

## UT-ORNL SCIENCE ALLIANCE July 1, 2009-June 30, 2010

# Creating opportunity FROM THE GROUND UP

This report to the Tennessee Higher Education Commission is a publication of the Science Alliance, a Center of Excellence at The University of Tennessee, Knoxville

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Science Alliance Span of Operation July 1984-2010



over photos by Jack Rose.
Rose, a freelance photographer, was chief photographer for the Knoxville *Journal* from 1987–1990 and taught basic photography in the UTK College of Communications during 1994–1996.

The front cover features the open stairwell in SERF (Science and Engineering Research Facility); on the back cover, floor tiles in Ferris Hall. Built in 1930, Ferris Hall is representative of many classic buildings on The University of Tennessee's campus. In contrast, SERF is a \$25 million, 120,000 sq ft building constructed in 1997 to house laboratories for both the College of Engineering and the College of Arts and Sciences.

Individual portraits for this report were taken by Jack Parker (http://jackparkerphoto.com/). Parker has worked as a freelance photographer in Knoxville since 1994, following graduation from UT in 1992 with a BFA in sculpture and photography.

Throughout this booklet you will find photos of architecture and grounds from across the Knoxville campus. Some have been cropped; others are displayed as taken. We challenge you to identify each image and where it appears on the university campus.

These images represent both old and new infrastructural support for research and education in Tennessee. In the context of this report, they symbolize what can be achieved through solid, consistent foundational backing. Science Alliance programs take a "ground-up" approach, encouraging and sustaining the ideas and talents of creative scientists and engineers.

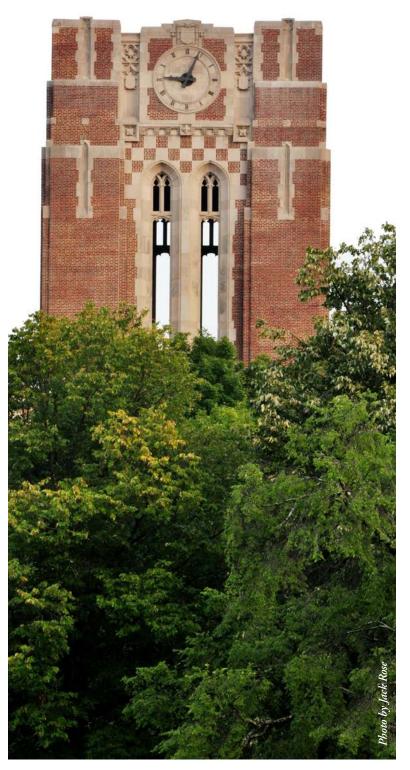
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Growth and energy are apparent across The University of Tennessee, Knoxville campus, in the classrooms and research laboratories; in the recent opening of the James A. Haslam II Business Building (2009) and Howard H. Baker Jr. Center for Public Policy (2003); not to mention the rising construction of the Min Kao Electrical Engineering and Computer Science Building that greets you on the corner of Estabrook Road and Cumberland Avenue and the mindful restoration of Ayres Hall, which, after 89 years, finally includes installation of clocks in its bell tower.

Most exciting are the results of all this activity—the new buildings, the Ph.D., Masters, and Bachelor's degrees awarded, the scientific discoveries and technological advances. Here is where the Science Alliance makes a significant contribution, laying groundwork and providing a framework to support creative ideas, train talented young scientists and engineers, and bring research leadership to UTK and ORNL.

## Spotlight on Research

# The Science Alliance creates opportunities from the ground up

In the midst of concern about economic stability, national stewardship of public funds for science and engineering calls for new initiatives in healthcare, sustainable energy, environmental protection, agricultural stability, homeland security, and many other areas of vital interest. The Science Alliance helps ensure that the public's investment in these ventures is well spent. Its programs build cross-disciplinary teams of scientists and engineers to address the most significant challenges of our time, in a trio of converging fields: nanotechnology, information technology, and biotechnology.

This annual report highlights initiatives sponsored by the Science Alliance during the fiscal year 2009–2010. In these pages is evidence of how we maximize the benefits of research funding, creating opportunities at the right time and in the right way to encourage the ideas and talents of our best scientists and engineers. It is our pleasure to share this year of success and accomplishments with you.



## 2010 Joint Directed Research and Development Projects

#### **IDRD** First-Year Awards

Paul Crilly & Seddik Djouadi, Department of Electrical Engineering and Computer Science: "Integrated navigation systems for GPS-denied environments" (Integrated navigation system for GPS-denied environments, Stephen Fulton Smith)\*

Joshua Fu, Department of Civil and Environmental Engineering: "Downscaling of global chemistry and climate predictions: regional analysis and local impacts" (Climate change impacts on energy infrastructure, David J. Erickson III)

Ivan Maldonado, Department of Nuclear Engineering: "Revolutionary radiation transport for next-generation predictive multi-physics modeling and simulation" (Revolutionary radiation transport for next-generation predictive multi-physics modeling and simulation, John C. Wagner)

**Stephen Paddison**, Department of Chemical and Biomolecular Engineering: "*Ab initio* studies of Li+ mobility in solid electrolytes and their interfaces" (Tough electrolytes for batteries—composites inspired by nature, Nancy Dudney)

**Edmund Perfect**, Department of Earth and Planetary Sciences: "Neutron imaging of fluids in rocks and soils" (Neutron imaging of fluids within plant-soil-groundwater Systems, Hassina Z Bilheux)

Mingjun Zhang, Department of Mechanical, Aerospace, and Biomedical Engineering: "A nature-derived nanoparticle and nanofiber-based scaffold for enhancing chemical detection and imaging" (Standoff detection and imaging of chemicals, Thomas George Thundat)

\*ORNL Laboratory Directed Research and Development (LDRD) project titles and principal investigators are listed inside parantheses.

#### **IDRD** Second-Year Awards

Itamar Arel, Department of Electrical Engineering and Computer Science: "A Semi-supervised learning system using deep belief networks for multi-modal medical data analytics" (Data analytics for medicine using semi-supervised learning [DAMSEL], Barbara Beckerman)

Michael Best, Department of Chemistry: "Synthesis and assembly of geometrically defined building blocks for dynamic covalent synthesis of robust higher order organic frameworks" (Controlled hierarchical self-assembly of robust organic architectures, Benjamin Hay and Radu Custelcean)

Aimée Classen & Nathan Sanders, Department of Ecology and Evolutionary Biology: "Developing a systems biology approach for linking genetic and environmental constraints to primary productivity—can patterns scale to the field?" (Developing a systems biology approach for linking genetic and environmental constraints to primary productivity in model and nonmodel species, David Weston)

Michael Gilchrist, Department of Ecology and Evolutionary Biology: "Integrating models of protein translation and gene fixation with experimental data in the archaeal system: *Ignicoccus-Nanoarchaeum*" (A systems biology approach to study metabolic and energetic interdependencies in the *Ignicoccus-Nanoarchaeum* system, Mircea Podar)

Arthur Ruggles, Department of Nuclear Engineering: "Molten salt cooled high temperature pebble bed reactor" (Investigation of molten salt thermal performance in pebble beds using unique heating techniques, Graydon Yoder)

Glenn Tootle, Department of Civil and Environmental Engineering: "Adaptation of water resource systems to climate change through weather modification" (Uncertainty assessment and reduction for climate extremes and climate change impacts, Auroop Ganguly)

**Zhili Zhang**, Department of Mechanical, Aerospace, and Biomedical Engineering: "Active control of surface plasmonics for nanoscale diagnostics" (Active control of surface plasmonics with ferroelectricity, Jian Shen)

## The Joint Directed Research and Development Program

oint Directed Research and Development (JDRD) projects are chosen for their potential to align the research interests of The University of Tennessee, Knoxville (UTK) and Oak Ridge National Laboratory (ORNL). Each project is linked independently to an ongoing ORNL Laboratory Development Research and Development (LDRD) project. JDRD grants concentrate on problems at critical developmental stages, where initial results, fruitful UT-ORNL connections, and joint publications make persuasive arguments for increased external awards. Now in its fifth year, we have clear evidence the program is making a difference. Current and former JDRD teams have reported 35 publications since the program began in 2006; four were published in 2009. In FY10, 15 proposals for external funds were submitted or planned; 2 have been awarded funding, to date.

#### Two success stories

In 2006 researchers Brian Edwards and David Keffer received the first of two-years' JDRD funding to work with their LDRD counterpart on a multi-scale simulation model, linking mechanical properties, such as strength and elasticity, to nanoscale structure. Keffer and Edwards addressed the technical difficulties of bridging known atomic-level physics to large-scale outcomes. Their models can slow, or freeze, simulated experiments, making it possible to examine nanoscale behavior at any instant in time.

Before the project ended in 2007, the Keffer-Edwards JDRD-LDRD collaboration led to a \$260,000 grant from the National Science Foundation (NSF).

Then, last fall, Shengting Cui and Bamin Khomami took advantage of a running start from their 2007–2008 JDRD funding, to apply for and win a \$600,000 DOE Nuclear Energy University Programs (NEUP) grant to improve nuclear fuel separation methods. Nuclear fuel reprocessing—a matter of selectively separating out valuable isotopes in spent fuel before sending them back to feed the reactor—reduces radioactive waste by 95 percent.

The JDRD team and their ORNL counterpart set out to develop scientific tools to understand and model the solvent extraction processes. Solvent extraction is the method widely used in aqueous-based reprocessing. It employs two liquids—a water-based solvent that dissolves the metal ions from spent nuclear fuel and a water-repelling (oily) organic solution containing an extractant agent such as tributyl-phosphate (TBP) in a dodecane solvent.

Cui says the TBP molecules at the aqueous-organic interface act as extracting agents. Sitting partly in the oily solution (organic phase) and partly in the water (aqueous phase), they capture and transport the valuable nuclear materials into the oily organic solution. The team's computer simulations detail how TBP attracts uranium—in the form of uranyl ([UO $_2$ ] $^{2+}$ )—and other targeted ions away from their watery surroundings and deposits them in the oily solution.

Now, he says, with the help of the NEUP grant they will push this simulation beyond its current, limited size and nanosecond boundary.

"Really, to be practical—to be useful to the experimental team at ORNL—we need a larger system of molecules and simulations that run for a microsecond or longer," Cui says, as opposed to the few nanoseconds usually done.

This research comes at an important time, given the recently abandoned plans for the Yucca Mountain repository and Secretary of Energy Steven Chu's charge to the new Department of Energy (DOE) Blue Ribbon Commission on America's Nuclear Future in early March, to review the "policies for managing the back end of the nuclear fuel cycle."

"JDRD funding gave us an early start," Cui says. The team, which includes Valmor de Almeida, Benjamin Hay and Kevin Felker of ORNL, has already published several papers. They lead the country in this research.

Like many JDRD ventures, both projects called upon extensive computing power, such as that supplied by Jaguar in the National Center for Computational Sciences at ORNL and Kraken in the UT-ORNL National Institute for Computational Sciences (NICS). Kraken, with 1.17 petaflops of computing capability and 147 terabytes of memory, is ideally designed to run computationally demanding scientific simulations.



## Paul Crilly & Seddik Djouadi

UTK electrical engineering and computer science

#### Engineering trustworthy navigation systems

Good engineering practice for critical applications demands both backup plans and redundancy in order to validate data.

Nearly a household word these days, GPS (Global Positioning System) has rapidly permeated our society and its systems for communication, information, and navigation. But it is not failsafe; typical rates of coverage are, at best, 85 percent, and it is also subject to deception or "spoofing" by an adversary or other interference. Canyons, urban areas, mountainous terrain, underground locations, and those deep inside large buildings pose significant challenges. For those instances, GPS can provide faulty information without even a clue that the location is inaccessible or the data is compromised by obstacles or obfuscated by intentional noise. Other technologies based upon radio frequencies—such as TPS (Terrestrial Positioning System) and LORAN-C—promise to correct and augment the increasingly popular GPS systems.

Together with UTK graduate students Zach Crane and Xiao Ma, and undergraduate Brian Doll, JDRD researchers Paul Crilly and Seddik Djouadi are developing a system called TRI-NAV with robust, low-cost capabilities to substantially improve location precision, accuracy, and reliability in a multitude of commercial, consumer, and military applications. To do so, they will also take advantage of the existing infrastructure, which has long supported other radio-based technologies, and make the case for keeping those in place for that purpose. Thus, their work is both timely and cost effective. Their investigations address both the mathematical foundation and practical implementation, in order to integrate and correlate data from both GPS and TPS systems.

In complement with LDRD work undertaken by Stephen Smith at the ORNL Position, Navigation, and Timing Program, this JDRD project will test the new integrated system in a variety of adverse conditions and benchmark its performance against conventional GPS receivers in typical field applications. Both teams expect to collaborate in future funding proposals to U.S. defense agencies as well as the Garmin Corporation.

## joint directed research & development

## Joshua Fu

UTK civil and environmental engineering

#### Predicting climate change and air pollution

In the early 1920s, Lewis Fry Richardson played with a mathematical weatherprediction scheme that divided the globe into checkerboard squares and required 64,000 people to calculate the forecast for the entire world.<sup>2</sup> Some 30 years later in the 1950s, meteorologists got their first real taste of computer forecasting with the advent of vacuum-tube computers.

Today's tera- and petascale supercomputers make it possible to run extraordinarily sophisticated simulations that incorporate everything from the effect of volcanic eruptions on temperature patterns to the influence of shifting sea ice on the sunlight reflected back into space.<sup>3</sup>

The collaborative JDRD-LDRD projects led by Joshua Fu of UTK and David Erickson of ORNL develop computational simulations that assess the impact climate change could have on future energy demands, looking for the best possible mix of resources to address our needs. Both take advantage of the Jaguar and Kraken peta-scale systems. Erickson's LDRD simulations provide a global-scale platform from which to assess the model's predictive ability and to identify critical gaps in their capacity to relate climate models to energy resources.

But, says Fu, "Research shows that the future conditions predicted by global models do not necessarily apply to regional observations or models."

His JDRD project downscales the output from the global model.

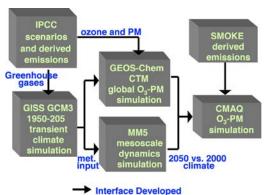
"[It is the] first fine-scaled analysis of the effects climate and energy demand have on precipitation and air quality in the United States," he says.

His team will evaluate detailed local climate/air quality conditions, such as drought, floods, and secondary ozone and aerosol formation.

Their results will be useful to air pollution control, water resource and health agencies. Regional rainfall predictions can help plan for adequate water supply and hydroelectric power. Fine scale, air quality data can be used to evaluate potential ozone and fine-particle matter pollution in the U.S.

Fu and Erickson will compare results to get a better understanding of how

global patterns actually relate to regional and local conditions.



Fu's group developed interface programs to integrate regional and global models into a coherent system for exploring future climate change and its effect on future air quality.



### first-year awards



## Ivan Maldonado

UTK nuclear engineering

#### Robust computational tools for nuclear power

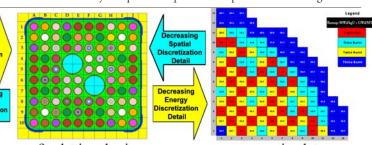
There can be little argument that what the world needs now are considerably more viable options for cost-effective, sustainable, carbon-free electrical energy.

Although no other country produces as much electricity from nuclear power as the U.S., that output comprises only 20 percent of our total requirement. In contrast, France produces 80 percent of its electricity from nuclear plants that have operated safely and reliably for many years. To achieve this higher percentage, the French take advantage of uniform management, operations, and safety systems for reactors with standardized designs that function as state utilities. If the U.S. is to boost growth of its own industry with emerging, competitive designs—while keeping efficiency and safety concerns paramount—it must address the critical need for a new generation of robust computational tools capable of predicting and tracking the status and performance of every single nuclear fuel pin in the core of a reactor—before, during, and after operation.

That is where the work undertaken by JDRD researcher Ivan Maldonado and graduate student Brenden Mervin comes in; and they are on course to bring about fundamental and radical change. Exploiting a unique approach and solution developed by their partnering LDRD team, led by John Wagner, they propose to develop and test highly accurate and fine-grained methods to analyze and predict the state of each fuel pellet from among the huge numbers found in the fuel core of modern nuclear power plants. Since these methods will eventually make it possible to precisely determine the composition of each fuel pin, they also have important implications for the larger issue of nonproliferation of nuclear material by providing for accounting, controls, and safeguards.

Maldonado brings to this collaboration exceptional research and industrial experience in computational reactor physics and nuclear fuel management that will readily enable transfer of the new method to production.

Cross sections of a fuel pin cell, a fuel assembly lattice, and quarter core. Instead of the current, multi-level, coarse-grained representations of the latter two figures, the collaborating research projects will employ the tremendous power of Jaguar's advanced petaflops processors at ORNL to model and simulate each and every fuel pellet and pin cell as depicted in the first figure.



 $\alpha = pin cell$ 

 $\beta$  = lattice physics

 $\gamma$  = core simulator

## joint directed research & development

#### Stephen Paddison

UTK chemical and biomolecular engineering

#### Better batteries

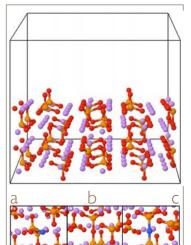
As researchers blaze new trails in discovering how to produce electricity from sources other than fossil fuels, high energy density storage devices—we call them batteries—become ever more critical components of power systems.

The high volatility of the liquid electrolyte used in today's state-of-the-art lithium batteries for applications such as hybrid and all-electric vehicles makes safety engineering both difficult and expensive. A better battery would be all solid state—based upon a robust, solid electrolyte—and rechargeable. (Oh, and did we mention low cost?)

Together with LDRD researchers led by Nancy Dudney—that project titled Tough electrolytes for batteries: composites inspired by nature—JDRD researchers Stephen Paddison and Brad Habenicht, a UTK postdoctoral researcher, propose to overcome current limitations by studying the option of replacing the liquid electrolyte with an efficient, solid lithium ion conducting electrolyte. For their part, Paddison and Habenicht will examine composites developed in experiments by the LDRD group and simulate those materials and their interfaces at a molecular level. Their theoretical results can then be used to guide further refinements of compositions and structures fabricated at ORNL.

The simulation technique to be used is known as AIMD (*Ab initio* Molecular Dynamics). It allows the JDRD team to directly model what is happening at the molecular level between the lithium ions and the solid composites (polymer or inorganic electrolytes) produced in the LDRD experiments. This work is significant because interactions in the interfacial regions between different materials in the composites are complicated and not well understood, while they have a substantial effect on the properties of the functioning storage device. As AIMD is computationally intensive, this project will make

use of an allotment of time on the Kraken Cray system of the UT-ORNL National Institute for Computational Sciences.



A schematic of a simulation cell used to investigate the interface between  $\rm Li_3PO_4$  and vacuum. Below that: Depictions of defects in the  $\rm Li_3PO_4$  lattice that increase lithium ion conductivity and define LiPON: a) is the  $\rm PO_3N$  defect; b) the  $\rm O_3P$ -O-PO $_3$  bridging structure; and c) the  $\rm O_3P$ -N-PO $_3$  bridging structure.

In both, the lithium (Li), nitrogen (N), oxygen (O), and phosphorus (P) atoms are purple, blue, red, and orange, respectively.



### first-year awards



## ED PERFECT

UTK earth and planetary sciences

#### High-tech water witching

A dowser scans the ground with a fresh-cut, y-shaped twig held taut in closed, upturned palms. When the stick turns down, water is said to lie below. What the twig is alleged to do for the dowser, neutrons do scientifically for soil hydrologist, Ed Perfect.

Sensitive to hydrogen, neutrons are attenuated (scattered and/or absorbed) as they pass through samples of moist soil. Patterns of attenuated neutrons create images of the distribution of water in pores throughout the soil. Images collected at varying water pressures reveal how air replaces water inside the sample during drying, or vice versa during wetting.

Soil scientists use hydraulic properties to determine the soil's water-holding capacity, the time it takes for soil to adsorb rainfall or irrigation, and the rate at which water moves through saturated or partially saturated soils. Traditionally, such properties are measured based on experiments run on samples in containers.

"But, inside the sample, it's essentially a black box," says JDRD team leader Ed Perfect. As a result, the data obtained must be combined with assumptions about the distributions of air and water in the sample in order to predict flow and transport.

