. Esai Selvan, S. Cui, B.J. Edwards, D.J. Keffer and W.V. Steele, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 13.** Rheological and entanglement characteristics of polyethylene liquids and visualization of conformational changes in shear and elongational flows, J.M. Kim, D.J. Keffer, M. Kröger and B.J. Edwards, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 14.** Reactive molecular dynamics of the thermal decomposition of  $CF_3OCF_3$ , B. Jiang, B.J. Edwards and D.J. Keffer, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 15.** Quantum mechanics study of decomposition of  $CF_3OCF_3$  and  $(CF_3CF_2)_2O$  catalyzed by  $AlF_3$ , B. Jiang, B.J. Edwards and D.J. Keffer, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 16.** Understanding the relationship between molecular architecture and thermophysical and rheological properties of perfluoropolyethers, B. Jiang, J.L. Adcock, N.J. Crawford, J.T. Fern, A.F. Pangloli, B.J. Edwards, W.V. Steele and D.J. Keffer, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 17.** Reactive molecular dynamics applied to proton transport in fuel cells, M. Esai Selvan, J. Liu, D.J. Keffer, B.J. Edwards, S. Cui and W.V. Steele, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 18.** Correlation-based coarse graining approach to multiscale materials modeling, C.Y. Gao, P.K. Nukala, B. Jiang, D.M. Nicholson, D.J. Keffer and B.J. Edwards, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 19.** Reactive molecular dynamics applied to proton transport in fuel cells, M. Esai Selvan, D.J. Keffer, B.J. Edwards, S. Cui, J. Liu and W.V. Steele, The Electrochemical Society Annual Meeting, Phoenix, Ariz., May 18-23, 2008.
- 20.** Molecular-Level modeling of the structure and wetting of electrode/electrolyte interfaces, J. Liu, S. Cui, D.J. Keffer, B.J. Edwards and M. Esai Selvan, The Electrochemical Society Annual Meeting, Phoenix, Ariz., May 18-23, 2008.
- 21.** A comparison of the aqueous phase structures of hydrated Nafion and short side-chain polymer electrolyte membranes through molecular dynamics simulation, J. Liu, S. Cui, D.J. Keffer, B.J. Edwards, S. Paddison and M. Esai Selvan, The Electrochemical Society Annual Meeting, Phoenix, Ariz., May 18-23, 2008.
- 22.** Elongational rheology of salt containing montmorillonite-PEO aqueous dispersions, E.A. Stefanescu, I.I. Negulescu, W.H. Daly and S. Petrovan, 235<sup>th</sup> ACS National Meeting, New Orleans, La., April 6-10, 2008.
- 23.** Investigation into the effect of bacterial chemotaxis on in-situ bioremediation rate, C.J. O'lenick, P.R. Beinkowski and P.D. Frymier, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 24.** Detection of alcohol with vertically aligned carbon nanofiber (VACNF), M.L. Weeks, T. Rahman, P.D. Frymier, S.K. Islam and T.E. McKnight, 6<sup>th</sup> Annual IEEE Conference on Sensors, Atlanta, Ga., October 28-31, 2007.
- 25.** Extraction of acetic acid from aqueous nitric acid waste streams in the UREX+ Process, J.A. Mitchell, J.A. Johnson, R.M. Counce, J.S. Watson, B.B. Spencer and G.D. DelCul, 32<sup>nd</sup> Actinides Separations Conference, Park City, Utah, May 12-15, 2008.
- 26.** Determination of water content and correlation to acid extraction for solvents in UREX+ Process, T.H. Russell, R.M. Counce, J.S. Watson, B.B. Spencer and G.D. DelCul, 32<sup>nd</sup> Actinides Separations Conference, Park City, Utah, May 12-15, 2008.
- 27.** Effects of electrolyte concentration on surfactant adsorption to a QCM immersed in surfactant + electrolyte solutions, S.J. Ray, S. A. Morton, III and R. M. Counce, 15<sup>th</sup> Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, Tenn., October 21-25, 2007.
- 28.** Removal of acetate from aqueous nitric acid waste streams, J.A. Mitchell, J.A. Johnson, R.M. Counce, J.S. Watson, B.B. Spencer and G.D. DelCul, 15<sup>th</sup> Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, Tenn., October 21-25, 2007.
- 29.** Thermodynamics of acetic acid (aq) calculated from the modified adsorption isotherm model for aqueous electrolytes, J.A. Johnson, J.A. Mitchell, R.M. Counce, J.S. Watson, B.B. Spencer and G.D. DelCul, 15<sup>th</sup> Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, Tenn., October 21-25, 2007.
- 30.\*** Sustainable Energy Education and Research Center (SEERC): University of Tennessee's response to the global energy challenge, B. Khomami, Knoxville Technical Society, Knoxville, Tenn., Sept. 15, 2007.
- 31.** Dynamics of single DNA molecules in oscillatory shear flow, D. G. Thomas and B. Khomami, 79<sup>th</sup> Annual Meeting of the Society of Rheology, Salt Lake City, Utah, October 15-18, 2007.
- 32.** Frictional drag properties of polymeric solutions in complex kinematics flows: a multiscale simulation approach, A. Koppol, R. Sureshkumar and B. Khomami, 79<sup>th</sup> Annual Meeting of the Society of Rheology, Salt Lake City, Utah, October 15-18, 2007.
- 33.** Modeling and simulation of solvent extraction in centrifugal contactors, V. de Almeida, S. Cui and B. Khomami, 15<sup>th</sup> Symposium on Separation Science and Technology for Energy Applications, Gatlinburg, Tenn., October 21-25, 2007.
- 34.** A computationally efficient reduced-order model for macromolecular solutions, V. Venkataramani, R. Sureshkumar and B. Khomami, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 35.** High throughput synthesis of visible-light-active nanostructured TiO<sub>x</sub> photocatalyst in a flame aerosol reactor, S. Dhumal, T. Daulton, J. Jiang, P. Biswas and B. Khomami, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 36.** Elucidation of molecular processes in liquid-liquid extraction of metal ions: a molecular dynamics study, S. T. Cui, V. de Almeida and B. Khomami, AIChE Annual Meeting, Salt Lake City, Utah, November 4-9, 2007.
- 37.** Tools for modeling and simulation of solvent extraction, V. de Almeida, S. Cui and B. Khomami, Nuclear Science & Technology Division Advisory Committee Review, ORNL, Oak Ridge, Tenn., Nov. 15, 2007.
- 38.** Surface attachment dynamics of photosystem-I self-assembly on thiol functionalized Au substrates for photovoltaic applications, D. Mukherjee, M. Vaughn, B. Khomami and B. Bruce, 17<sup>th</sup> Western Photosynthesis Conference, Asilomar, Calif., Jan. 8-12, 2008.
- 39.** Reversible and irreversible flow-induced phase transition in micellar solutions, M. Vasudevan, E. Buse, R. Kalyanaraman, A. Shen, B. Khomami and R. Sureshkumar, APS March Meeting, New Orleans, La., March 17-21, 2008.
- 40.** Understanding the deposition dynamics of Photosystem I (PSI) onto thiol-activated Au substrates, D. Mukherjee, M. Vaughn, B. Khomami and B. D. Bruce, International Scanning Probe Microscopy, Seattle, Wash., June 9-13, 2008.
- 41.\*** Multiscale modeling of the proton exchange membrane, 3<sup>rd</sup> Summer Workshop of the Center for Nanomaterials Design and Assembly, Lansing, Mich., June 22-26, 2008.
- 42.\*** Multiscale modeling of polymer electrolyte membranes, Physical and Chemical Sciences Division, Sandia National Laboratory, Albuquerque, N.M., May 21, 2008.
- 43.\*** The energetics of proton transfer in phosphoric and substituted phosphonic acids, 213<sup>th</sup> National Meeting of the Electrochemical Society, Phoenix, Ariz., May 18-22, 2008.
- 44.\*** Multi-scale modeling of proton exchange membranes, New York University, New York, N.Y., January 18, 2008.
- 45.\*** The proton exchange membrane: mesoscale and molecular modeling, Workshop of the Israel Science Foundation, Eilat, Israel, January 13-17, 2008.
- 46.\*** Multi-scale modeling of proton exchange membranes, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel, January 9, 2008.
- 47.\*** Modeling of anhydrous proton conductors, CARISMA School on Proton Conductors: Materials & Mechanisms, Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany, November 8-10, 2007.
- 48.\*** Modeling water and transport in hydrated ionomers, CARISMA School on Proton Conductors: Materials & Mechanisms, Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany, November 8-10, 2007.
- 49.\*** Multi-scale modeling of proton exchange membranes, Department of Chemistry, University of Alberta, Edmonton, Canada, October 30, 2007.
- 50.\*** Ab initio modeling of structure, reactivity and transfer at water/ionomer and water/catalyst interfaces, 212<sup>th</sup> National Meeting of the Electrochemical Society, Washington, D.C., October 7-12, 2007.
- 51.\*** Multi-scale modeling of proton exchange membranes, 7<sup>th</sup> NSF-MEXT Joint Symposium: Fuel Cell and Related Nanotechnologies, NSF and the Ministry of Education, Culture, Sports, and Technology of Japan, Washington D.C., October 5-7, 2007.
- 52.\*** Proton transfer in anhydrous polymeric membranes for fuel cells: an ab initio study, 58<sup>th</sup> Annual Meeting of the International Society of Electrochemistry, Banff, Canada, September 9-14, 2007.
- 53.\*** Multi-scale modeling of proton transport, water distribution and methanol permeability in proton exchange membranes (PEMs), Progress in Advanced Energy Conversion, sponsored by the ARO, The University of North Carolina at Chapel Hill, Chapel Hill, N.C., September 6-7, 2007.
- 54.\*** Molecular-level modeling of polymer electrolyte membranes, 234<sup>th</sup> National Meeting of the American Chemical Society, Boston, Mass., August 19-23, 2007.
- 55.** Mesoscale modeling of the hydrated morphology of PFSA membranes, 213<sup>th</sup> National Meeting of the Electrochemical Society, Phoenix, Ariz., May 18-22, 2008.
- 56.** Multi-scale materials modeling of function and failure of minimally hydrated and dry PEMs, Department of Energy 7 Review, Colorado School Mines, Colo., March 10-11, 2008.
- 57.** Proton transfer in anhydrous polymeric membranes for fuel cells: an ab initio study, 57<sup>th</sup> Canadian Chemical Engineering Conference, Edmonton, Canada, October 28-31, 2007.
- 58.** Molecular dynamics simulations of proton and water diffusion in the short-side-chain perfluorosulfonic acid ionomer, 212<sup>th</sup> National Meeting of The Electrochemical Society, Washington D.C., October 7-12, 2007.
- 59.** Molecular modeling of proton diffusion in the short-side-chain perfluorosulfonic acid ionomer, 58<sup>th</sup> Annual Meeting of the International Society of Electrochemistry, Banff, Canada, September 9-14, 2007.