A newcomer to neutron imaging, Perfect joined forces with LDRD team leader Hassina Bilheux to develop neutron-imaging techniques to improve predictions of the behavior of fluids in plant-soil groundwater systems. Ultimately, the two teams hope to build a community of users to benefit from a future neutron imaging facility at the Spallation Neutron Source at ORNL.

Currently, Perfect conducts neutron imaging studies at ORNL's HFIR facility and at the National Institute of Standards and Technology in Gaithersburg, MD. His JDRD study combines data from both two-dimensional (radiography) and three-dimensional (tomography) analyses. When plotted the data form a water-retention curve, from which he can glean those all-important hydraulic properties. The results will be used to strengthen mathematical models for predicting flow and transport in soil, and oil-water displacement in underground petroleum reservoirs.

Neutron radiography images of water (blue) displacing air (green) as a soil column is wetted up from below (Time 1 = initial dry state, Time 6 = final wet state). Note the filter paper at the bottom of the column which remains saturated with water throughout.

## joint directed research & development

## Mingjun Zhang

UTK mechanical, aerospace, and biomedical engineering

#### Stuck

Tiny drops of glue glitter on a sundew's hair-like tentacles. A mosquito flies too close, its wing grazing the sticky bubbles. When the mosquito tries to fly away the glue stretches and pulls it back to the leaf. The vibrations from the insect's struggle to escape generate a mechanical response in the leaf, and it curls around the prey to lock it inside.

In addition to helping the sundew capture lunch, bioadhesives secreted by plants and animals help flies walk upside down on the ceiling, ivy climb straight up a brick wall, marine barnacles cling to a ship's hull, and *giardia* protozoa attach to intestine walls.

"Sundew's amazing natural adhesive distinguishes it among carnivorous plants," says JDRD project leader Mingjun Zhang. "The glue stretches up to a meter long.

"The elasticity is crucial because it allows strong contact with the prey and helps to transport the insect to the inner leaf surface."

Curious about the sundew glue's nanoscale characteristics, Zhang's team examined it under atomic force microscopy and found a nanofiber-nanoparticle scaffolding structure deep inside the elastic adhesive.

Inspired by the structure, Zhang immediately began to think about practical uses. Could this adhesive be made into a strong, easily identified nanoscaffold, for anchoring the sensors used in signal detection and imaging systems, for example?

The JDRD program gave Zhang a chance to test this idea on a new standoff chemical screening system being developed by LDRD team leader Thomas Thundat. Standoff detection is done at distances that reduce the danger to humans or other vital resources. Thundat's goal is to develop a screening device capable of identifying the molecular signature of chemicals at distances as great as 100 meters.

"Background interference is a major challenge for long-distance screening," Zhang says. "The sundew nanoscaffold's molecular signature will be easy to identify and eliminate from Thundat's screening results."

Zhang also sees a future for the adhesive nanoscaffold in image labeling, cell-growth guidance in tissue engineering and regenerative medicine applications, coatings to enhance biofuel cell conductivity, and solar cells with better optical properties.

Below left: the entire sundew plant structure; its numerous leaves with attached tentacles.



Plants were typically 3.4 cm tall and 5.3 cm wide. On the right: a higher magnification of the leaf showing the unique structure of the tentacles, including the sticky mucin attached to the head of each tentacle.





#### ITAMAR AREL

UTK electrical engineering and computer science

#### Detection deep inside medical data

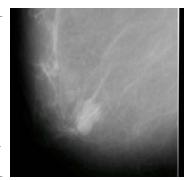
Mammography, a special form of x-ray imaging, is a tool used by radiologists in the challenging task of detecting masses or calcifications that may be indicators of breast cancer. To make mammography an even more powerful technique in the arsenal of busy, highly skilled practitioners, scientists have begun to investigate computer-aided diagnostic methods to more accurately and efficiently recognize patterns of interest and significance in the imaging data of patients.

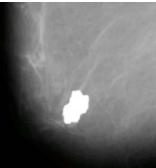
Now in its second year of funding, the JDRD research of Itamar Arel—with doctoral students Derek Rose and Steven Young—incorporates a novel system developed at UTK for classifying mammographic images. Based on a unique biologically-inspired technology for classifying visual content, the approach derives from recent neuroscience research that discovered how the cortex of the brain captures spatial and temporal information by maintaining a "deep" hierarchical neural network. In effect mimicking the way in which the brain interprets visual patterns, the system can cope better with the "noisy" data encountered in detecting abnormalities.

In just its first year as a JDRD project, a powerful new deep machine learning modeling engine called DeSTIN (Deep SpatioTemporal Inference Network) has been developed and used successfully on mammography data sets consisting of images, as well as pathology data and textual reports. Together with the corresponding LDRD research of Barbara Beckerman and her team in the ORNL Biomedical Science and Engineering Center (BSEC), DeSTIN will be used to examine additional data sets and explore alternative analysis schemes for comparison and validation in this second year of collaboration.

Initial results are promising and have led to publication in the *IEEE Computational Intelligence Magazine* and papers delivered at the BSEC Conference and the International Conference on Information Technology (ITNG). The team is also preparing a large-scale joint National Institutes of Health (NIH) proposal, due in October 2010.

The visual display on the right demonstrates how DeSTIN aids in highlighting the presence of the mass depicted in the mammography image on the left





## joint directed research & development

#### MICHAEL BEST UTK chemistry

#### Nice crystals—nice properties

Chemists use the simple term "nice" to indicate stable crystals with highly ordered structures. Those tend also to offer beneficial properties for vital applications.

However, there is nothing that is simple or easy about predicting and controlling structure at the molecular level, in order to develop the "nice" new materials that exploit these desirable properties. Fortunately, JDRD scientist Michael Best's team—comprising graduate students Chi-Linh Do-Thanh, Heidi Bostic, and Meng Rowland—excels at employing the challenging tools and methods of synthetic organic chemistry required to create such materials.

The JDRD research employs a novel strategy to control the assembly of robust architectures in high-quality crystal engineering, using a technique called dynamic covalent chemistry (DCC). This approach not only retains the advantages of reversible self-assembly of materials, including adaptability and self healing, but also generates materials with increased stability.

The JDRD team's efforts to design good molecular building blocks exploits computational methods developed by Benjamin Hay, distinguished scientist in the ORNL chemical sciences division (CSD). He collaborates in the corresponding LDRD project with Radu Custelcean, also of ORNL/CSD.

The computational methods identify building blocks that will self-assemble into predictable shapes. Then the chemists at UTK propose a synthesis method, synthesize the material, and finally study the result in terms of satisfying the criteria for a robust, ordered framework. Working in parallel, as well as together on both design and synthesis, the two teams are able to experiment with different approaches to maximize the scope of new building blocks and the subsequent assemblies that will be generated from them.

As the two teams continue their partnership in their second year of funding, they have also prepared a number of proposals for additional programmatic support to continue research through the Department of Energy and other sources.



Best and his graduate students recently reported research results at an American Chemical Society conference in San Francisco. Left to right: Chi-Linh Do-Thanh, Heidi Bostic, Professor Best, and Meng Rowland.





### Aimée Classen & Nathan Sanders

UTK ecology and evolutionary biology

#### Do genes respond to climate change?

We can see that plant species respond differently to varied environments. Cacti do better in deserts than they do in tundra, and spruce trees do better at the tops of mountains than in tropical forests, says JDRD team leader Aimée Classen.

On a global scale, altered precipitation patterns and warming trends bring large shifts in species distribution, say Classen and co-team leader Nathan Sanders. But is there any evidence that individuals of the same species respond differently to different environments?

"Individuals in the same species can be very different—just look around at a room of people—and have very different traits, such as leaf size and leaf color. We are interested in knowing if these trait variations alter the way an individual responds to environmental change," Classen says

Classen, Sanders, and their LDRD counterpart David Weston speculate that one way to get at that information would be to link genes to ecosystem functions, such as the quantity of carbon absorbed by a plant or the amount of energy produced by photosynthesis.

Global warming aside, the Earth's geological processes responsible for fluctuating ecosystems have caused glaciers to advance and retreat and turned great inland seas to grassy plains. In their wake, as plants and animals evolved they developed and retained a core of physiological mechanisms to protect themselves from stressful changes in the environment. These two projects help identify the genetic controls underlying those adaptive traits.

"If we can associate gene modules with environmental stress, such as warming, and correlate these modules to plant traits, we might be able to use that information to identify and relate same-species responses to the environment," Classen says.

During year one, Weston's group began to identify evolutionarily conserved groups of heat-stress-and-recovery genes that are associated with assimilating  $\mathrm{CO}_2$  and absorbing energy in three well-know (model) plant species. Classen and Sanders extended the approach to a non-model species, *Solidago altissima* (goldenrod).

"If we can specify the genetic controls underlying adaptive traits, then we might be able to use genetic indicators as an analogue to predict whether, and how, particular species can adapt to changing climates," Classen says.

Undergraduate Lauren Breza measures ecosystem carbon exchange in the study's goldenrod garden.



## joint directed research & development

## MICHAEL GILCHRIST

UTK ecology and evolutionary biology

#### Those ever-so discriminating genes

Nobel Laureate Frederick Sanger developed the basic technique used for DNA sequencing in 1975. Today, after 35-plus years, the number of sequenced genomes stands at 3000 and climbing.

This wealth of information, says JDRD team leader Michael Gilchrist, extends beyond the basic codes living cells use to make proteins.

"For example, many genes show distinct preferences among the multiple codons available to encode a given amino acid," Gilchrist says.

Basically, he says, the genes encode amino acids using triplets of nucleotides called codons. Since there are four types of nucleotides, adenine (A), guanine (G), cytosine (C), and thymine (T), the nucleotide-triplets can create 64 different codons (4x4x4=64). But, cells only use 20 different types of amino acids. As a result, the genetic code is inherently redundant, with some amino acids having as many as six possible codon choices.

"The genes don't use these redundant codons equally, though," says Gilchrist. "They show what we refer to as 'codon usage bias'.

"Our goal is to use the genomic sequence data to make quantitative inferences about how often a gene is expressed based on how picky it is in its choice of codons," Gilchrist says.

An evolutionary biologist, Gilchrist turned to computing power to pull information out of the data. He and LDRD team leader Mircea Podar combine experimental and computational methods to learn how natural selection has influenced the subtle codon preferences within specific genes and the affect these preferences have on the energetic cost of gene expression.

Two organisms provide the data for their projects, *Ignicoccus hospitalis* and its obligate symbiont *Nanoarchaeum equitans*. The JDRD team will help Podar unravel the tightly woven energetics between host and obligate symbiont and understand how these interactions evolved.

Similarly, Gilchrist's group will use the experimental data Podar provides to test and refine their mathematical and computational models. In year two, the team resolved a difficult statistical problem, simplifying their approach to achieve unbiased estimates. They will now expand this method to extract additional information on how often a gene is used based on its choice of codons.



## second-year awards



#### **ARTHUR RUGGLES**

UTK nuclear engineering

#### Safe, efficient, affordable nuclear power

While most people in the U.S. have forgotten the sustained level of public investment that went into building the existing fleet of nuclear power plants, they will certainly be reminded soon. The next generation of power production plants, with the much greater efficiency required to reduce our carbon footprint, will not come cheaply or quickly.

Now in its second year of funding, this JDRD research is a leading indicator for the larger scale of development that will be necessary to produce a commercially viable, very-high-temperature power plant. Operation at the maximum temperatures possible in the thermodynamic power cycles that generate electricity plays a significant part in improving this efficiency.

Consequently, fundamental research in thermal-fluid transport is once again a "hot topic," and UTK's nuclear engineering department, with its longstanding expertise in this area, is well positioned to make use of work and partnerships in a number of applications, including high-temperature hydrogen production and solar collecting systems with high-temperature energy storage.

An LDRD project team headed by Graydon Yoder of the Nuclear Science and Technology Division built a small molten salt loop system to reestablish and advance this much needed technology. In the companion JDRD research, Arthur Ruggles and his graduate research assistant John Ritchie have identified, developed, and tested instrumentation capable of withstanding the high temperatures, testing both experimentally and in the molten salt-based energy production systems themselves. One sensor design, in particular, shows significant promise. In its second year, the JDRD project will fabricate and test five high temperature pressure measurement devices for the molten salt flow loop with the expectation that practical instrumentation will be achieved.

Both ORNL's loop and UT'Ks instrumentation constitute a substantial commitment on the part of the collaborating, experienced thermal-fluid researchers at both

institutions. Together these projects are already attracting interest as a means for integrating storage in power systems and are prime candidates for additional funding.

Graduate student John Ritchie beside the experimental pressure instrumentation setup at ORNL.



## joint directed research & development

## GLENN TOOTLE

UTK civil and environmental engineering

#### Let it snow!

Beijing's claim to have dispersed looming rain clouds for the opening ceremonies of the twenty-ninth Olympic games in 2008 fell on skeptical ears. Who can say it wouldn't have remained dry without their efforts?

Thirty-seven countries around the globe practice some form of weather modification,<sup>4</sup> as do eleven of our western states. California's Department of Water Resources estimates a conservative 4 percent increase in runoff from their enhancement projects. A Utah Department of Natural Resources study in 2000 claimed an average increase of 7 to 20 percent in their April snowpack's water-content; the data came from a group of weather modification projects in operation from nine to 22 years.<sup>5</sup>

Amidst these claims of success, a 2003 National Research Council report concludes that while weather modification shows "strong indications of induced changes" in some cases, "[the] evidence has not been subjected to tests of significance and reproducibility."

"A tremendous amount of dense hydrological data are needed, before and after, to evaluate the performance of modification experiments," says JDRD team leader Glenn Tootle. "Unfortunately, the data are not readily available, so we turn to hydrologic models to estimate surface and subsurface runoff."

Tootle and LDRD team leader Auroop Ganguly are helping the National Center for Atmospheric Research (NCAR) conduct an independent study for the state of Wyoming to see if cloud seeding significantly increases snowfall runoff.

Wyoming began the five-year, \$8.8 million project in 2006, targeting snowfall in the Sierra Madre and Wind River mountain ranges. Both feed the North Platte River basin and have excellent locations for ground seeding and experimental control areas.

The two teams use meteorological, soil, and vegetation data to estimate whether increased snowfall brought on by weather modification will actually make a difference to the farmers and ranchers in the watershed.

Given the forecasts of increasing temperatures, Tootle says, "the project also has far-reaching potential in the Tennessee Valley where heat and flat-line

precipitation could alter water supplies and hydroelectric power."

Sally Rose Anderson, Ph.D. student in civil and environmental engineering, and Professor Tootle at a Weather Modification generator in the Wyoming Wind River Range.





## second-year awards



#### ZHILI ZHANG

UTK mechanical, aerospace, and biomedical engineering

#### Controlling nanoscale surfaces

A little remarked discovery occurred in the last decade when scientists succeeded in "squeezing" spectral light into sub-wavelengths, revolutionizing conventional optics for the purpose of studying nanoparticles. If current experimentation is successful, this breakthrough promises dramatic innovations in many applications, such as biosensors for health care or concentrating light for solar energy.

In this JDRD research, nanoparticles are inserted into an impressive new material (LuFe $_2$ O $_4$ ) recently engineered and fabricated at ORNL. Then small amounts of voltage are applied, in a sense "tuning" the surface spectral response. In this way the specially-engineered surfaces can adapt to different environments such that diverse applications are possible with a single device. For example, in third generation photovoltaic devices, nanostructures on the surface could automatically track solar spectra from ultraviolet to infrared and adjust to changing conditions for maximum efficiency.

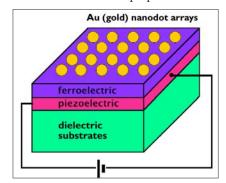
While previous investigations along these lines have been limited to static (passive) structures, calibrating by applying voltage to the surface material allows for far greater active control and discernment of nanoparticles, both in changing environments and in diagnoses of the special, dynamic characteristics of flow.

In its first year of funding, JDRD researcher Zhili Zhang and his students, including undergraduate research assistants Jeremy Petersen and Matt Elder, have used the tools of Surface Enhanced Raman Scattering (SERS) spectroscopy and a new fiber optic laser purchased specifically in support of this project for both experimental validation and computer modeling of the new material fabricated by ORNL. The results provided a comprehensive materials analysis to the corresponding LDRD project, Active control of surface plasmonics with ferroelectricity, under the direction of Jian Shen.

In its second year of funding, undergraduates Matt Elder and Zach Dixon joined post doctoral research associate Scott Lenaghan on Zhang's JDRD team. Several papers have already been published, and additional proposals

are in preparation for grants in this emerging frontier of research in nanoscale photonics and plasmonics.

The proposed Au (gold) nanodot/ ferroelectric structures. The ferroelectric to paraelectric transition can be achieved by changing the external electric field applied on the peizoelectric layer.





## Science and the Expanding Envelope

Of the many phrases used to describe high-profile research, the most common refer to the work as leading- or cutting-edge; ground- or path-breaking; or research on the frontiers of science. Some opt for "pushing the outside of the envelope," a phrase with roots in mathematics but popularized by Tom Wolfe in *The Right Stuff.*7 Wolfe writes: "... probing the outer limits of the envelope seemed to be the great challenge and satisfaction of flight test" for Navy test pilots in 1955.

Realistically, these expressions can't convey the constancy required of the men and women whose work chips away at the perimeters of known science; nor, for that matter, can they communicate the cautious excitement felt by a research team as it compiles evidence to support a new idea.

## UT-ORNL DISTINGUISHED SCIENTISTS

The individuals in the UT-ORNL Distinguished Scientist Program fit this profile. All are internationally recognized leaders in their respective fields.

The Distinguished Scientist Program anchored the Science Alliance in its partnership-building role during the center's early years. Today, UT-ORNL appointments of this caliber are being made through the Governor's Chair Program (see pages 29–38).

#### Elbio Dagotto

UTK physics and astronomy; ORNL materials science and technology

#### Nanoscale dimensions and correlated electronic behavior

nanoscale<sup>8</sup> or smaller object behaves differently from its larger-scaled counterpart. Logically, this makes sense; even if you know only a little about atoms and electrons, or the mathematical constructs and complex experiments that define them.

Visualize a film, one-atom or one-molecule thick. Spread it out across a flat surface, with the atoms distributed like marbles on a tray. The film's increased surface area in relation to volume creates a different dynamic than you would expect to find in a three-dimensional material of the same substance, where the atoms surround each other. The one-dimensional film's electronic and atomic movements are confined (restrained) to the interior of the nanoscale surface—a fact that changes the material's mechanical, thermal, and catalytic characteristics. Physicists use the phrase "strongly correlated electronic behavior" to describe this phenomenon.

Elbio Dagotto develops computational models and numerical techniques that predict how strongly correlated electronic materials will respond in the presence or absence of an electronic or magnetic field. His research group studies transition metal oxides, a family of materials with promise for improved memory devices, solid-state batteries and other energy-saving electronics.

Building on new scientific ability to prepare multilayered materials with atomically perfect interfaces between alternating layers of oxides, Dagotto's group began studying the electronics inside these substances. Their models help explore how differences in chemical composition might be exploited to transfer charge from one layer to another.

Dagotto also models materials that are simultaneously ferroelectric<sup>9</sup> and magnetic (multiferroic). "Multiferroics are rather rare 'creatures', . . . [I]t is difficult to combine ferroelectricity and ferromagnetism in the same material<sup>10</sup>," write the editors of *Nature Materials* in an issue dedicated to the topic. Dagotto's group is looking for methods that will stabilize these materials for use as long- and short-term computer data storage and other electronic applications.

In related work the group investigates colossal magnetoresistant manganite materials and iron-arsenic superconductors. Recently they also developed a technique for studying correlated electronic materials in real-time as opposed to calculating averages over time.

In 2009 Dagotto was elected a Fellow of the American Association for the Advancement of Science.

#### Atomic-scale dynamics of metallic glass

Takeshi Egami

UTK materials science and engineering and physics and astronomy; ORNL materials science and technology

e've used glasses for millennia, yet their atomic-level physics remains poorly understood.

While many liquids transform into crystalline structures at their melting temperature,

glasses do not; they solidify into amorphous (noncrystalline) structures. The temperature at which a liquid becomes a glass is called the glass transition temperature (Tg). For amorphous solids, whether oxide (common) glasses, organic polymer glasses, or even the new metallic glasses, Tg is the critical temperature that separates their glassy and rubbery behaviors.<sup>11</sup>

"The glass transition was the key in understanding the cause of the Challenger disaster, as was pointed out by Richard Feynmann," Takeshi Egami says.

Especially intriguing to Egami is a new family of glasses made from metals. In spite of being tougher and less brittle than ordinary glasses and more resilient than conventional metal, 12 metallic glasses have not fared as well in toughness. 13 Scientists have not been able to discover how the failures occur. Initially they thought that the heat dissipated by the deformation caused the glass to melt.

"More recent evidence suggests the heat is simply a by-product of deformation," says Egami, "not the cause."

Egami's research team set about discovering exactly what happens to the atoms and molecules when metallic glass fails. Their computer simulation showed the material's viscosity (fluidity) came from both temperature and stress in a relationship where the effect of stress reduced the glass transition temperature, leading to stress-induced softening.

"In other words, the mechanical failure is nothing more than a stress-induced glass transition," Egami says.

#### High-temperature superconductivity

1987 Nobel Prize winners Bednorz and Müller discovered high-temperature superconductivity 24 years ago for copper oxide compounds (cuprates). But their electron correlations present a formidable challenge; scientists are still looking for the underlying microscopic mechanism.



While the microscopic origin for conventional low-temperature superconductivity comes from coupling between electrons and the lattice vibration (phonons), the effect is too weak to explain high-temperature superconductivity in cuprates or the electronically and structurally

#### Takeshi Egami, cont.

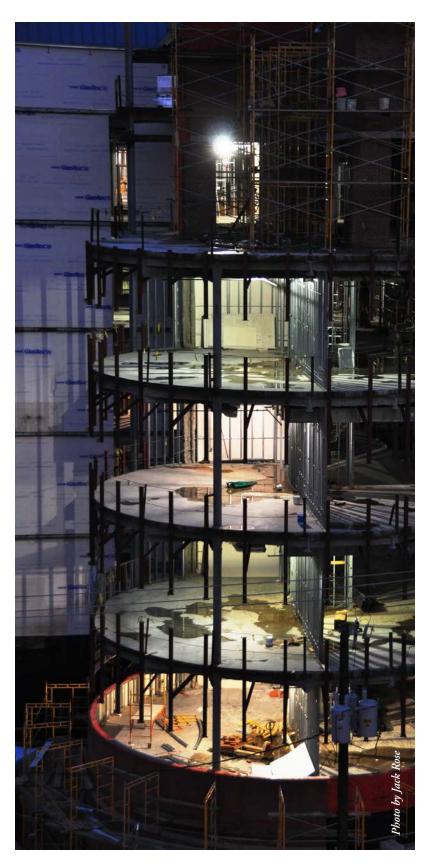
simpler—and hopefully easily understood—family of iron-pnictides<sup>14</sup> found, two years ago, to possess this phenomenon.

Most researchers, Egami says, look at electron-phonon coupling via the conventional coupling that comes from interaction between the phonon's electrical charge and the electrons, rather than the electron-phonon coupling via the spin, the quantum property that refers to the magnetic orientation of electrons and atoms on which Egami focuses.

Egami's team uses neutron scattering to study coupling between electrons and phonons. In this case they are looking at the interaction between the electron's spins and phonons.

Spin effects are much stronger in cuprates and pnictides than in conventional superconductors, Egami says. They could hold the key to understanding high-temperature superconductivity in these mateirals.

Egami received the 2010 J.D. Hanawalt Award from the International Union of Crystallography, with S. J. L. Billinge. The Hanawalt Award is given for important contributions to the field of x-ray powder diffraction. He also organized a threemonth workshop on the physics of glasses at the Kavli Institute for Theoretical Physics (KITP) at the University of California, Santa Barbara—a high honor, as KITP is the focal center for theoretical physicists.



# Separation science: determining chemical processes in living organisms

GEORGES GUIOCHON

UTK chemistry

iving cells, going about their daily business, metabolize food into fats, which they store to satisfy further energy needs, and provide other vital cell-building chemicals. The process involves nearly 1000 metabolites (low molecular weight compounds).

Scientists have been investigating the cells that make and store fats, to see if they might be harvested for biodiesel fuels. Algae are particularly attractive because they do not make cellulose but only fats and need only water, sunlight, and a few minerals to survive. But researchers need to understand the details of the metabolism of these fats if they are to select the algae with the highest productivity and the most favorable conditions for their culture.

Georges Guiochon says, "The complexity of these mixtures of metabolites defies the most powerful combinations of analytical methods currently available."

A single simple step in the metabolism of fatty acids, triglycerides, glucose, or cholesterol involves several hundred different metabolites. Unraveling the successive steps involved requires identification and quantitative analysis of each.

Biochemists and molecular biologists turn to liquid chromatography (HPLC) to fractionate the mixtures of compounds isolated from cells. HPLC percolates a steady stream of solvent through a long tube packed with fine adsorbent particles. Samples are injected at the column inlet, and their composition monitored at the exit. Given the proper

solvent and adsorbent, each compound will migrate along the column at its own velocity, depending upon the molecular interaction with the adsorbent surface. The eluted fractions are analyzed by mass spectrometry (MS), which identifies the molecular structure, and/or nuclear magnetic resonance (NMR), which identifies spatial relationships within individual compounds.



But each of these methods has limitations, says Guiochon. MS requires relatively simple mixtures of six to 12 compounds; NMR is only useful if the sample is pure. HPLC will separate complex mixtures into fractions

#### Georges Guiochon, cont.

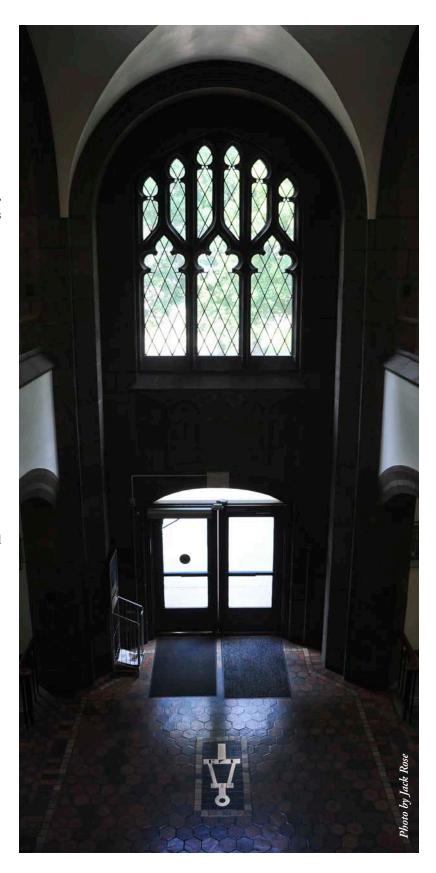
simple enough to be identified with these spectrometric methods but it is limited to a few hundred chemicals per column.

To address the problem, Guiochon's group couples together two successive separations.

This can be done in a number of ways. The most powerful collects a few hundred fractions at the exit of one column and separates these fractions on a second column, according to different characteristics. Success requires the development of fast methods of chromatography, which recently led to a rapid evolution of chromatographic column technology. The new columns are packed with finer and finer porous particles, which makes them faster and more powerful; but this also increases the inlet pressures, and temperatures rise from the friction of the liquid stream percolating through the column. The escaping heat cools the column wall faster than the center. As a result the center stream is faster than flow at the wall because heat decreases viscosity. So, the bands of compound leaving the column are not uniform.

Guiochon's investigations found a solution to this problem. They replaced the conventional packing with particles that have a solid core surrounded by porous shell. The chromatographic properties of the shell are the same as the fully porous ones, but they conduct heat out from the center far more quickly, reducing the loss in efficiency.

A leading expert in multidimensional chromatography, Guiochon received the 2010 Lifetime Achievement Award for contribution to separation science from the *LCGC Magazine* at the recent Pittsburg conference and the 2009 Professor Andrzej Waksmundzki Medal from the Polish Chemical Society.



#### Structural geology and tectonics of continental crust

Robert Hatcher

UTK earth and planetary sciences

oday's continental crust is a product of some 4-billion years interaction of the solid Earth, oceans, and atmosphere. Nearly modern continental crust first appeared about

crust first appeared about 3 billion years ago when Earth's plate-tectonic processes began. It has grown in mass—with parallel changes in composition—to its present configuration, mostly by the addition of mountain chains along the flanks of continents.

Bob Hatcher has investigated the processes that generate and change continental crust for more than four decades. He studies the Appalachians both in the field and in the laboratory and compares them with other ancient and modern mountain chains in Europe and North America to determine how the mountain-building process varies both in time and with respect to position.

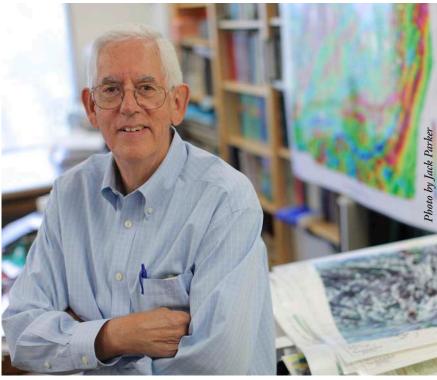
We understand the process of mountain building reasonably well

from studies of chains that are still under construction, like the Andes and Himalayas, Hatcher says. But numerous unanswered questions remain, particularly about the deeper parts of the crust that are best exposed in some of the older chains like the Appalachians.

He says, today we also understand the relationships of earthquakes and volcanoes to the boundaries where the tectonic plates collide with each other. The numerous large earthquakes and volcanoes that occur on the west coasts of North and South America are direct products of plate collision.

One of the great, unresolved problems in tectonics, however, is the cause of large, damaging earthquakes in interiors of plates, such as those in West Tennessee (1811-12) and at Charleston, SC (1886). The New Madrid seismic zone in West Tennessee and adjacent states produces more earthquakes per year than any other region in the eastern U.S. It and other seismically active regions like Charleston, SC, and New England have been intensely studied for years.

The second most active seismic zone in the eastern U.S., however, is the East Tennessee seismic zone (ETSZ), which extends from just north of Knoxville southward into northwestern Georgia and northeastern Alabama. But, until



recently, no extensive study has been done because no historic earthquakes greater than magnitude 4.6 have occurred there. Nevertheless, the U.S. Geological Survey has rated the ETSZ as being capable of a magnitude 7.5 earthquake, based on the large size of the area where earthquakes occur and their frequency. Eastern U.S. earthquakes commonly originate some 5- to 15-miles deep in the crust, and while there are numerous surface faults in eastern Tennessee, none of these have been active for millions of years.

During 2009-10 Hatcher led a group of geologists and earth scientists in a one-year Nuclear Regulatory Commission-funded pilot study of the ETSZ to determine if there is evidence of prehistoric, large earthquake activity. The results were

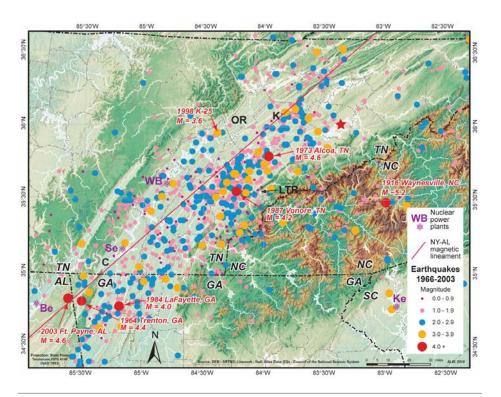
#### Bob Hatcher, cont.

outstanding: numerous fractures and small faults have been found in stream deposits, along with some indications of liquefaction of water-saturated sand. These secondary effects from earthquake shaking confirm that prehistoric greater-thanmagnitude 5.5 earthquakes have occurred in the ETSZ.

Questions remain about when the ancient earthquakes occurred and how often large earthquakes have occurred in the ETSZ. The answers have a direct bearing on the hazards and design of engineered structures, such as buildings and roads, as well as the overall seismic hazard in the eastern U.S. These questions will be addressed in the coming years.

(a) Bottom left: Large fracture in weathered shale bedrock that was later filled with stream gravel (dark material down the middle of the photo). Hatcher's colleague Dr. Steve Obermeier stands at the lower end of the fracture for scale.

(b) Bottom right: A closeup of light orange weathered shale in (a) shows that the large gravel-filled fracture was displaced about 2.5 inches by a small, younger fault, produced by an earthquake.



East Tennessee seismic zone earthquakes from 1966–2003 superposed on a Digital Elevation Model of the region. The red line is the New York-Alabama lineament; the red star is the area near Dandridge, Tennessee, where most of the data confirming extensive prehistoric earthquake damage has been found. It is clear that additional work should be concentrated in the area of greatest earthquake frequency southwest of Knoxville (K), as well as in the cluster of earthquakes in northwestern Georgia.

C–Chattanooga. LTR–Little Tennessee River, OR–Oak Ridge. Nuclear power plants: Be–Bellefonte. Se–Sequoia. WB–Watts Bar. Ke–Keowee. Streams and reservoirs are shown in white.



#### Hydrogen fuel-cell conductivity

UTK biochemistry and cellular and molecular biology and materials science and engineering; ORNL materials science and technology

DAVID OY

getting the most out of their semipermeable membranes.

David Joy, along with others involved with the STAIR project (see page 39), is studying the physical, electrical, and mechanical properties of Nafion™ membranes (the membrane of choice used in most fuel cells today).

ne of the trickiest problems in developing hydrogen fuel cells is

We know generally how fuel cells work. Hydrogen enters the anode side of the cell and, aided by a catalyst, splits into electrons and protons. On the other side of the cell a catalyst-coated cathode attracts oxygen from the air to its surface, creating a kind of electrical pressure called a potential. A thin membrane separating the anode and cathode allows the protons to pass through but rebuffs the electrons, hydrogen gas, and oxygen. Electrons attracted to the oxygen on the other side of the membrane flow through an external circuit and back into the cell, supplying power for electrical motors or equipment along the way. To complete the circuit, the protons pass through the membrane, pair off, and bond with the oxygen and incoming electrons to form water.

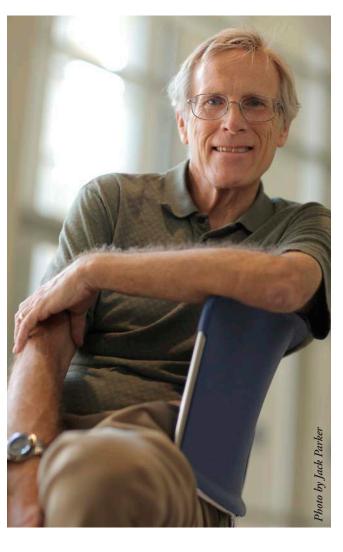
"The current of protons through the Nafion™ produces the desired electrical output, but the microscopic details of their transmission through the membrane remain unknown," Joy says.

Joy develops techniques to improve the accuracy and performance of electron and ion-beam imaging tools. His team set up a system in the ORNL Center for Nanophase Materials Sciences to measure the conductivity of pure membrane samples and correlate it with Nafion's™ microstructure and other physical attributes. Initially, they will map the actual conduction pathways along which the

protons travel to see how they are affected by the membrane's topography and thickness. Following that, the team will examine the material's performance under more realistic conditions of humidity, air pressure, and temperature.

#### Focused ion beam tool

An ongoing project studying the affect of cerium oxide (CeO) nanoparticles on living tissue (E. coli) brought an interesting auxiliary discovery. Thought to be the material of choice for next generation catalytic converters, CeO particles can assume a long, sharp, needle-like shape, potentially capable of penetrating cell walls. Scanning transmission and electron microscopies revealed the CeO rarely penetrated the study's living E. coli cells.



Joy's group found their focused ion beam tool was an excellent scalpel, capable of cutting E. coli in half without any mechanical damage or distortion. Ph.D. student Jetana Kittisenee also found the ion-beam tool useful for turning tree branches, roots, dried leaves, etc., into ethanol. Her work shows that irradiating the biomass with ions enhances their ethanol yield because it breakes down the tough, insoluble lignin component prior to immersion in water.

#### IOSEPH MACEK

UTK physics and astronomy; ORNL physics

#### Electron vortices in simple atomic systems

magine water swirling around a drain or a tornado snaking across the landscape. According to Joseph Macek's three-dimensional models, something like this happens when a proton punches its way into atomic hydrogen. A vortex forms as electrons respond to the collision, leaving

evidence of the original proton-hydrogen impact in their wake.

The probabilities of finding electrons at given points in space are described mathematically in quantum mechanics by wave functions. Macek relies on this theory to study what happens to simple fragmented atomic systems when atoms collide.

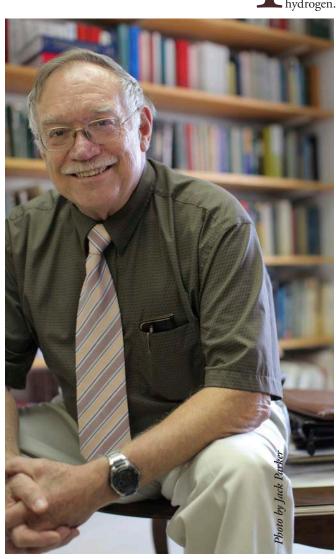
In 2007, his research group discovered the evidence for vortices in the measurements from electrons ejected during impacts of charged particles and photoabsorption (where photon energy transfers to atoms and molecules).

Hoping to confirm the existence of the theorized vortex structures, Macek's team joined forces with an experimental group from Frankfurt, Germany, which had data from electron impact ionization (e,2e) processes—a technique used to ionize and fragment the sample molecules before analysis by mass spectroscopy. The term e,2e is shorthand for the phenomenon that occurs when electrons strike an atom or molecule and eject two electrons simultaneously.

Macek says the atomic-scale vortices can explain these interesting structures. Studies probing electron correlations show circumstances where two electrons are completely absent from the atomic system. Computations by Macek's group confirmed that the absent electrons (zero measurements) correspond to vortices in the underlying two-electron wave function.

The evidence for atomic-scale vortices in this context has implications for control and manipulation of atomic processes, for example, in the known velocity limits of charged particles used to probe atomic, molecular, and solid-state structures by fast electron beams.

Macek received the Ioffe medal and diploma from the Ioffe Physical Technical Institute in October 2008. The institute is affiliated with the Russian Academy of Sciences.



Computed ring vortices produced by photon interactions with atomic hydrogen. The red rings are regions of space in a hydrogen atom wave function where the probability for finding an electron vanishes. The green translucent region shows where the electron probability is largest. The vortices encircle the atom and move according to the hydrodynamic representation of quantum mechanics.

#### Synthesizing new polymers

IMMY MAYS

UTK chemistry; ORNL chemical sciences

he plastic, rubber, adhesives, fiber, and coating industries all rely on polymers. So it's no surprise, then, that Jimmy Mays's fundamental interest in macromolecular structures and their influence on

polymer characteristics has its practical side.

In their simplest form, polymers are one long chain of repeating molecular units. Branched polymers are macromolecules with side chains dangling from a backbone.

"Long-chain branching, even when it is present at very low levels, can have a dramatic impact on how a polymer flows," Mays says. This is critical because many products are manufactured from melted material under high shear conditions.



The discovery of metallocene catalysts for making the world's two most common plastics, polyethylene (PE) and polypropylene (PP), made it possible to spin the polymer into fibers or blow it into films at much faster rates, and without the surface defects that mar their appearance, Mays says.