Mrs. Ann B. Anderson  
 Mrs. Susan Kay Arensman and Mr. Michael Arensman  
 Mr. Bernie Lemuel Arnold and Mrs. Christina E. Arnold  
 Mr. Dewayne P. Atchley  
 Mr. William Ralph Ayers, III and Mrs. Christy S. Ayers  
 Mr. Clyde Hermon Bell and Mrs. Kazue Mameda Bell  
 Ms. Linda R. Bell  
 Mr. Robert G. Bell and Mrs. Eunice Bell  
 Ms. Debra A Bennett  
 Mr. William Michael Bennett and Ms. Patti Bennett  
 Ms. Sydney E. Bonham  
 Mr. Mark Benjamin Boone and Mrs. Donise C. Boone  
 Dr. Louis P. Bosanquet and Mrs. Janine Bosanquet  
 Mr. Daniel James Bouch and Ms. Brenda Bouch  
 Mrs. Pamela E Bowen and Mr. Kenneth E. Bowen  
 Mr. Burton N. Boyd and Ms. Jane Adams  
 Mr. Tommy L. Brumfield and Mrs. Sally B. Brumfield  
 Mr. Walter P. Bussart and Mrs. Elizabeth W. Bussart  
 Mrs. Lucille R. Buttram and Mr. Claude E. Buttram, Jr.  
 Dr. Joseph A. Byington and Mrs. Connie Byington  
 Mr. Bill A. Cabbage and Mrs. Judy K. Cabbage  
 Mr. Thomas H. Clark and Mrs. Ruth L. Clark  
 Mr. Fred L. Collier, Jr. and Mrs. Jacqueline G. Woods Collier  
 Mrs. Sandra E. Counce and Dr. Robert M. Counce  
 Dr. Richard L. Cox and Mrs. Kathleen J. Cox  
 Mrs. Constance S. Denihan and Mr. Dennis A. Denihan  
 Ms. Amanda W. Duncan  
 Mrs. Harriet F. Eddlemon  
 Mr. Kenneth M. Elliott and Mrs. Virginia Elliott  
 Mr. A. Phil Farrow, Jr. and Mrs. Sandra Farrow  
 Mr. Kirk D. Firestone  
 Mr. Ted P. Fix and Mrs. Carol J. Fix  
 Mr. Jeffery A. Gamble and Ms. Susan Finch Gamble  
 Mr. J. Leonard Garland and Mrs. Marsha Garland  
 Mr. Terry T. Godsey and Ms. Kathleen Godsey  
 Mr. Anthony Perry Gouge and Ms. Leslie Gouge  
 Mr. Malcolm B. Hale and Mrs. Ellen Kelly Hale  
 Mr. William T. Hall and Mrs. Linda Hall  
 Mr. Hobart B. Hansard III and Mrs. Audrey C. Hansard  
 Mr. Bradley J. Harris  
 Mr. Everette Kerby Harris, Jr.  
 Dr. William B. Harrison, III and Mrs. Josephine M. Harrison