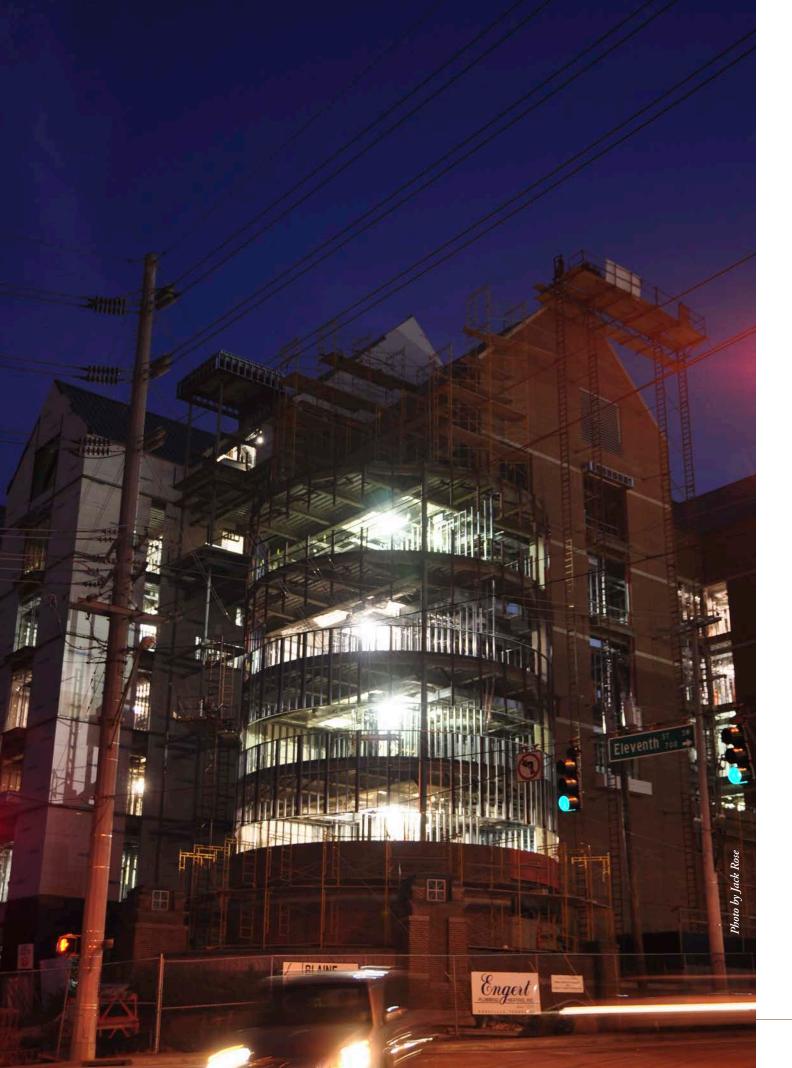
Unfortunately, the PE and PP produced using these catalysts are complex mixtures of linear, single branch, and more highly branched chains with substantially different lengths, which makes reliable structural-property relationships difficult to pin down.

"For 20 years, groups have tried to gain insight into the effects of branching through synthesis and study of 'model branched polymers'—ideal materials with equal chain lengths and only one type of branching architecture. But the different groups report varying results, and no consensus on the quantitative effects of branching exists," Mays says.

In fact, says Mays, a new technique called temperature gradient interaction chromatography (TGIC) recently revealed that many branched polymers, previously viewed as models for that type, contained substantial impurities, which could not be identified by other chromatographic processes.

Mays's group invented new synthetic strategies to avoid the impurities. Incorporating TGIC into their work, they now produce several series of welldefined and characterized models of branched polymers available for studies of deformation and flow (rheology). Ron Larson (Michigan) and John Dealy (McGill) collaborate with Mays on the National Science Foundation project.

Other research by the group explores a new class of versatile, potentially low-cost membranes for hydrogen fuel cells and lithium-ion batteries. Effective, low-cost membranes are desperately needed to limit release of carbon dioxide into the environment. The new material has up to ten times the proton conductivity of Nafion™ (currently the favored choice for fuel cells) at one-tenth the cost. The UTK-ORNL team will now explore the material's potential for carbon-capture membranes.



# Governor's Chair appointments (in order of arrival)

Jeremy Smith (2006) molecular biophysics

Alexei Sokolov (2009) polymer science

Howard Hall (2009) global nuclear security

Yilu Liu (2009) power electronics

Tom Zawodzinski (2009) electrical energy storage

**Robert Williams** (2009) genetics of central nervous system disease and addiction

**Frank Loeffler** (2009) microbiology and civil and environmental engineering

**William Weber** (2010) radiation interactions with materials

**Brian Wirth** (2010) computational nuclear engineering

## Tennessee Governor's Chair Program

Exceptional opportunities to combine the best talent with the resources of both a notable research university and distinguished national laboratory don't come along every day.

The university, founded in 1794, and ORNL, which grew out of the federal program to develop nuclear weapons in World War II, have always shared academic and research interests and infrastructure; never more so than when UT-Battelle, LLC, was established in 2000 as a private not-for-profit company to manage and operate the national laboratory for the U.S. Department of Energy. This partnership and the increasing importance of research and technology to the state's economic and environmental well being led Governor Phil Bredesen to invest significant additional state resources in the joint venture.

Initiated in 2005, the UT-ORNL Tennessee Governor's Chair program takes advantage of the synergy between the state's flagship university and the nation's leading multipurpose laboratory. The program recruits exceptionally accomplished researchers, worldwide, to help solve global problems. A first appointment came in 2006, when Jeremy Smith accepted a Governor's Chair in molecular biophysics. So far, nine individuals have joined the program.



#### Supercomputing and Neutrons—Jeremy Smith

eremy Smith has assembled a team of four UT professors and three ORNL staff scientists to probe biological mechanisms at the molecular level, using high-performance computing and neutron scattering.

Generally speaking, says Smith in a 2007 interview for the *ORNL Review*, "we want to understand enzyme reactions and how enzymes use chemical energy to make molecular machines work, such as the proteins in muscle contraction, vision, or cancer-cell growth."

Enzymes are selective catalysts, only working on specific molecules, from which they take the first part of their name and add the suffix "ase" to indicate their enzymatic status. They bind temporarily to the substances involved in a chemical reaction, lowering the amount of energy needed to activate that reaction.

In our bodies, enzymes accelerate numerous reactions, including DNA replication and the digestion of food. Elsewhere in nature microbial enzymes such as hydrogenase and cellulase help turn plant stems and leaves into sugar.

In one project, Smith's computer simulations and neutron scattering experiments examine the position and motion of atoms during the enzymatic digestion of cellulose.

Working out how to release the sugar subunits from the cellulose is a challenge.

"Humans want to make alcohol [ethanol] out of plants, but plants do not want to be made into alcohol," Smith says. 16

The sugars needed for fermentation are trapped inside lignocellulose, which is extremely resistant to hydrolytic degradation—the reaction that occurs before cellulose is broken down into glucose.

Smith says that little is known about how the enzymes interact with the biomass, an important aspect of understanding lignocellulosic resistance to hydrolysis.

His team uses molecular dynamics simulation to calculate how the parts of the lignocellulosic biomass are arranged and how strongly they are bonded to one another at the atomic level. The natural enzyme complexes found in cellulose act as catalysts to break it down. The team's massively parallel code running on UT's petascale computing system Kraken makes it possible to see how the enzymes react with each other and with cellulose. Kraken is housed in the National Institute for Computational Sciences (NCIS) at ORNL,

## Tennessee governor's chairs

#### Designing polymer molecules—Alexei Sokolov

mong the variety of materials around us, polymers occupy a special and important place. Synthetic or natural, they are everywhere in our daily lives; moreover, life itself essentially relies on polymers—consider proteins, DNA, and cellulose, for example.

Alexei Sokolov's group studies the fundamental properties of polymers. They use what they learn to design molecules and materials with the properties desired for various applications.

"Our specific expertise is actually in molecular motion," Sokolov says. "Molecular motion is the key to many materials properties.

"We study both synthetic and biological polymers: for fuel, for batteries and fuel cells, for nano- and biotechnologies.

"We are after different properties, simply depending on their applications," he says.

For example, his group helps design lightweight polymeric-based composites with greater mechanical strength and toughness than metal.

"If we can replace metals with materials that are three to five times lighter, we can improve significantly the fuel efficiency of our cars and planes. The new Boeing 'Dreamliner' is actually made from this kind of material. As a result it can fly longer and consume less fuel," he says.

Another direct application for Sokolov's group is in creating polymers for batteries and fuel cells.

"We target polymeric membranes that increase power and reduce the weight of batteries. This might finally open the door for electrical vehicles that go -200 to 300 miles without charge," he says.

Sokolov's group also identifies the motion and activity of biological polymers such as proteins, DNA, and RNA.

"One application for our results is in bio-preservation—that is how to preserve activity of biological systems for a long enough time," Sokolov says.

This problem is important to pharmaceutical companies (drug and vaccine preservation) and medical applications (tissue and organ preservation). In one case Sokolov's group designed a solvent that preserves proteins at room temperature for years without any significant degradation.

"For the lightweight polymeric materials, we want good mechanical properties (strength, toughness)—good or even better than metals," he says. "For batteries we are looking for materials with good ionic conductivity (fast ionic motions). For questions of biopreservation we look for the opposite behavior—materials that can strongly suppress any kind of biomolecular motion."

# JEREMY SMITH UT-ORNL Center for Molecular Biophysics; UTK biochemistry and cellular and molecular biology; ORNL biosciences



ALEXEL SOKOLOV

UTK chemistry; ORNL chemical sciences





### Nuclear security—Howard Hall

he odds of a nuclear attack or accident in the United States are not in our favor," says nuclear chemist and national security expert Howard Hall. "Most experts put the chances of a nuclear event in the next five years at around 25 percent." 18

Hall is a member of an elite team of scientists, law enforcement experts, policy advisors, and politicians assigned the task of protecting the U.S. from nuclear threats. He says global nuclear security involves two fundamental issues: opportunistic threats and arms-control negotiations.

Hall says: "The ability to detect radioactive material in realistic scenarios, such as within the flow of commerce or at crowded events, is critical to preventing radiological terrorism, let alone detecting and measuring radioactive material to verify compliance with arms control treaties and to keep the material from being diverted into dangerous, illegal pursuits.

"We can have terrific technology for detecting special nuclear materials, but if we can't differentiate between legitimate and illicit radioactive material, it won't be useful," Hall says.

Roughly one of every 1,000 to 2,000 individuals in the U.S. has detectable radioactive signatures from nuclear medicine, such as heart and thyroid scans and cancer treatments. This means that if we could detect all the radioactive signals from Neyland Stadium on game day, we'd get between 50 and 100 alerts, just from the crowd alone, he says.

The challenge is to identify the source and do away with threatening situations.

Hall is training future engineers to meet that challenge. This spring, his nuclear engineering class carried out a practical exercise in developing strategies against theft of stored nuclear materials. The drill took place at the Y-12 National Security Complex, a weapons-grade uranium storage and processing facility in Oak Ridge.

In the hypothetical face-off, a blue team of students was assigned the task of protecting weapons-grade uranium secretly stored by a fictional government inside Pasqua Hall; a red team endeavored to infiltrate the facility and detonate the material.

"The students get real, practical training in putting together a system—or rather a system of systems—to keep that material out of the hands of the bad guys," Hall says.

## Tennessee governor's chairs

#### Smart grid technology for electrical power—Yilu Liu

magine being able to tell exactly how much electrical power it takes to run your dishwasher and then use that information to move power-hungry tasks to times when electricity is less expensive. Or, what if you were not only compensated for saving energy but also allowed to sell excess self-generated power back to the grid with few technological or regulatory barriers.

This and more is what developers of the Smart Grid propose.

While our electrical power system has become quite effective at supplying power to homes and businesses (so much so that the National Academy of Engineering called it the engineering achievement of the twentieth century), technology has outstripped the grid's capabilities. Its communications systems are too slow and localized to support the kind of integrated communication needed for a fully automated, reliable, secure, interactive Smart Grid.<sup>19</sup>

"I think the Smart Grid will definitely change the way we use electricity as individual customers," Yilu Liu says.

But, she says, "There are a lot of areas we [in the research community] haven't yet explored."

For their part, Liu's team develops new and better ways to monitor and understand large-scale flow of electrical energy through the nation's power grid.

"Right now we can only observe the system and try to digest what we see.

"Once we have more understanding we will be able to develop a theory and tools to control the system," she says.

Liu expects her research group to gain the kind of understanding necessary to contribute to the Smart Grid's development, most especially in preventing blackouts and other failures.

HOWARD HALL
UT nuclear engineering; ORNL global nuclear
security technology



YILU LIU

UTK electrical engineering and computer science;

ORNL energy and transportation science



Photos of Howard Hall, Yilu Liu, Tom Zawodzinski, William Weber and Brian Wirth courtesy of Kim Cowart and the UTK College of Engineering:



## Storing electrical energy—Tom Zawodzinski

hile fuel cells and batteries serve a similar purpose, they are not the same thing. To be sure, both are electrochemical devices, but fuel cells have an external fuel source; batteries do not.

Batteries store chemical energy in a closed system, then convert and release it as electrical energy on demand. A rechargeable battery uses an external energy source to reverse the electrochemical reaction. In contrast, this same oxidation-reduction reaction in a fuel cell is powered internally.<sup>20</sup>

"A fuel cell is a device that takes in a fuel and burns it—but without burning it. It actually converts the chemical energy inside the fuel into electrical energy," Thomas Zawodzinski says.

Zawodzinski studies the basic mechanics of elementary chemical processes occurring in materials used in batteries and fuel cells.

"You've got ions and electrons moving around inside there," Zawodzinski says, "and I want to know how to make them move faster and how to make the reactions occur faster; how to design materials to make that happen.

"[Industry]—especially Toyota, Honda, GM—are pushing very, very hard to put [fuel cells] in cars," he says, adding that "at least one company will release a fuel cell car by 2015, if not sooner.

"This is far and away the hardest application because basically the cost you pay for an [automobile] engine is extremely low relative to any fuel cell we can make right now.

"But as we scale up in manufacturing there's a possibility we can lower those costs to where they can be competitive. That's certainly what the projections show."

Zawodzinski's work explores how to make the fuel cells and other energy storage technologies more durable and ensure that they function properly at the high temperatures often present in these devices.

## Tennessee governor's chairs

#### Computational genomics—Robert Williams

e are now venturing into new genomic territory made possible by ultra-high throughput sequence," writes Robert Williams in a recent commentary for *Frontiers in Neuroscience.*<sup>21</sup>

To date, most studies to discover the role of genes in various diseases have relied on mutagenesis techniques pioneered at ORNL using the common house mouse. More recently, single genes have been targeted in mice using so-called "knock out" technology. Both methods fundamentally disrupt gene function. Scientists then study the mutant offspring and track down the genes that were hit to determine exactly what went wrong.

But Rob Williams says: this single shot approach doesn't tell us much about the most common and pervasive diseases—heart disease, neurodegeneration, psychiatric disorders—which usually come from an accumulation of small, detrimental effects of many normal genes that for one reason or another just don't work together well.

These complex and, unfortunately, common human diseases often correspond roughly to an equivalent mouse trait or disease; even autism and schizophrenia have mouse models. To study the genetics of these types of diseases, Williams and colleagues can cross breed mice with specific, but different, ancestries (strains) and then compare the risk in the offspring.

Through tricks of breeding, mice can be bred to be genetically identical—like human identical twins; except it is possible to have hundreds of these identical mice.

"The beauty of using genetically 'fixed' mice is that they are not only identical but they are also in a sense immortal. It is possible to reproduce the same type of mouse for many years and study it in many environments and in many different labs," Williams says.

It is as if each of us had one hundred identical "twin" brothers or sisters who had been studied for over 10 generations and in many situations.

"Imagine what you could do with that kind of information," he says. "Scary, but powerful."

Williams uses many different sets of identical mice (up to 100 sets) to study the genetics of diseases that range from high blood pressure to aging to impaired brain function. His group combines mouse resources with new, highly efficient DNA sequencing technologies and sophisticated computational methods to determine just how far we are likely to get with personalized human health care.

## Tom Zawodzinski

UTK chemical and biomolecular engineering; ORNL materials science and technology



ROBERT WILLIAMS
UT Health Science Center anatomy and
neurobiology





#### Environmental microbiology—Frank Loeffler

hen it comes to countering the damage humans do to the environment there's no silver-bullet. We need all the help we can get.

Frank Loeffler is one of the "good guys" in the fight to restore our environmental health, amidst the needs and desires of exploding global populations.

Loeffler's team studies the intricate biological processes that naturally occurring bacteria use to break down toxic contaminants, such as chlorinated solvents; immobilize radioactive wastes; and reduce greenhouse gas emissions. His is one of several research teams around the globe that correlate microbial ecology with function to predict and, if necessary, enhance pollutant detoxification.

Loeffler's group is interested in novel microbes with unusual enzymes and genes. He says: of all the microbes out there less than one percent has been characterized, so that we know what they do. Which means the undiscovered potential for engineering and medical applications is enormous.

"There's a lot of promise in the microbial world for new antibiotics, for new pathways that degrade environmental pollutants, for generating energy. We have just scratched the surface," he says.

"And now we have new tools that allow us to study this unexplored diversity and functionality [what they do] in much greater detail," Loeffler says. "So, there are many great opportunities to make new, important discoveries; it's a very, very exciting time to do microbiology."

His group's innovative discoveries form the basis for collaborations with others in microbiology and engineering, developing useful molecular monitoring tools and testing them in real-world situations.

Loeffler says UTK and ORNL are attractive because they have a strong cross-disciplinary base for doing fundamental research in his field, not to mention their close proximity to one another.

"Many people here are pursuing similar goals, and we [the university and national laboratory] have great opportunities to lead research efforts in the area of environmental biotechnology" he says.

## Tennessee governor's chairs

#### Radiation interactions with materials—William Weber

nvision how a billiard ball collides with other billiard balls on a pool table," William Weber suggests.

"That is how radiation reacts with the atoms in materials.

Basically it knocks them about in their structure; sometimes they come back together, sometimes they don't."

When an electrically charged atom (an ion) hits a solid, it either knocks the atoms about or transfers energy to the electrons. The first reaction is becoming fairly well understood; the second is less so.

Weber and ORNL collaborator Yanwen Zhang developed an experimental approach to measure the energy lost to the electrons in such collisions, a vital step in understanding what happens to the ions, as well as the material it hits.

Energetic ions are the primary mode of energy dissipation from nuclear reactions and radioactive decay. So understanding how the materials react is key to maintaining today's, and designing tomorrow's, reactors.<sup>22</sup>

Weber's research uses both direct measurement of materials and extremely powerful computer simulation. It has broad applications, touching areas from nuclear energy to environmental remediation, and even space exploration.

"We want to be able to predict the performance of the materials in nuclear reactors for 30 to 60 years; or in nuclear waste products, where we may need to predict the behavior of the material over 10,000 or one-million years, depending on what the regulators eventually decide," he says.

Weber's group is building a new ion accelerator laboratory at UTK. Once that comes online, his group will have a unique niche for training researchers and contributing to university and national laboratory research.

# FRANK LOEFFLER UTK microbiology and civil and environmental engineering; ORNL biosciences



WILLIAM WEBER
UTK materials science and engineering;
ORNL materials science and technology



## Tennessee governor's chairs

#### BRIAN WIRTH

UTK nuclear engineering; ORNL computer science and mathematics





rom solar powered homes to plug-in hybrid cars, the search for safe and reliable energy sources marches on. Nuclear power, too, is back on the table as a viable energy resource, as the U.S. strives to become more energy independent and lower its carbon footprint. Of course nuclear power is already in use, but to date, none of the U.S. plants use recycling techniques to reclaim the uranium and plutonium remaining in the spent fuel.

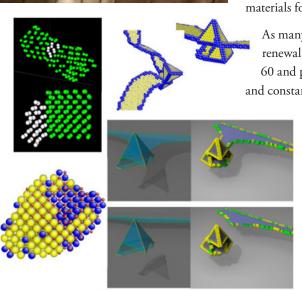
Today's nuclear power plants obtain energy through fission (splitting atomic nuclei); however we can't write off nuclear fusion (the process by which lightweight atoms under pressure are fused to form heavier atoms, releasing energy) as another possible future energy resource. For example, Steven Crowley, director of the United Kingdom's Culham Fusion Science Center<sup>23</sup> (their national laboratory for fusion research), believes that in spite of the high-temperatures required (some 150 million Kelvin) and the extremely complex technology, we will have real electric power from fusion sometime in the 2030s.<sup>24</sup>

Brian Wirth investigates the performance of nuclear fuels and structural materials in nuclear environments. He expects this research will lead to improved predictions about the longevity of nuclear reactor components and ultimately to the development of high-performance, radiation-resistant materials for advanced nuclear fission and fusion energy power plants.

As many of the nation's aging nuclear reactors' licenses come up for renewal, Wirth will have the opportunity to examine the effects of 40 to 60 and perhaps as much as 80 years of exposure to extreme temperatures and constant bombardment from radiation.

"Some may not be tough enough to withstand future use, creating the danger of vessel failure or even meltdown," Wirth says.

Wirth's research group uses high-fidelity computer simulation to study the lifetime of nuclear reactor components and the physical processes responsible for material defects and the degradation of reactor performance. Along with better reliability assessments, the group can use what they learn to develop new, more durable materials, ultimately capable of containing the energy from nuclear fusion reactors.



Results from computer simulations of irradiated material show how defects affect behavior at nanoscales.

## support for students



## SUPPORT FOR STUDENTS

## Integrative Graduate Education and Research Traineeship

The Science Alliance contributes to two IGERT projects. The STAIR project (Sustainable Technology though Advanced Interdisciplinary Research) trains graduate students for research careers exploring alternative energy resources. SCALE-IT (Scalable Computing and Leadership Edge Innovative Technologies) teaches future biologists to be adept at combining computing and experimental resources. IGERT awards from the National Science Foundation are for innovative programs that train graduate students to use an interdisciplinary approach.

STAIR (Sustainable Technology through Advanced Interdisciplinary Research)

Program directors—David Keffer & Paul Frymier (both of UTK chemical and biomolecular engineering)

#### Growth

STAIR training for graduate students is bearing fruit. A total of 18 UTK faculty members and seven ORNL researchers have joined at least one of three interdisciplinary research teams. Ten students joined the program in the fall of 2009; 13 are currently in the program.

In FY10, two new interdisciplinary courses, a new interdisciplinary graduate certificate in sustainability science, and a seminar series were added to the STAIR curriculum. STAIRMaster introduces the fundamental concepts in biology, chemistry, and materials science, and

STAIR IGERT trainees created a new panel exhibit, "STAIRing at Resource Conservation: Reduce, Reuse, Recycle," for the American Museum of Science and Energy in Oak Ridge. They then gave copies of the exhibit posters to visitors at the city's Earth Day festivities. At the table from left to right (in orange t-shirts) are Jeff Bunn, Michelle Everett, Shawn Buckley, and Rosemary He. Dr. Claudia Rawn is in the far right background (blue blouse).

engineering essential for research in sustainable technology. STAIRCase uses case studies as a platform for training teams to solve energy and manufacturing challenges. STAIRWise offers weekly seminars with speakers from government, industry, academia, and national laboratories.

#### Research

Harvesting hydrogen from photosynthetic bacteria

Biofuel production is expensive, energy-wise. Essentially the closer you are in the process to the solar energy source, the more efficient the fuel production. But, many processing methods take place too far from the source, losing a good bit of the plants' photosynthetically converted energy along the way.<sup>25</sup>

Paul Frymier and Barry Bruce (biochemistry, and cellular and molecular biology) have been searching for an efficient way to capture solar energy early in the photosynthetic process. To do this they must "trick" the photoreaction center of plants, algae, or bacteria into giving up some of their electrons, then bond the captured electrons with protons to form hydrogen gas (H<sub>2</sub>).

They found, however, that the large systems designed to harness sunlight operated at temperatures too high for most photosynthetic resources to be efficient, let alone survive. So they wondered what would happen if they used a thermophillic (heat-loving) life form similar to those found thriving in hot springs?

When the team joined thermophillic photosynthetic bacteria to a platinum catalyst and exposed this to sunlight the combination produced a steady supply of hydrogen (H<sub>2</sub>). In fact, the STAIR team found their new process was ten times more efficient as temperatures increased.

#### Improving fuel cells

The efficiency of a fuel cell depends upon its ability to transport both protons (H+) and electrons. Jimmy Mays and David Joy worked on two aspects of this problem. Mays's team synthesized a new proton-exchange, fuel-cell membrane. Their blend exceeds the proton conductivity requirements specified by DOE's Year 3 Milestone. Joy's group assembled an experimental system for scanning electron microscopy. Their work makes it possible to characterize all the key physical aspects of the membrane (including liquid layers) with one instrument.

SCALE-IT (SCALABLE COMPUTING AND LEADERSHIP EDGE INNOVATIVE TECHNOLOGIES)

Program manager—Harry Richards

#### Growth

Interdisciplinary research means interdisciplinary know-how. SCALE-IT graduate students need a diverse range of skills to be successful. Often, though, new trainees lack skills in one or more areas of computational biology. This is to be expected, given the typical focus and organization of undergraduate programs and early career experience. Computer scientists typically lack a solid background in life science; biologists know little about programming.

In the first case, SCALE-IT brings computer science students to campus early in the summer to audit an undergraduate course in biochemistry, organic biology, genetics, or another life-sciences course. They also work in a research laboratory to learn basic lab skills.

Training life science students to use computational analysis is by far the greater hurdle. Many SCALE-IT students do not have base-line computer-programming skills or the expertise required for parallel-processing analyses of huge biological data sets. The Electrical Engineering and Computer Science Department solved the dilemma, offering a course taylored to the needs of the SCALE-IT graduate students. This has benefits well beyond the needs of the IGERT program. This and a course on fundamental programming tools for

science are on their way to becoming regular course offerings.

A total of 44 faculty members from UTK and ORNL and 15 students participated in the SCALE-IT research and educational program. The program will recruit and fund another 15 doctoral level students.

#### Research

SCALE-IT trainees are already influencing biocomputational research. Sally Ellingson, a computer science major with little biological experience, began the SCALE-IT doctoral program by taking two months in the summer to audit organic chemistry and work in a biochemistry lab. Learning about nitrogen fixation in soybeans and the importance of adequate ammonia permeability measurements to examine this process, she identified a potentially more accurate method to calculate this parameter. She is now part of an interdisciplinary team evaluating the technique.

Biocomputational research is data intense, most especially when it comes to genetics. Scientists use microarray<sup>26</sup> data analysis to study the details of gene correlations; however Ellingson was struck by the inability of manual or simple clustering tools to cope with the vast data sets collected from full transcription microarrays. Her team created a code linking several types of clustering analyses together and looked for correlations among data in an existing mouse brain database. The team discovered several gene relationships that were missed in previous analyses. They believe their

## support for students

methodology could unlock the real power behind high throughput analysis.

Future protein-folding studies could benefit from the work of Jason Harris. His background in biophysics, and the computing skills gained through the IGERT-sponsored programming class, made it possible to build the code necessary to analyze the thousands of protein interactions involved.

LIVING LIGHT

# Team Tennessee builds UT's Solar Decathlon house

Low energy use, small footprint, maximum use of daylight, and passive solar design strategies: Team Tennessee will spend the next 18 months building a house with all these features for the DOE 2011 Solar Decathlon.

Entry into the event is by invitation only; and the slots are few. The 2011 competition received so many qualified entries that, for the first time since the program began in 2002, DOE held a

preliminary round. Team Tennessee, one of 34 to make it into the second round, received notice in April 2010 that they were one of 20 finalists slated to build and display their Living Light house on the National Mall

in Washington, D.C., in the 2011 competition.

The Solar Decathlon is a competition among student teams from around the world to design, construct, and operate a 1000-sq-ft, fully functional, energy

Left to right: Doug Beasley, Thinh Nguyen, Steven Coley, Megan Chafin, and Bialu Xiao pose for a photo on the National Mall, snapped during their ORNL-sponsored trip to Washington, D.C., for the DOE Schematic Design Review in May 2010.







Biophysics workshop participants engaged in a collaborative discussion. The workshop was held July 7-10, 2010, at the UTK Conference Center.

efficient home. The teams earn points in a series of ten contests that ultimately test the home's ability to function off the power grid. The houses are on display for a week; visitors can tour them for free and learn how energy-saving features can help them save money in their own homes.

The cantilever barns of Southern Appalachia inspired Living Light's design. The floor plan organizes space for bathroom, kitchen, and laundry on the two ends, framing an open living space in between. The home is designed to be energy efficient in southern U.S. climates.

"We kept returning to the phrase Living Light for inspiration," says UTK faculty advisor James Rose, "[and] incorporated multiple interpretations of this concept into the design, including transparency and open space, low energy use, and built-in storage to reduce clutter."

So far, 60 architecture, 12 engineering, and 6 graphic design students have worked on the project. Involved faculty advisors from the College of Architecture are Edgar Stach, Barbara Klinkhammer and Amy Howard, from the School of Art, Debora Shmerler, and from the Collage of Engineering, Leon Tolber. Following the competition the team plans to take the home on tour in Tennessee and to the European Solar Decathlon in 2012.



## Summer fellows: research experiences for undergraduates in mathematics, chemistry, and physics

In past years the Science Alliance has co-sponsored an NSF summer program to provide Research Experiences for Undergraduates (REU). Highly competitive, these programs attract top-performing students, many of them from excellent colleges too small for substantial research programs. REU mentors are faculty with active research agendas who work with the students on projects and in associated mini courses over a nine-week session. Many forge relationships and secure reputations with students that later bring them back to UTK to continue their studies as graduate students.

In 2010, the Science Alliance helped fund a pilot REU program in the Department of Biochemistry and Cellular and Molecular Biology. The pilot program provides the groundwork for submission of a full REU proposal to the National Science Foundation.

/bttp://www.olcf.ornl.gov/2010/07/30/)

The organizing theme for this year's program, held June 7 to July 30, 2010, was "Sensing and Signaling" with emphasis on introducing students to cutting-edge research in this broad area, bringing them in contact with a multidisciplinary group of cell biologists, geneticists, biochemists and biophysicists. A full listing of topics, faculty researchers/mentors and students selected for the program in 2010 can be found at http://web.bio. utk.edu/bcmb/reu/index.shtml.

# Summer school in biophysics

The goal of the annual Summer School in Biophysics—Computation and Experimental Challenges is twofold and transitive: to spark interest in interdisciplinary problems and "grand challenges" in biology among students and scientists in the "exact sciences," such as physics, chemistry, mathematics, materials science, and computer science. At the same time the program provides an outlet for



Trey Green and John Gardner prepare to run their Junkyard Challenge device at the 2010 National Science Olympiad Tournament.

the biological sciences community to acquaint the "exact science" community with problems that require a multidisciplinary approach and advanced technical solutions.

The workshop targets senior undergraduates, graduate students, and postdoctoral fellows in physical and computational sciences who are interested in considering biosciences as a future career and area of research. Invitation to the conference is based on a personal statement of interest, as well as a strong academic record and grade point average. In only two years, the summer program has proven immensely successful, attracting a capacity roster of distinguished presenters from around the world and students from schools with outstanding reputations. Particularly popular this year was a "Meet the Prominent" session where students were able to interact with specialists in biophysics.

Speakers also highlighted the importance of ORNL's high-performance computing capabilities in addressing biological challenges, based

upon examples of research using both Jaguar and Kraken supercomputers.

Held at the UTK Conference Center in Knoxville July 7-10, the 2010 event involved many ORNL and UTK divisions and departments, in addition to the Science Alliance—especially the UT-ORNL Joint Institute for Computational Sciences (JICS), the ORNL Spallation Neutron Source, Physical Sciences Directorate, Biological and Environmental Sciences Directorate, and the National Center for Computational Sciences (NCCS), and the UT National Institute for Computational Sciences (NICS), the Office of Research, the Genome Science and Technology Graduate Program, and the departments of Physics and Biochemistry and Cellular and Molecular Biology. Full details of the program can be found at http:// biophysics.ornl.gov/program.html.

# Tennessee Science Olympiad State Tournament and Tennessee Junior Science and Humanities Symposium

The Science Alliance contributes to two academic outreach programs, as part of national and state initiatives to increase the number and caliber of students in science, technology, engineering, and mathematics (STEM) and to enrich science and mathematics education in our schools. Building upon base funding from the Academy of Applied Science, the programs reinforce ongoing recruitment efforts and serve to give Tennessee's brightest young students the opportunity to get to know, first hand, about the exceptional reputation of the university's scientists and research facilities.

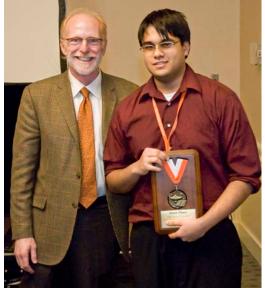
## support for students

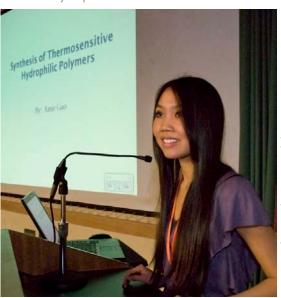




Highlights of the Tennessee Junior Science and Humanities Symposium

Clockwise from the top left: Joanna Nyland and Orlando Hollett at the Smyrna High School poster session; Demonstration tour of robots from computer science professor Lynn Parker's laboratory; Amy Guo's paper presentation; and Arts and Sciences College Dean Bruce





Courtesy of Lynn Champion and the 2010 Tennessee Junior Science and Humanities.

Bursten with TJSHS first-place winner Yajit Jain.

## Tennessee Science Olympiad

On March 27, 2010, UTK was host to 36 middle school and high school Olympiad teams with more than 800 participants. Held at the Knoxville campus since 1994, this state tournament brings winners from

seven regional Olympiads to compete for trophies and medals. The winning teams in each division receive travel support to advance on to the national competition. Not unlike the Olympics athletic games, the trials intrigue and challenge talented students and are well distributed over a wide range of scientific disciplines.

Placing first at UTK in their respective divisions of high school and middle school were Montgomery Bell Academy of Nashville and Bearden Middle School of Knoxville. Both teams went on to represent Tennessee in the national tournament held at the University of Illinois at Urbana-Champaign, May 20-22, 2010, where



they ranked 32 and 21, respectively, among the 60 teams.

The annual Tennessee State Science Olympiad is sponsored by the College of Engineering and the Science Alliance. It is administered by the College of Arts and Sciences Office of Academic Outreach, which obtains funding for team travel and arranges access to facilities and mentors/coaches from among faculty and graduate students on the university campus. A special initiative planned for October 2, 2010, is a statewide workshop for team coaches.

## Tennessee Junior Science and Humanities Symposium (TISHS)

The TJSHS requires top-notch students to 1) conduct original research in collaboration with a scientist at UT, or another research facility in the state, who serves as their mentor and 2) summarize their research findings in a formal paper that is then submitted for review by a faculty jury. Selected papers are presented at a state symposium held at UTK. The top three are invited to present their papers at the national symposium, where they may win scholarship awards.

Tennessee's 45<sup>th</sup> annual TJSHS was held on February 25-26, 2010, with 67 students and 26 teachers representing 21 Tennessee high schools, including seven schools new to the competition. Thirty-one young scholars submitted original research papers, spanning a variety of topics and scientific disciplines. Students also visited a number of laboratories at both UTK and ORNL and consulted with

scientists in a wide range of fields. Over the many years of this outstanding program, previous students have gone on to win signal achievements in several other advanced competitions—including invitations to work in notable laboratories and to submit papers for presentation and publication with full-fledged scientific societies.

This year's first place winner was Yajit Jain, a junior at Oak Ridge High School; second place Niral Sheth, a senior at Farragut High School; and third place Ariel Buehler, also a senior at Farragut High School. Two honorable mention awards were presented to Lillie Brown, a senior at Cleveland High School, and Ashley Fuqua, a senior at Greenbrier High School. The best poster award was presented to Cristen Peterson, a senior at Farragut High School. The 2010 Award of Excellence in Science Teaching was presented to Ronnie Nixon of Greenbrier High School in recognition of his tireless and sustained effort in providing research opportunities, sparking the interest of his students in the sciences, and mentoring their progress.

The subject fields of winning research papers in the 2010 Symposium included mathematics and computer science; engineering; life science; environmental science; and physics.

Additional information on both of these exemplary student programs, as well as other STEM outreach initiatives, can be found at http://www.artsci.utk.edu/outreach/CEESTEM.asp.

## OTHER VENTURES

Each year the Science Alliance contributes matching funds for new research ideas, joint institutes, support services in the university's Research Office, and conferences that fall within the scope of its mission.

# UT-ORNL JOINT SEED MONEY

# Exploring obesity-related inflammation with three-dimensional microscopy

In 2010, Ph.D. student Ben Curry joined John Biggerstaff (UTK Center for Environmental Biotechnology) and Michael Zemel (UTK nutrition) on a project, investigating the biological mechanisms of obesity-related inflammation.

Formerly thought to be primarily a matter of fat deposits, atherosclerosis actually involves an ongoing inflammatory response. The adiposcytes (adipose tissue) serve as a significant source of the chronic inflammatory conditions that precede atherosclerosis.

A growing body of evidence indicates that dairy foods confer protection against cardiovascular disease, independently of other beneficial effects on obesity and blood pressure.

Biggerstaff and Zemel received Science Alliance matching seed money to expand their work on an ORNL Seed Money project led by Christopher Mann. The two teams combined fluorescent and holographic techniques in a timesaving microscope

#### other ventures

The effects of treating adipocytes with calcitriol, leucine, and calcitriol+leucine on subsequent monocyte adherence to vascular endothelial cells under physiological flow and shear conditions.

Monocytes are labeled in red and endothelial cells in green.

that produced threedimensional images of biological specimens.

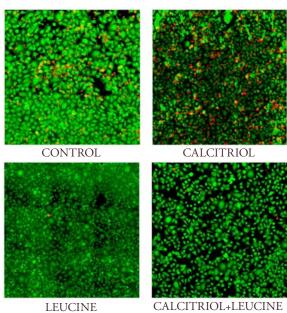
Curry used the
new microscope to
study immune-cell infiltration into
inflammatory tissues found in obese
individuals. His work showed that key
dairy components, including calcium
and leucine, reduce the ability of
monocytes to adhere to the cells that
line blood vessels. Monocytes are the
blood cells that cross the vascular wall
and trigger atherosclerosis.

Eating a low-calcium diet markedly increases the number of monocytes adhering to the vessel wall, Biggerstaff says, the first step in the formation of an atherosclerotic lesion.

Curry's finding support the hypothesis that dairy foods attenuate the risk of athrosclerosis and subsequent cardiovascular disease.

## New biodiesels and fuelchemical biosynthesis genes

Imagine powering your truck with diesel-like fuel produced by a tree. While unusual, accounts of engines being run on oleoresin collected from



diesel trees (*Copaifera*) in Brazil were reported by Nobel Prize-winning Melvin Calvin in the 1980s.

Better known for unraveling the secrets of photosynthesis, Calvin says the fuels collected directly from trees were filtered beforehand, but that's all. One caveat, though; the observations were actually based on anecdotes from Brazilian farmers in the 1970s.

Still, given their chemistry, the cyclic hydrocarbons in the diesel tree's oleoresin deserve more study to determine their usefulness as a fuel



Copaifera langsdorfii (also known as the diesel tree) in a park in São Paulo, Brazil.

source and as a means to identify key genes responsible for chemical biosynthesis, says C. Neal Stewart (UTK plant molecular genetics).

Neal, UTK collaborator Feng Chen, and graduate student Blake Joyce, (both of UTK plant sciences) have identified three additional plants that synthesize combustible metabolites (common names: kukui nut, gas plant and petroleum nut). In a partnership with ORNL, the team will study the plants' usefulness as direct sources of biodiesel or for crop improvement through introduction of transgenes into other well-known biodiesel plants. The Science Alliance contributed seed funding to this project.

Compared with petroleum diesel, biodiesels do not flow well in cold temperatures. Researchers are attempting to change this by altering the fatty acid biodiesels from oilseed crops.

"We are investigating new hydrocarbons that are not derived from fatty acids," Neal says. "They have myriad structures and conformations, so we hope they will give the same chemical variety to biodiesels that make petroleum diesels attractive and effective fuels."

Ultimately, he says, they hope to match the chemical diversity of petroleum diesel, which allows it to be modified to flow at winter temperatures in northern climates.

Essentially, Neal says, these new compounds could rewrite the ASTM International standard definition of biodiesel, which specifically requires the use of methyl esters of fatty acids derived from biological sources.



# UT-ORNL JOINT INSTITUTES

Five joint institutes link distinct complementary resources in select, high-priority scientific and engineering fields at UTK and ORNL. Science Alliance support for UT-ORNL joint institutes began with the Joint Institute for Heavy Ion Research. Organized in 1982, JIHIR opened joint facilities on the ORNL campus in 1984. In 2000, UT-Battelle used the JIHIR model to organize an additional four joint institutes in computational science (JICS), advanced materials (JIAM), neutron sciences (JINS), and biological sciences (JIBS). Detailed information on the joint institutes can be found at http://research.utk.edu/orus/.