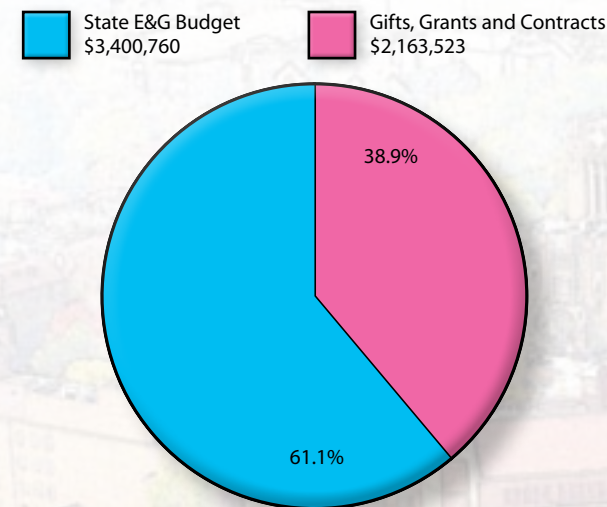
Dr. James H. Haynes and Mrs. Mary A. Haynes  
 Mrs. Janice Franklin Hensley  
 Mr. William B. Hickam and Mrs. Christine Hickam  
 Mr. Thomas M. Hobbs and Ms. Lori Stephenson  
 Mr. Lawrence S. Hood  
 Mr. Paul N. Horne and Mrs. Julia S. Horne  
 Ms. Patricia A. Houser  
 Dr. Craig A Hoyme and Ms. Debra P Hoyme  
 Mrs. Helen Marie Hunt and Dr. Paul Payson Hunt  
 Mr. George Andrew Huttick and Ms. Julie Ann  
 Mr. William L. Johnson  
 Mr. Jobie L Jones and Ms. Terri L Jones  
 Dr. Robert T. Jubin and Mrs. Sandra K. Jubin  
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 Mrs. Susan Elizabeth Rawlston