In FY10 the Science Alliance contributed research and administrative funds and website management support to JIHIR and gave leadership support to JINS through Takeshi Egami's Distinguished Scientist appointment.

This year, several headline-making research teams were led by, or included, JIHIR-affiliated investigators: Thomas Papenbrock (UTK physics and astronomy, ORNL physics), Kate Jones (UTK physics and astronomy), Robert Grzywacz (UTK physics and astronomy, ORNL physics) and Joseph Hamilton (JIHIR co-director; Vanderbilt physics and astronomy).

#### Element 117

In April a team led by Yuri Oganessian of the Joint Institute for Nuclear Research in Dubna, Russia, reported the first observed occurrence of heavy element 117. The team, which included JIHIR co-director Hamilton, created

the new element by smashing together calcium-48 and the radioactive element berkelium-249. The collision spit out neutrons to create two isotopes of an element with 117 protons: one with 176 neutrons and the other with 177. The data supports what theorists have long suspected: that as these artificially produced elements acquire more neutrons they will become more stable and long-lived.

At first, as researchers created heavier and heavier elements, their lifetimes shortened. Then, when the elements became still heavier, their lifetimes began to climb, Hamilton told James Glanz of the *New York Times*.<sup>27</sup> That could mean they are approaching a theorized "island of stability," where lifetimes might go from fractions of a second to days or even years.

Hamilton was the primary U.S. spokesperson on the project, coordinating ORNL collaboration with the team from Russia.

## Doubly-magic tin

Atomic nuclei—protons and neutrons held together by the strong (nuclear) force—make up 99 percent of the mass of all visible matter in the universe. In the 1950s Maria Goeppert-Mayer and J. Hans D. Jensen discovered that nuclear architecture arranges those particles (known collectively as nucleons) into shells, akin to the orbits of electrons.

Once the shell of a nucleus is full, or "closed," it becomes much more difficult to add or subtract a proton or neutron. Magic numbers of nucleons—2, 8, 20, 28, 50, 82, 126—result in extra binding of the nucleus.

"Doubly magic" nuclei have magic numbers of both protons and neutrons.

In an experiment performed at the ORNL Holifield Radioactive Ion Beam Facility, Kate Jones and her colleagues, including researchers from ORNL and UTK, demonstrated that the neutron-rich isotope tin-132 is one of the "favored-few" observed doubly-magic isotopes.

Jones says tin-132, which has 50 protons and 82 neutrons, is one of only 10 observed doubly-magic nuclei.

"And now with our measurement, seven of these are well studied," she says.

Doubly-magic nuclei are particularly interesting because they provide a standard by which to assess nuclear structure. Jones' team's results promise a greater understanding of the r- (rapid) process, in which a nucleus captures a large number of neutrons in rapid succession. This process occurs in supernovae explosions and is thought to be responsible for the formation of elements heavier than iron.

"All the precious metals in your jewelry box—gold, silver, and platinum—are produced in the r-process," Jones says.

# JINS building nearing completion

Takeshi Egami reports that the construction of the JINS building begun in the fall of 2008 is complete, and they are moving in this August 2010. In 2008, JINS received a DOE EPSCoR grant of \$1M per year for three years to support neutron scattering collaboration among researchers from the EPSCoR states, UTK, and the Spallation



Neutron Source (SNS) and High Flux Isotope Reactor (HFIR). JINS shares postdoctoral fellows with the SNS and HFIR, collaborating on projects in biology, polymer science, condensed matter physics, and other areas that cross-cut these disciplines, such as glass transition research.

#### Conference support

# UT-ORNL-KBRIN Bioinformatics Summit

The Ninth Annual Bioinformatics Summit was held at Lake Barkley State Resort Park in Cadiz, western Kentucky, March 19-21, 2010. The regional summit has acquired a welldeserved reputation for enhancing collaborative links and integrating multidisciplinary research effortsresulting in numerous new, cooperative projects in bioinformatics research and education. A total of 269 participants included 81 faculty, 31 postdoctoral researchers, 63 staff and 94 students. The conference was jointly sponsored by UTHSC Center of Genomics & Bioinformatics and Molecular Resource Center, and the UTK Innovative Computing Laboratory; the Kentucky Biomedical Research Infrastructure Network (KBRIN); and the Science Alliance.

Scientific presentations were organized in formal sessions under the major headings of next-generation sequencing, epigenetics, and medical informatics. Workshops focused on introductory and advanced microarray data analysis. Mike Hawrylycz, of the Allen Institute in Seattle, Washington, delivered the keynote address on the informatics of creating large-scale digital atlases in

neuroscience. Proceedings are available online at http://www.biomedcentral.com/1471-2105/11/S4/I1.

#### Publications support

# Trace (Tennessee Research and Creative Exchange)

Administered by the University of Tennessee Libraries, Trace is a new, web-based digital archive containing the full text of creative and scholarly work produced by the UT community, thereby preserving and sharing the intellectual capital that makes Tennessee a leader in research and teaching. Content is easily identified and accessed worldwide.

When contributors upload their work to Trace, they grant the university a non-exclusive, perpetual right to use the digital assets for noncommercial use. Because authors retain the copyright for all content posted, they are free to reuse it elsewhere, and hold all proprietary rights in the work. Descriptive information about each item in the collection generates metadata that facilitates access through both local and worldwide library catalogs and internet harvesters.

Contributors receive automatically generated reports of usage. Trace resources proving to be the most popular are Selected Works—pages highlighting the research and scholarship of UT authors—and Electronic Theses and Dissertations. Other services offered include hosting both conference publications and online journals.

In addition to author pages and publications, Trace allows for access

to information such as data sets. As an example, see David Keffer's file of molecular simulations at http://trace.tennessee.edu/utk\_molecularsimulation/.

In its first year Trace added more than 3,000 resources produced in over 50 academic departments and other university units. In the same period, the archive received nearly 30,000 visits from users in all 50 states of the U.S. and many other parts of the world. Nearly half of the visitors used Trace multiple times.

Trace uses the Digital Commons platform of Berkeley Electronic Press, founded by academics in 1999 to explore new avenues for scholarly communication and publication, with emphasis on accessibility, experimentation, innovation, and outreach. At UT, sponsors are the UT Office of the Provost and the Office of Research, along with the University Libraries and the Science Alliance.

## Proposal development and grant-writing support

In FY08 the Science Alliance began to offer proposal development and grant writing support to UTK Office of Research teams. This continued in FY10 and was extended to include web development services and science writing support for articles featuring UT-ORNL research.

The following professional contractors were involved: Carmen Trammell, Jayne Dadmun, Darlene Casey, Theresa Pepin, and Lisa Carroll.

Carmen Trammell leads proposal development teams that provide management, editorial, budgetary, and other forms of assistance to PIs in the development of large, complex, or strategically important research proposals.

Jayne Dadmun supports the proposal development team, developing and completing a Quest Online Research Capacity Catalog, which supplies background information on foundations and their relationship to Tennessee and the university; federal funding agency opportunities; and alumni ties with the university that may aid the mission of the Office of Research in its service to UTK faculty.

Darlene Casey helped create a more uniform and up to date web image and presence for various departments, including the Science Alliance. She helped develop new websites/pages and UTK-standardized templates that would allow for greater flexibility and functionality, while at the same time bolster the image and efficiency of overall UTK web presence.

Theresa Pepin and Lisa Carroll completed work on the federal stimulus-related Broadband Technology Opportunities Program (BTOP) in the late summer of 2009, followed by presentations in the fall and winter to professional and public interest groups. A second, smaller grant proposal in early 2010 proved successful and will fund expanded broadband in 13 public library systems in Tennessee. While the original, comprehensive proposal for nearly \$85 million was not immediately successful, the Science Alliance's leadership role with the State of

Tennessee's Recovery Act Management Team (TRAM) was instrumental in allowing for a much wider and deeper appreciation of the problems and solutions for extending affordable broadband to the large rural areas of the state.

Pepin also supports the Science Alliance annual report preparation team, interviewing and writing brief science features and organizing photo sessions with the scientists involved.

## In Conclusion

he Science Alliance has an exceptional record of success in cultivating senior leadership, increased funding, strategic new research, superior graduate education, and dependable postdoctoral support.

Its efforts to increase and strengthen UT-ORNL partnerships make a significant contribution to the university and national laboratory. As a result, the center helps secure UTK's place in the worldwide science and engineering community, which ultimately also contributes to the economic growth of Tennessee.

## References

- 1. "Blue Ribbon Commission on America's Nuclear Future Charter," US Department of Energy, March 2, 2010, (http://www.energy.gov/news/8698.htm).
- 2. "Scientific Computation on SIMD and MIMD Machines," D. J. Wallace, *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences*, Vol. 326, No. 1591, Solving Scientific Problems on Multiprocessors, The Royal Society, Sep. 26, 1988, pp. 481-498 (http://www.jstor.org/stable/38058); and "Lewis Fry Richardson. 1881-1953" by E. Gold, *Obituary Notices of Fellows of the Royal Society*, The Royal Society, Vol. 9, No. 1 (Nov., 1954), pp. 216-235 (http://www.jstor.org/stable/769208).
- 3. "Picturing Climate's Complexity," National Center for Atmospheric Research, University Corporation for Atmospheric Research (UCAR) (http://www.ucar.edu/communications/CCSM/history.html)
- 4. "Weather Modification Multimedia Gallery," National Center for Atmospheric Research (NCAR) and University Corporation for Atmospheric Research (UCAR) (http://www2.ucar.edu/news/weathermodification-multimedia-gallery).
- 5. Weather Modification for Precipitation Augmentation and its Potential Usefulness to the Colorado River Basin States, Tom Ryan, Metropolitan Water District of Southern California, p. 14, October 2005.
- 6. Critical Issues in Weather Modification Research (2003) Committee on the Status and Future Directions in U.S Weather Modification Research and Operations, National Research Council, National Academy of Sciences Board on Atmospheric Sciences and Climate and Earth and life Studies (http://dels.nas.edu/), Executive Summary, p 3, (http://www.nap.edu/catalog.php?record\_id=10829).
- 7. The Right Stuff, Tom Wolfe, Farrar, Straus and Giroux, 1979.
- 8. A nanometer is a billionth of a meter (10-9 meter). Individual atoms measure about 0.1 to 0.3 nm, depending upon the element. By comparison the average human hair measures 100,000 nm in diameter.
- 9. Ferroelectricity is a spontaneous electric polarization of a material that can be reversed by the application of an external electric field.
- 10. "Editorial: The best is yet to come" *Nature Materials*, 6(1):1 2007 Nature Publishing Group (http://www.nature.com/nmat/journal/v6/n1/full/nmat1811.html).
- 11. *SiliconFarEast.com*, a comprehensive, online reference on semiconductor manufacturing (http://www.siliconfareast.com/tg.htm).
- 12. "Metallic Glass Yields Secrets Under Pressure," *Condensed Matter News*, March 16, 2010, Physorg.com (http://www.physorg.com/news187964555. html).
- 13. Fatigue occurs when a material is subjected to fluctuating stress and strain.

- 14. Pnictides are compounds formed from the nitrogen group on the periodic table.
- 15. "Metabolism Basics," *KidsHealth*, Nemours: A Children's Health System (http://kidshealth.org/parent/general/body\_basics/metabolism.html).
- 16. "Enzymes in motion" and "A closer look: Jeremy Smith," Carolyn Krause, *ORNL Review*, 40(1):20, and 40(1):22, 2007.
- 17. "The Next Generation of Ethanol," Elizabeth Storey, National Institute for Computational Sciences news (http://www.nics.tennessee.edu/next-generation-ethanol).
- 18. "Spotlight on Howard Hall" Kim Cowart, *Quest*, Spring 2010, pp 8-9; and "UT and Y-12 Team-Up for Nuclear Engineering Class Project," Whitney Holmes, *Tennessee Today*, (http://www.utk.edu/tntoday/2010/05/19/ut-y12-teamup-nuclear-engineering-class-project/).
- 19. "Smart grid basics," *smartgrid.gov*, Federal Smart Grid Task Force website (http://www.smartgrid.gov/basics).
- 20. "How cells work," *Electropedia*, Woodbank Communications Ltd, a battery consultancy based in Chester, U.K. (http://www.mpoweruk.com/chemistries.htm#redox and http://www.mpoweruk.com/fuel\_cells.htm).
- 21. "Headlond into a genomic singularity," by Robert W. Williams, *Frontiers in Neuroscience*, Neurosci. doi: 10.3389/neuro.15.001.2010 (http://frontiersin.org/neurogenomics/10.3389/neuro.15.001.2010/full).
- 22. 'Collision Science: How fast was that ion going when it hit?' contacts: Kathryn Long and Christine Novak, Chemical and Materials Sciences Division Research Highlights, Pacific Northwest National Laboratory, August 2009.
- 23. (http://www.ccfe.ac.uk/CCFE.aspx).
- 24. (http://www.ted.com/talks/steven\_cowley\_fusion\_is\_energy\_s\_future. html).
- 25. "Using photosynthesis to power hydrogen production" by Casey Johnston, ars technical, Nov.13, 2009, http://arstechnica.com/science/news/2009/11/photosynthesis-proves-to-be-a-powerful-source-for-hydrogen.
- 26. Microarray: Sets of miniaturized chemical reaction areas that may also be used to test DNA fragments, antibodies, or proteins, by using a chip having immobilized target and hybridizing them with probed sample. After hybridization, the color from the chip is and the data is analyzed by a soft ware to find the expression level.
- 27. "Scientists Discover Heavy New Element," James Glanz, *The New York Times*, April, 6, 2010.

## **PUBLICATIONS**

#### Elbio Dagotto

ORNL Materials Science and Technology; UTK Department of Physics and Astronomy

Dias da Silva, L.G.G.V., M.L. Tiago, S.E. Ulloa, F.A. Reboredo, and E. Dagotto, "Many-body electronic structure and Kondo properties of cobalt-porphyrin molecules," *Phys. Rev. B*, 80:155443 (2009).

Dong, S., R.Yu, S. Yunoki, J.-M.Liu, and E. Dagotto, "Double-exchange model study of multiferroic RMnO3 perovskites," *Eur. Phys. J. B*, 71:339-344 (2009).

Dong, S., R.Yu, J.-M. Liu, and E. Dagotto, "Striped multiferroic phase in double-exchange model for quarter-doped manganites," *Phys. Rev. Lett.*, 103:107204 (2009).

Dong, S., K. Yamauchi, S. Yunoki, R. Yu, S. Liang, A. Moreo, J.-M. Liu, S. Picozzi, and E. Dagotto, "Exchange bias driven by the Dzyaloshinskii-Moriya interaction and ferroelectric polarization at G-type antiferromagnetic perovskite interfaces," *Phys. Rev. Lett.*, 103:127201 (2009).

Heidrich-Meisner, F., A.E. Feiguin, and E. Dagotto, "Real-time simulations of nonequilibrium transport in the single-impurity Anderson model," *Phys. Rev. B*, 79:23533 (2009).

Heidrich-Meisner, F., S.R. Manmana, M. Rigol, A. Muramatsu, A.E. Feiguin, and E. Dagotto,, "Quantum distillation: Dynamical generation of low-entropy states of strongly correlated fermions in an optical lattice," *Phys. Rev. A*, 80:041603(R) (2009).

Moreo, A., M. Daghofer, A. Nicholson, and E. Dagotto, "Interband pairing in multiorbital systems," *Phys. Rev. B*, 80:104507 (2009).

Salafranca, J., G.Alvarez, and E. Dagotto, "Electron-lattice coupling and partial nesting as the origin of Fermi arcs in manganites," *Phys. Rev. B*, 80:155133 (2009).

Ye, F., S. Chi, J.A. Fernandez-Baca, A. Moreo, E. Dagotto, J.W. Lynn, R. Mathieu, Y. Kaneko, Y. Tokura, and P.Dai, "Electronic self-organization in the single-layer manganite  $Pr_{l-x}Ca_{l+x}MnO_4$ " *Phys Rev. Lett.*, 103:167202 (2009).

Yu, R., S. Yunoki, S. Dong, and E. Dagotto, "Electronic and magnetic properties of RMnO3/AMnO3 heterostructures," *Phys. Rev. B*, 80:125115 (2009).

#### Takeshi Egami

ORNL Materials Science and Technology; UTK Department of Materials Science and Engineering and Department of Physics and Astronomy

Egami, T., "Recent advances in the study of complex materials by neutron scattering," in *Diffuse Scattering and the Fundamental Properties of Materials*, eds. R.I. Barabash, G.E. Ice, and P.E.A. Turchi, *Springer-Verlag, Berlin*, p. 317 (2009).

Kaatz, F.H., A. Bultheel, and T. Egami, "Real and reciprocal space order parameters for porous arrays from image analysis," *J. Mater. Sci.*, 44:40 (2009).

Braiman, Y., and T. Egami, "Nanoscale oscillatory fracture propagation in metallic glasses," *Physica A*, 388:1978 (2009).

Lumsden, M.D., A.D. Christianson, D. Parshall, M.B. Stone, S.E. Nagler, H.A. Mook, K. Lokshin, T. Egami, D.L. Abernathy, E.A. Goremychkin, R. Osborn, M.A. McGuire, A.S. Sefat, R. Jin, B.C. Sales, and D. Mandrus, "Two-dimensional resonant magnetic excitation in BaFe<sub>1.84</sub>Co<sub>0.16</sub>As<sub>2</sub>," *Phys. Rev. Lett.*, 102:107005 (2009).

Parshall, D., K. Lokshin, J. Niedziela, A.D. Christianson, M.D. Lumsden, H.A. Mook, S.E. Nagler, M.A. McGuire, M.B. Stone, D.L. Abernathy, A.S. Sefat, B.C. Sales, D.G. Mandrus, and T. Egami, "Spin excitations in BaFe<sub>1.84</sub>Co<sub>0.16</sub>As<sub>2</sub> superconductor observed by inelastic neutron scattering," *Phys. Rev. B*, 80:012502 (2009).

Seo, S.S.A., Z. Marton, W.S. Choi, G.W.J. Hassink, D.H.A. Blank, H.Y.Hwang, T.W. Noh, T. Egami, and H.N. Lee, "Multiple conducting carriers generated in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures," *Appl. Phys. Lett.*, 95:082107 (2009).

Reznik, D., K. Lokshin, D.C. Mitchell, D. Parshall, W. Dmowski, D. Lamago, R. Heid, K.-P- Bohnen, A.S. Sefat, M.A. McGuire, B.C. Sales, D.G. Mandrus, A. Asubedi, D.J. Singh, A. Alatas, M.H. Upton, A.H. Said, Yu. Shvyd'ko, and T. Egami, "C-axis phonons in Fe-As based superconductors investigated by inelastic x-ray scattering," *Phys. Rev. B*, 80:214534 (2009).

Morris, J.R., R.S. Aga, T. Egami, and V.A. Levashov, "Simulating the effect of poisson ratio on metallic glass properties," *Int. J. of Mod. Phys. B*, 23:1229 (2009).

#### Georges Guiochon

UTK Department of Chemistry

Abia, J.A., K.S. Mriziq, and G. Guiochon, "Radial heterogeneity of some analytical-type columns for high performance liquid chromatography," *Journal of Chromatography A*, 1216:3185–3191(2009).

Abia, J.A., K.S. Mriziq, and G. Guiochon, "Radial distribution of the contributions to band broadening of a silica-based semi-preparative monolithic column," *Journal of Separation Science*, 32:923–930 (2009).

Andrzejewska, A., K. Kaczmarski, and G. Guiochon, "Theoretical study of the accuracy of isotherms measured by frontal analysis, frontal analysis by characteristic point, and the pulse methods," *Journal of Chromatography A*, 1216:1067–1083 (2009).

Andrzejewska, A., F. Gritti, and G. Guiochon, "Investigation of peptide adsorption mechanism in controlled and uncontrolled pH of the sample by reverse phase chromatography," *Journal of Chromatography A*, 1216:3992–4004 (2009).