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 Mrs. Sue T. Utley  
 Mr. Frank Watkins, Jr.  
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 Mr. Bobby F. Williams and Mrs. Carol Williams

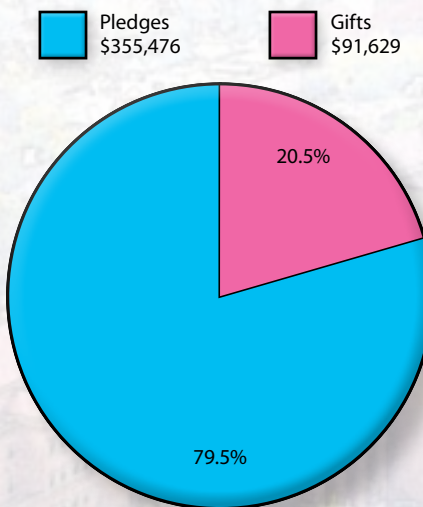
**Corporations**

Dow Chemical Company Foundation  
 Bridgestone/Firestone Americas  
 Ball Corporation  
 Johnson & Johnson Family of Companies  
 Merck & Co., Inc. Foundation  
 Rohm and Haas Company  
 Shell Oil Company Foundation  
 Eastman Chemical Company  
 Bristol-Myers Squibb Foundation, Inc.  
 ExxonMobil Foundation  
 ExxonMobil Corporation  
 Williams Companies Foundation, Inc.  
 3M General Offices

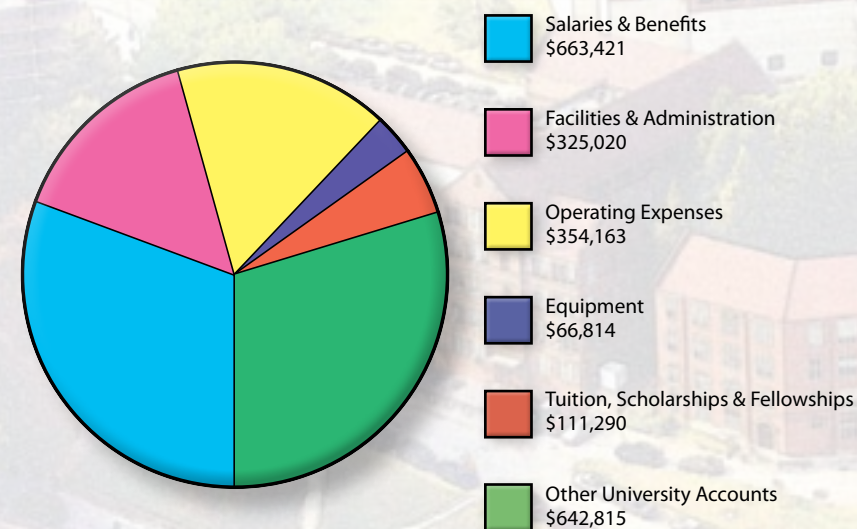
**Total Income/Revenue for FY 2008 - \$5.56 Million**



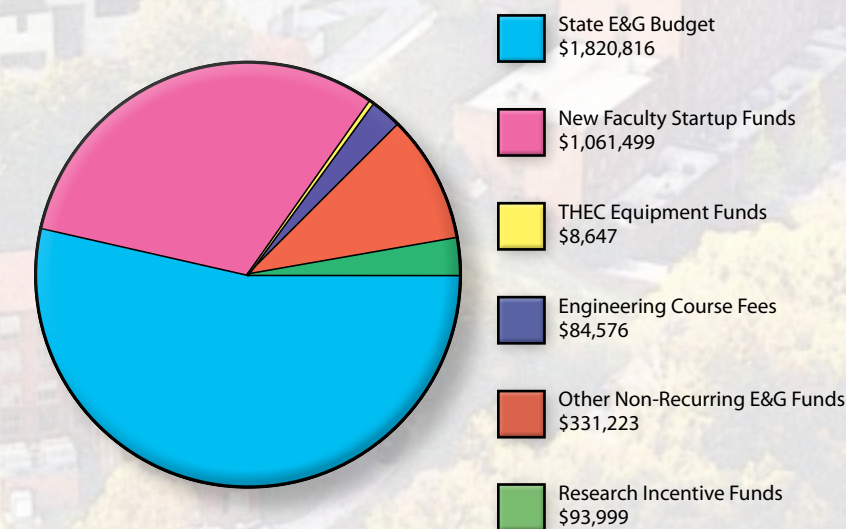
**Gifts and Pledges for FY 2008 - \$447,105 Thousand**



**Gifts, Grants and Contract Expenditures for FY 2008 \$2.16 Million**



**Educational and General Income Revenue for FY 2008 \$3.40 Million**



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