Chen, F., E.C. Drumm, G. Guiochon, and K. Suzuki, "Discrete element simulation of 1D upward seepage flow with particle-fluid interaction using coupled open source software," *Paper # 730098903*, *Proceedings of The 12th International Conference of the International Association for Computer Methods and Advances in Geomechanics (IACMAG)*, Goa, India, 1-6 October (2008).

Fairchild, J.N., K. Horváth, and G. Guiochon, "Approaches to comprehensive two-dimensional liquid chromatography systems," *Journal of Chromatography A*, 1216:1363–1371 (2009).

Fairchild, J.N., K. Horváth, and G. Guiochon, "Theoretical advantages and drawbacks of on-line, multidimensional liquid chromatography using multiple columns operated in parallel," *Journal of Chromatography A*, 1216:6210–6217 (2009).

Gritti, F., A. dos S. Pereira, P. Sandra, and G. Guiochon, "Comparison of the adsorption mechanisms of pyridine in hydrophilic interaction chromatography and in reversed phase aqueous liquid chromatography," *Journal of Chromatography A*, 1216:8496–8504 (2009).

Gritti, F., and G. Guiochon, "Adsorption behavior of the three species of the biprotic peptide Phe-Ala onto an endcapped  $C_{18}$  -bonded organic/inorganic hybrid stationary phase," *Analytical Chemistry*, 81:9871–9884 (2009).

Gritti, F., and G. Guiochon, "Adsorption mechanism of acids and bases in RPLC in weak buffered mobile phases designed for Liquid Chromatography/Mass Spectrophotometry," *Journal of Chromatography A*, 1216:1776–1788 (2009).

Gritti, F., and G. Guiochon, "Band profiles of reacting acido-basic compounds with water-methanol eluents at different w pH and ionic strengths in reversed-phase liquid chromatography," *Journal of Chromatography A*, 1216:3175–3184 (2009).

Gritti, F., and G. Guiochon, "Characteristics of the adsorption mechanism of acido-basic compounds with two p $K_a$  in reversed-phase liquid chromatography," *Journal of Chromatography A*, 1216:6917–6930 (2009).

Gritti, F., and G. Guiochon, "Determination of the adsorption energy distribution of neutral and charged compounds onto endcapped silica-C<sub>18</sub> adsorbent from polar liquid phases," *Colloid Journal (Kolloidnyi zhurnal)*, 71(4):479–485 (2009).

Gritti, F., and G. Guiochon, "Isosteric heat of adsorption in liquid-solid equilibria. Theoretical determination and measurement by liquid chromatography/mass spectrometry," *Journal of Chromatography A*, 1216:4745–4751(2009).

Gritti, F., and G. Guiochon, "Mass transfer equation for proteins in very high pressure liquid chromatography," *Analytical Chemistry*, 81:2723–2736 (2009).

Gritti, F., and G. Guiochon, "Mass transfer kinetic mechanism in monolithic columns and application to the characterization of new research monolithic samples with different average pore sizes," *Journal of Chromatography A*, 1216:4752–4767(2009).

Gritti, F., and G. Guiochon, "Optimization of the thermal environment of columns packed with very fine particles," *Journal of Chromatography A*, 1216:1353–1362 (2009).

Gritti, F., and G. Guiochon, "Peak compression factor of proteins," *Journal of Chromatography A*, 1216:6124–6133 (2009).

Gritti, F., and G. Guiochon, "Peak shapes of acids and bases under overloaded conditions in reversed phase liquid chromatography, with mobile phases of various buffer pH. A thermodynamic interpretation," *Journal of Chromatography A*, 1216:63–78 (2009).

Gritti, F., and G. Guiochon, "Simultaneous measurement of  $_{\rm w}{}^{\rm S}{\rm pH}$  and overloaded band profiles of small peptides in insufficiently buffered mobile phases used in preparative liquid chromatography," *Journal of Chromatography A*, 1216:8874–8882 (2009).

Gritti, F., M. Martin, and G. Guiochon, "The influence of viscous friction heating on the column HETP," *Analytical Chemistry*, 81:3365–3384(2009).

Horváth, K., J. Fairchild, and G. Guiochon, "Optimization of on-line two-dimensional chromatography," *Analytical Chemistry*, 81:3879–3888 (2009).

Horváth, K., J. Fairchild, and G. Guiochon, "Optimization strategies for off-line two-dimensional liquid chromatography," *Journal of Chromatography A*, 1216:2511–2518 (2009).

Horváth, K., J.N. Fairchild, and G. Guiochon, "Detection issues in two-dimensional liquid chromatography," *Journal of Chromatography A*, 1216:7785–7792 (2009).

Kaczmarski, K., J. Kostka, W. Zapała, and G. Guiochon, "Modeling of thermal processes in high pressure liquid chromatography. I - Onset of thermal heterogeneity," *Journal of Chromatography A*, 1216:6560–6574 (2009).

Kaczmarski, K., F. Gritti, J. Kostka, and G. Guiochon, "Modeling of thermal processes in high pressure liquid chromatography. II - Thermal heterogeneity at very high pressures," *Journal of Chromatography A*, 1216:6575–6586 (2009).

Miyabe, K., N. Ando, and G. Guiochon, "Peak parking method for measurement of molecular diffusivity in liquid phase systems," *Journal of Chromatography A*, 1216:4377–4382 (2009).

Miyabe, K., Y. Matsumoto, Y. Niwa, N. Ando, and G. Guiochon, "An estimation of the column efficiency made by analyzing tailing peak profiles," *Journal of Chromatography A*, 1216:8319–8330 (2009).

Putnam, J., and G. Guiochon, "Characterizing the memory effect on the CHIRALPAK® AD® stationary phase," *Journal of Chromatography A*, 1216:8488–8495 (2009).

Shalliker, R.A., and G. Guiochon, "Understanding the importance of the viscosity contrast between the sample solvent plug and the mobile phase and its consequence in two-dimensional HPLC," *Journal of Chromatography A*, 1216:787–793 (2009).

#### Robert D. Hatcher, Jr.

UTK Department of Earth and Planetary Sciences

Thigpen, J. R., and R.D. Hatcher, Jr., "Geologic map of the western Blue Ridge and portions of the eastern Blue Ridge and Valley and Ridge provinces in southeastern Tennessee, southwestern North Carolina, and northern Georgia: Geological Society of America Maps and Charts Series," scale 1:200,000 (2009).

Wunderlich, A. L., and R.D. Hatcher, Jr., Rescuing legacy digital data: Maps stored in Adobe Illustrator<sup>™</sup> format, *in* Soller, D. R., ed., *Digital Mapping Techniques '08—Workshop Proceedings: U.S. Geological Survey Open-File Report* 200 1298, p. 85–100 (2009).

#### David C. Joy

ORNL Materials Science and Technology; UTK Department of Biochemistry, Cellular and Molecular Biology & Department of Materials Science and Engineering

Cord, B., J. Yang, H. Duan, D.C. Joy, J. Klingfus, and K.K. Berggren, "Limiting Factors in sub-10nm scanning electron beam lithography," *J Vac Sci Techol. B*, 27(6):2616-2621 (2009).

Hildebrand, M., G. Holton, D.C. Joy, M. J. Doktycz, and D.P. Allison, "Diverse and conserved nano-and mesoscale structures of diatom silica revealed by atomic force microscopy," *J. Microscopy*, 235(2):172-187 (2009).

Joy, D. C., "Scanning electron microscopy: second best no more," *Nature Materials*, 8,(10):76-777 (2009).

Peckys, D.B., G.M. Veith, D.C. Joy, and N. de Jonge, "Nanoscale imaging of whole cells using a liquid enclosure and a STEM," *PLoS ONE*, 4(12):1-7 (2009).

#### Joseph Macek

ORNL Physics Division; UTK Department of Physics and Astronomy

Jansen, K., S. J. Ward, J. Shertzer, and J. H. Macek, "Absolute cross-section for positron impact ionization of hydrogen near threshold," *Phys. Rev. A.*, 79:022704 (2009).

Macek, J.H., "Multiparticle interactions of zero-range potentials," *Few-Body Syst.*, 46:207 (2009).

Macek, J.H., J.S. Sternberg, S.Y. Ovchinnikov, T-G. Lee and D.R. Schultz, "Origin, evolution, and imaging of vortices in atomic processes," Phys. Rev. Lett, 102:143201 (2009).

Ovchinnikov, S.Y., J.H. Macek, J.S. Sternberg, T-G. Lee, and D.R. Schultz, "Evolution of quantum systems from microscopic to macroscopic scales," *CAARI 2008 Proceedings AIP Conference Proceedings*, 1099:164 (2009).

#### Jimmy Mays

ORNL Chemical Sciences Division; UTK Department of Chemistry

Alonzo, J., J.W. Mays, and S.M. Kilbey, II, "Forces on interaction between surfaces bearing looped polymer brushes in good solvent," *Soft Matter*, 5:1897-1904 (2009).

Ashcraft, E., H. Ji, J. Mays, and M. Dadmun, "A novel reactive processing technique: Using telechelic polymers to reactively compatibilize polymer blends," *ACS Applied Materials & Interfaces*, 1: 2163-2173 (2009).

de Anda, C., G. Morales, P. Acuña, J. Sosa, D. Knoeppel, and J.W. Mays, "Evaluation of the final morphology of HIPS based on the architecture of the compatibilizer graft copolymer PBd-g-PS," *Macromolecular Symposia*, 283:27-33 (2009).

Duan, Y., M. Thunga, R. Schlegel, K. Schneider, E. Rettler, R. Weidisch, H. Siesler, M. Stamm, J. W. Mays, and N. Hadjichristidis, "Morphology and deformation mechanisms and tensile properties of tetrafunctional multigraft copolymers," *Macromolecules*, 42:4155-4164 (2009).

Hinestroza, J.P., J. Alonzo, J.W. Mays, and S.M. Kilbey, II, "Role of surface reorganization on preferential adsorption of macromolecular ensembles at the solid/fluid interface," *Macromolecules*, 42:7913-7918 (2009).

Marchal, F., P. Guenoun, J. Daillant, D.W. Holley, and J.W. Mays, "Unprecedented microemulsion boosting effect induced by a charged diblock copolymer: Bending modulus and curvature frustration of the surfactant film," *Soft Matter*, 5:4006-4014 (2009).

Park, J.Y., M. Liu, J.W. Mays, M. Dadmun, and R. Advincula, "Nano-donuts from pH-dependent block restructuring in amphiphilic ABA triblock copolymer vesicles at the air-water interface," *Soft Matter*, 5:747–749 (2009).

Priftis, D., G. Sakellariou, D. Baskaran, J.W. Mays, and N. Hadjichristidis, "Polymer grafted janus multi-walled carbon nanotubes," *Soft Matter*, 5:4272–4278 (2009).

Priftis, D., N. Petzetakis, G. Sakellariou, M. Pitsikalis, J.W. Mays, and N. Hadjichristidis, "Surface initiated titanium-mediated coordination polymerization from catalyst-functionalized single and multi-walled carbon nanotubes," *Macromolecules*, 42:3340-3346 (2009).

Sakellariou, G., J.R. Dunlap, N. Hadjichristidis, J.W. Mays, and D. Baskaran, "Controlled functionalized organic nanoparticles from diblock copolymer micelles," *Polymer*, 50:6202-6211 (2009).

Schlegel, R., U. Staudinger, M. Thunga, R. Weidisch, G. Heinrich, D. Uhrig, J.W. Mays, H. Iatrou, and N. Hadjichristidis, "Investigation on mechanical properties of PI-PS multigraft copolymers," *Eur. Polym. J.*, 45:2902–2912 (2009).

Schlegel, R., D. Wilkin, Y. Duan, R. Weidisch, G. Heinrich, D. Uhrig, J.W. Mays, and N. Hadjichristidis, "Stress softening of multigraft copolymers," *Polymer*, 50:6297-6304 (2009).

Winoto, W., S. Tan, Y. Shen, M. Radosz, K. Hong, and J.W. Mays, "High-pressure micellar solutions of polystyrene-block-polybutadiene and polystyrene-block-polyisoprene solutions in propane exhibit cloud-pressure reduction and distinct micellization end points," *Macromolecules*, 42:3823-3826 (2009).

Winoto, W., S. Tan, Y. Shen, M. Radosz, K. Hong, and J.W. Mays, "High-pressure micellar solutions of symmetric and asymmetric styrene—diene diblocks in compressible near critical solvents: Micellization pressures and cloud pressures respond but micellar cloud pressures insensitive to copolymer molecular weight, concentration, and block ratio changes," *Macromolecules*, 42:7155-7163 (2009).

Winoto, W., Y. Shen, M. Radosz, K. Hong, and J.W. Mays, "Deuteration can impact micellization pressure and cloud pressure of polystyrene-block-polybutadiene and polystyrene-block-polyisoprene in compressible propane," *J. Phys. Chem. B*, 113:15156-15161 (2009).

#### Joint Directed Research and Development

#### Shengting Cui and Bamin Khomami

UTK Department of Chemical and Biomedical Engineering

Xianggui, Y., S. Cui, V. de Almeida, and B. Khomami, "Interfacial complex formation in uranyl extraction by tributyl phosphate in dodecane diluent: A molecular dynamics study," *Journal of Physical Chemistry*, 113:9852-9862 (2009).

#### Hong Guo

UTK Department of Biochemistry and Cellular and Molecular Biology

Guo, H., A. Gorin, and H. Guo, "A Peptide-linkage deletion procedure for estimate of energetic contributions of individual peptide groups in a complex environment: Application to parallel ?-sheets," *Interdiscip Sci Comput Life Sci* 1:12–20 (2009).

#### Janice Musfeldt

UTK Department of Chemistry

Sun, Q.-C., X.S. Xu, L.I. Vergara, R. Rosentsveig, and J.L. Musfeldt, "Dynamical charge and structural strain in inorganic fullerene-like MoS2 nanoparticles," *Phys. Rev. B*, 79:205405 (2009). This paper was reprinted in the May 18, 2009 issue of the *Virtual Journal of Nanoscale Science and Technology*.

Xu, X.S., Q.-C. Sun, J.L. Musfeldt, and R. Rosentsveig, "Evaluating born and effective charges in unoriented materials from vibrational spectra," *Phys. Rev. B.*, 80:014303-1 - 014303-8 (2009)

#### Joint Institute for Heavy Ion Research

Adare, A., T.C. Awes, V. Cianciolo, A. Enokizono, K.F. Read, Jr., D.O. Silvermyr, S.P. Sorensen, P.W. Stankus, and G.R. Young, "High-pT pi $^0$  production with respect to the reaction plane in Au+Au Collisions at sqrt( $s_{\rm NN}$ ) = 200 GeV," PHENIX Collaboration, *Phys. Rev. C*, 80:054907 (2009).

Adare, A., T.C. Awes, V. Cianciolo, A. Enokizono, K.F. Read, Jr., D.O. Silvermyr, S.P. Sorensen, P.W. Stankus, and G.R. Young, "Gluon-spin contribution to the proton spin from the double-helicity asymmetry in inclusive pi<sup>0</sup> production in polarized p + p collisions sqrt S = 200 GeV," PHENIX Collaboration, *Phys. Rev. Lett.*, 103:012003 (2009).

Adare, A., T.C. Awes, V. Cianciolo, A. Enokizono, K.F. Read, Jr., D.O. Silvermyr, P.W. Stankus, S.P. Sorensen, and G.R. Young, "Erratum: Cold nuclear matter effects on J/psi production as constrained by deuteron-gold measurements at  $\operatorname{sqrt}(s_{NN}) = 200$  GeV," PHENIX Collaboration, [*Phys. Rev. C*, 77:024912 (2008)], *Phys. Rev. C*, 79:059901 (2009).

Adare, A., T.C. Awes, V. Cianciolo, A. Enokizono, K.F. Read, Jr., D.O. Silvermyr, S.P. Sorensen, P.W. Stankus, and G.R. Young, "Measurement of bottom versus charm as a function of transverse momentum with electron-hadron correlations in p+p collisions at sqrt(s) = 200 GeV," PHENIX Collaboration, *Phys. Rev. Lett.*, 103:082002 (2009).

Adare, A., T.C. Awes, V. Cianciolo, and A. Enokizono, "Photon-hadron jet correlations in p+p and Au+Au collisions at  $sqrt(s_{NN}) = 200 \text{ GeV}$ ," PHENIX Collaboration, K.F. Read, Jr., D.O. Silvermyr, S.P. Sorensen, P.W. Stankus, and G.R. Young, *Phys. Rev. C*, 80:24908 (2009).

Afanasiev, A., T.C. Awes, V. Cianciolo, Y. Efremenko, A. Enokizono, K.F. Read, Jr., D.O. Silvermyr, S.P. Sorensen, P.W. Stankus, and G.R. Young, "Charged kaon interferometric probes of space-time evolution in Au+Au collisions at sqrt  $^{\rm S}_{\rm NN}$  = 200 GeV," PHENIX Collaboration, *Phys. Rev. Lett.*, 103:142301 (2009).

Afanasiev, S., T.C. Awes, V. Cianciolo, A. Enokizono, K.F. Read, Jr., D.O. Silvermyr, S.P. Sorensen, P.W. Stankus, and G.R. Young, "Photoproduction of J/psi and of high mass e+e- in ultra-peripheral Au+Au collisions at sqrt  $^{S}_{NN}$  = 200 GeV," PHENIX Collaboration, *Phys. Lett. B*, 679:321 (2009).

Afanasiev, S., T.C. Awes, V. Cianciolo, A. Enokizono, K.F. Read, Jr., D.O. Silvermyr, S.P. Sorensen, P.W. Stankus, and G.R. Young, "Systematic studies of elliptic flow measurements in Au+Au collisions at sqrt(s\_NN) = 200 GeV," PHENIX Collaboration, *Phys. Rev. C*, 80:024909 (2009).

Bacca, S., A. Schwenk, G. Hagen, and T. Papenbrock, "Helium halo nuclei from low-momentum interactions," Fifth International Conference on Exotic Nuclei and Atomic Masses (ENAM'08), Ryn, Poland, Sept. 7-13, 2008, *Eur. Phys. J. A*, 42:553 (2009).

Baran, A., J.A. Sheikh, A. Staszczak, and W. Nazarewicz, "Fission quadrupole mass parameters in HF+BCS and HFB methods," 15th Nuclear Physics Workshop, Kazimierz Dolny, Poland, Oct. 23-27, 2008, *Int. J. Mod. Phys. E*, 18:1049 (2009).

Baran, A., J.A. Sheikh, and W. Nazarewicz, "Adiabatic mass parameters for spontaneous fission," 15th Nuclear Physics Workshop, Kazimierz Dolny, Poland, Oct. 23-27, 2008, *Int. J. Mod. Phys. E*, 18:1054 (2009).

Bardayan, D.W., K. Chipps, R.P. Fitzgerald, J.C. Blackmon, K. Chae, A.E. Champagne, U. Greife, R. Hatarik, R.L. Kozub, C. Matei, B. Moazen, C.D. Nesaraja, S.D. Pain, W. Peters, S. Pittman, J.F. Shriner, Jr., and M.S. Smith, "Direct measurements of (p, gamma) cross sections at astrophysical energies using radioactive beams and the daresbury recoil separator," 5th International Conference on Exotic Nuclei and Atomic Masses, Ryn, Poland, Sept. 7-13, 2008, Eur. Phys. J. A, 42:457 (2009).

Batchelder, J.C., J.L. Wood, P. Garrett, K.P. Rykaczewski, J. Bilheux, C.R. Bingham, H.K. Carter, D. Fong, R. Grzywacz, J. Hamilton, D.J. Hartley, J. Hwang, W. Krolas, D. Kulp, Y. Larochelle, A. Piechzczek, A. Ramayya, E. Spejewski, D. Stracener, M. Tantawy, J. Winger, and E. Zganjar, "Collective and non-collective states in <sup>116</sup>Cd studied via the beta-decays of <sup>116</sup>Ag<sup>m1,m2,gs</sup>," *Phys. Rev. C*, 80:054318 (2009).

Chipps, K., D.W. Bardayan, J.C. Blackmon, K. Chae, U. Greife, R. Hatarik, R.L. Kozub, C. Matei, B. Moazen, C.D. Nesaraja, S.D. Pain, W. Peters, S. Pittman, J.F. Shriner, Jr., and M.S. Smith, "The <sup>17</sup>F(p,gamma)<sup>18</sup>Ne resonant cross section," *Phys. Rev. C*, 80:065810 (2009).

Grigorenko, L., T. Wiser, K. Miernik, R. Charity, M. Pfutzner, A. Banu, C. Bingham, M. Cwiok, I. Darby, W. Dominik, J. Elson, T. Ginter, R. Grzywacz, Z. Janas, M. Karny, A. Korgul, S. Liddick, K. Mercurio, M. Rajabali, K.P. Rykaczewski, R. Shane, L. Sobotka, A. Stolz, L. Trache, R. Tribble, A. Wuosmaa, and M. Zhukov, "Complete correlation studies of two-proton decays: <sup>6</sup>Be and <sup>45</sup>Fe," *Phys. Lett. B*, 677:30 (2009).

Hagen, G., T. Papenbrock, and D.J. Dean, "Solution of the center-of-mass problem in nuclear structure calculations," *Phys. Rev. Lett.*, 103:062503 (2009).

Hagen, G., T. Papenbrock, D.J. Dean, M. Hjorth-Jensen, and B. V. Asokan, "Ab initio computation of neutron-rich oxygen isotopes," *Phys. Rev. C*, 80:021306 (2009).

Jones, K.L., S.D. Pain, R.L. Kozub, A.S. Adekola, D.W. Bardayan, J.C. Blackmon, W.N. Catford, K. Chae, K. Chipps, J. Cizewski, L. Erikson, A. Gaddis, U. Greife, R. Grzywacz, C.W. Harlin, R. Hatarik, J.A. Howard, J. James, R. Kapler, W. Krolas, J.F. Liang, Z. Ma, C. Matei, B. Moazen, C.D. Nesaraja, P. O'Malley, N. Patterson, S. Paulauskas, D. Shapira, J.F. Shriner, Jr., M. Sikora, D. Sissom, M.S. Smith, T. Swan, J.S. Thomas, and G.L. Wilson, "Studies of nuclei close to <sup>132</sup>Sn using single-neutron transfer reactions," FUSION08: New Aspects of Heavy Ion Collisions Near the Coulomb Barrier, Chicago, Illinois, Sept. 22-26, 2008, *Am. Inst. Phys. Conf. Proc.*, 1098:153 (2009).

Liang, J.F., J.R. Beene, A.L. Caraley, H. Esbesnen, A. Galindo-Uribarri, C.J. Gross, P.E. Mueller, K. Schmitt, D. Shapira, D.W. Stracener, and R.L. Varner, Jr., "Dynamic polarization in the coulomb breakup of loosely bound <sup>17</sup>F," *Phys. Lett. B*, 681:22 (2009).

McDonnell, J.D., W. Nazarewicz, and J. Sheikh, "Thermal fission pathways in <sup>232</sup>Th," *4th International Workshop on Nuclear Fission and Fission Product Spectroscopy* (Fission 2009), Cadarache, France, May 13-16, 2009, *Am. Inst. Phys. Conf. Proc.*, 1175:371 (2009).

Michel, N., W. Nazarewicz, M. Ploszajczak, and T. Vertse, "Shell model in the complex energy plane," *J. Phys. G: Nucl. Part. Phys.*, 36:013101 (2009).

Miernik, K., W. Dominik, Z. Janas, M. Pfutzner, L. Grigorenko, C. Bingham, H. Czyrkowski, M. Cwiok, I. Darby, R. Dabrowski, T. Ginter, R. Grzywacz, M. Karny, A. Korgul, W. Kusmierz, S. Liddick, M. Rajabali, K. P. Rykaczewski, and A. Stolz, "Two-proton radioactivity of <sup>45</sup>Fe," International Conference on Exotic Nuclei and Atomic Masses ENAM 2008, Ryn, Poland, Sept. 7-13, 2008, *Eur. Phys. J. A.*, 42:431 (2009).

Papadimitriou, G., N. Michel, W. Nazarewicz, M. Ploszajczak, and J. Rotureau, "Description of charge radii in halo nuclei within the gamow shell model," 5th ANL/MSU/JINA/INT FRIB Workshop on Bulk Nuclear Properties, East Lansing, Michigan, Nov. 19-22, 2008, *Am. Inst. Phys. Conf. Proc.*, 1128:11 (2009).

Pei, J., W. Nazarewicz, and M. Stoitsov, "Coordinate-space hartree-fock-bogoliubov description of superfluid fermi systems," 5th International Conference on Exotic Nuclei and Atomic Masses (ENAM '08), Ryn, Poland, Sept. 7-13, 2008, *Eur. Phys. J. A*, 42:595 (2009).

Pei, J., W. Nazarewicz, J.A. Sheikh, and A.K. Kerman, "Fission barriers of compound superheavy nuclei," *Phys. Rev. Lett.*, 102:192501 (2009).

Pittman, S., D.W. Bardayan, J.C. Blackmon, R.L. Kozub, and M.S. Smith, "Analysis of <sup>25</sup>Al energy levels observed in the <sup>28</sup>Si(p,alpha)<sup>25</sup>Al reaction," *Phys. Rev. C*, 80:038801 (2009).

Rotureau, J., N. Michel, W. Nazarewicz, M. Ploszajczak, and J. Dukelsky, "Density matrix renormalization group approach to two-fluid open many-fermion systems," *Phys. Rev. C*, 79:014304 (2009).

Satula, W., J. Dobaczewski, W. Nazarewicz, and M. Rafalski, "Isospin mixing in nuclei within the nuclear density functional theory," *Phys. Rev. Lett.*, 103:012502 (2009).

Sheikh, J., G.H. Bhat, R. Palit, Z. Naik, and Y. Sun, "Multi-quasiparticle gamma-band structure in neutron-deficient Ce and Nd Isotopes," *Nucl. Phys. A*, 824:58 (2009).

Sheikh, J.A., W. Nazarewicz, and J. Pei, "Systematic study of fission barriers of excited superheavy nuclei," *Phys. Rev. C*, 80:011302 (2009).

Stoitsov, M., J. More, W. Nazarewicz, J. Pei, J. Sarich, N.F. Schunck, A. Staszczak, and S. Wild, "Towards the universal nuclear energy density functional," SciDAC 2009 Conference, San Diego, California, June 14-18, 2009, *J. Phys.: Conf. Ser.*, 180:12082 (2009).

Wong, C., "Momentum kick model analysis of PHENIX near-side ridge data and photon jet," *Phys. Rev. C*, 80:034908 (2009).

Wong, C., "The wigner function of produced particles in string fragmentation," *Phys. Rev. C*, 80:054917 (2009).

#### Integrative Graduate Education and Research Traineeship

#### SCALE-IT

Scalable Computing and Leading Edge Innovative Technologies

Baker, E.J., J.J. Jay, V.M. Philip, Y. Zhang, Z. Li, R. Kirova, M.A. Langston, and E.J. Chesler, "Ontological discovery environment: A system for integrating gene-phenotype associations," *Genomics*, 94:377-387 (2009).

Gothandaraman, A., R. Weber, G.D. Peterson, R.J. Hinde, and R.J. Harrison, "Architectural comparisons for a quantum Monte Carlo application," *Symposium on Application Accelerators in High Performance Computing*, Champaign, IL (2009).

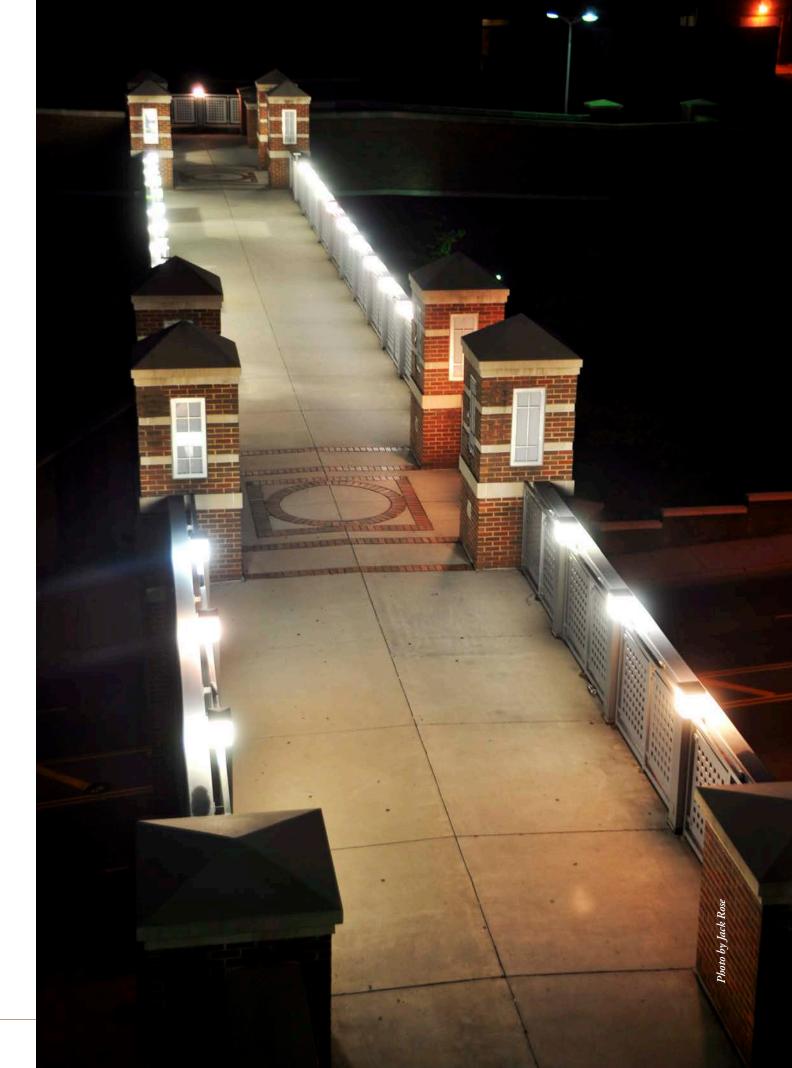
Weber, R., A. Gothandaraman, R.J. Hinde, and G.D. Peterson, "Comparing hardware accelerators in scientific applications: A case study," *IEEE Transactions on Parallel and Distributed Systems*, 6:1 (2009.

Weber, R., R.J. Harrison, and G.D. Peterson, "Programmability: Design costs and payoffs using AMD GPU streaming languages and traditional multi-core libraries." *Symposium on Application Accelerators in High Performance Computing*. Champaign, IL, (2009).

#### **STAIR**

Sustainable Technology through Advanced Interdisciplinary Research

Mulder, C., L. Theogarajan, M. Currie, J.K. Mapel, M.A. Baldo, M. Vaughn, P. Willard, B.D. Bruce, M.W. Moss, C.E. McLain, and J.P. Morseman, "Luminescent solar concentrators employing phycobilisomes," *Advanced Materials*, 21:1-5, (2009).



## UT-ORNL joint faculty

Appointee	ORNL Appointment in	Based at		Field	Appointment Title
Dagotto, Elbio	ORNL/MSTD	UTK/Physics		Materials	Distinguished Scientist/Professor
Egami, Takeshi	ORNL/MSTD	UTK/MSE		Materials	Distinguished Scientist/Professor
Joy, David	ORNL/MSTD	UTK/BCMB		Neutrons	Distinguished Scientist/Professor
Macek, Joseph	ORNL/PD	UTK/Physics		Atomic Physics	Distinguished Scientist/Professor
May, Jimmy	ORNL/CSD	UTK/Chemistry		Neutrons	Distinguished Scientist/Professor
Hall, Howard	ORNL/GNSD	UTK/Nuclear Engr		Nuclear	Governor's Chair
Liu, Yilu	ORNL/ETSD	UTK/EECS		Electrical	Governor's Chair
Loeffler, Frank	ORNL/Biosciences	UTK/Microbiology			Governor's Chair
Smith, Jeremy	ORNL/Biosciences	UTK/BCMB*		Molecular Biophysics	Governor's Chair
Sokolov, Alexei	ORNL/CSD	UTK/Chemistry		Materials	Governor's Chair
Webber, William	ORNL/MSTD	UTK/MSE			Governor's Chair
Williams, Robert		UTHC			Governor's Chair
Zawodzinski, Thomas	ORNL/CSD	UTK/Chemistry		Materials	Governor's Chair
Name	Joint Appointment at	Based at	ORNL Contact	Field	
Adhern, Shaun	UTK/EECS	ORNL/NCCS			
Almeida, Valmor	UTK/Chem & Bio	ORNL/NSTD			
Banks, David	ORNL/NCCS	UTK/EECS	Ricky Kendall	Computing	
Barnes, Ted	UTK/Physics	ORNL/PD	Glenn Young	Nuclear Physics	
Bjornstad, David	UTK/Enviro Sci	ORNL/Enviro sci			
Britton, Charles	UTK/EECS	ORNL/ESTD	Ted Fox	Detectors	
Cardall, Christian	UTK/Physics	ORNL/PD	Anthony Mezzacappa	Astrophysics	
Choo, Hahn	ORNL/MSTD	UTK/MSE	Steven Zinkle	Materials	
Dadmun, Mark	ORNL/CSD	UTK/Chemistry	Mike Simonson	Neutron Scattering	
Dai, Pencheng	ORNL/NSSD	UTK/Physics	Stephen Nagler	Neutrons	
Dai, Sheng	ORNL/CSD	UTK/Chemistry			
Efremenko, Yuri	ORNL/PD	UTK/Physics	Glenn Young	Neutrons	
Ericson, M. Nance	UTK/EECE	ORNL/ESTD	Ted Fox	Electrical Engineering	g
Fahey, Mark	UTK/CSMD	ORNL/NCCS		Computational Science	ces
Gao, Yanfei	ORNL/CSMD	UTK/MSE	Thomas Schulthess	Materials	
George, Easo	UTK/MSE	ORNL/MSTD	Steven Zinkle	Materials	
Graham, David	UTK/Biosciences	ORNL/Biosciences			
Greene, David	UTK/ETSD	ORNL/ETSD			
Greene, Geoffrey	ORNL/PD	UTK/Physics	Glenn Young	Neutrons	
Harrison, Robert	UTK/Chemistry	ORNL/CSMD	Jeff Nichols	Computing	
Hayward, Jason	ORNL/NSTD	UTK/Nuclear Engr	James Rushton		
Hayward, Jason Hix, Ralph	ORNL/NSTD UTK/Physics	UTK/Nuclear Engr ORNL/Physics	James Rushton		

Name	Joint Appointment at	Based at	ORNL Contact	Field
Kilbey, S. Michael	UTK/Chemistry	ORNL/CNMS	Linda Horton	
Klasky, Scott	UTK/Comp Sci	ORNL/NCCS		
Larese, John	ORNL/CSD	UTK/Chemistry	Phillip Britt	Neutrons
Maldonado, Ivan	ORNL/NSTD	UTK/Nuclear	James Rushton	
Mandrus, David	UTK/MSE	ORNL/MSTD		
Mezzacapa, Anthony	UTK/Physics	ORNL/PD		
Miller, Bill	UTK/ETSD	ORNL/ETSD		
Moreo, Adriana	ORNL/MSTD	UTK/PD	Peter Tortorelli	Materials
Morris, Jamie	UTK/MSE	ORNL/MSTD	Steven Zinkle	Materials
Ostrouchov, George	UTK/CSMD	ORNL/CSMD		
Papenbrock, Thomas	ORNL/PD	UTK/PD	Glenn Young	Nuclear Physics
Pharr, George M.	ORNL/MSTD	UTK/MSE	Steven Zinkle	Materials
Plechac, Petr	ORNL/CSMD	UTK/Mathematics	Jeff Nichols	Computing
Rack, Philip	ORNL/CNMS	UTK/MSE	Linda Horton	Materials
Rawn, Claudia	UTK/MSE	ORNL/MSTD	Steven Zinkle	Materials
Read, Ken F.	UTK/Physics	ORNL/PD	Glenn Young	Nuclear Physics
Sankaran, Ramanan	UTK/MABE	ONRL/NCCS		
Sayler, Gary	ORNL/Biology Sci	UTK	Berry Berven	
Simpson, Michael	UTK/MSE	ORNL/CNMS	Linda Horton	Materials
Simunovic, Srdjan	UTKL/CSMD	ORNL/CSMD		
Vass, Arpad	UTK/Biosciences	ORNL/Biosciences		
Vazhkudai, Sudharshan	UTK/CSMD	ORNL/CSMD		
Wang, Fred	ORNL/ETSD	UTK/ETSD		
Weitering, Hanno	ORNL/MSTD	UTK/PD	John Wendelken	Materials
Wilson, Bruce E	UTK/Enviro sci	ORNL/Enviro Sci		
Xing, Yulong	UTK/CSMD	ORNL/CSMD		
Zhang, Yanwen	UTK/MSE	ORNL/MSTD		
Zhang, Zhenyu	UTK/Physics	ORNL/MSTD	Steven Zinkle	Materials

#### Key:

BCMB--Biochemical and Cellular and Molecular Biology

CNMS--Center for Nanophase Materials Sciences

CSD--Chemical Sciences Division

CSED--Computer Science and Engineering Division

CSMD--Computer Science and Mathematics Division

EECS--Electronical Engineering and Computer Science

ESTD--Engineering Science and Technology Division

ETSD - Energy and Transportation Science Division

GNSD - Global Nuclear Security Division

JICS--Joint Institute for Computational Sciences

MABE--Mechanical Aerospace and Biomedical Engineering

MSE--Materials Science and Engineering

MSTD--Materials Science and Technology Division

NCCS--National Center for Computational Sciences

NSSD--Neutron Scattering Science Division

NSTD--Nuclear Science and Technology Division

PD--Physics Division

ORNL--Oak Ridge National Laboratory

UTK--University of Tennessee Knoxville



## external funding

EXTERNAL
RESEARCH FUNDS
AWARDED TO
UT-ORNL
DISTINGUISHED
SCIENTISTS
DURING FY10

The table that follows lists the research funding brought in to The University of Tennessee from external sources by UT-ORNL Distinguished Scientists designated as principal investigators on the projects. These individuals also appear as investigators on many other funded research proposals, including large research grants awarded to Oak Ridge National Laboratory. A few examples are bulleted below.

• Elbio Dagotto is principal investigator of an ORNL Field Work Proposal/project with a budget of \$1.3 million, which also supports the work of R. Fishman and S. Okamoto, and UT-ORNL joint faculty professor A. Moreo. A renewal proposal was prepared during the summer of 2009 and orally defended during a DOE

site visit in November 2009. The team awaits a final answer.

- Takeshi Egami is principal investigator of \$1.05 million, DOE-BES: KC020103 for ORNL Field Work Proposal/project number ERKCM40, *Atomistic Study of Bulk Metallic Glasses*. The project team also includes J.R. Morris, E. George, D. Nicholson and G.M. Stocks. Project dates—8/01/04-7/31/11.
- Joseph Macek brought \$65,000 to ORNL's research budget again in FY10.
- David Joy was responsible for bringing ORNL a DOE Stimulus Grant of \$1.5 million for microscopes. His LDRD project *SEM imaging in Liquids* is in its final year (\$340,000 in FY10).

Principal Investigator	Project Name	Project Title	Start Date	End Date	FY 10 Award Amount Expenditu	
Dagotto	NSF-IMR-0716020	Correlated Electrons in Complex Oxides and Nanoscopic Systems	08/15/2007	07/31/2010	\$ 408,000	\$ 113,224
Egami	UT-B 4000039517	Atomistic Study of Bulk Metallic Glasses	03/01/2005	12/31/2010	\$ 642,164	\$ 116,596
Egami	UT-B 4000080940	Summer Assistantship	05/05/2009	12/31/2009	\$ 5,036	\$ 1,728
Egami	UT-Battelle 4000039718	Atomistic Study of Bulk Metallic Glasses	03/14/2005	03/14/2011	\$ 508,451	\$ 20,765
Egami	UT-Battelle 4000071951	Atomistic Structure of Gold Nano-Particles	07/31/2008	07/30/2010	\$ 76,148	\$ 4,482
Egami	NSF DMR-0602876	Materials Research Network: Structure and Dynamics of Complex Ferroelectrics	07/01/2006	06/30/2011	\$ 264,000	\$ 58,930
Egami	DOE-DE-FG02- 08ER46528	Neutron Scattering Research Network for Epscor States	09/01/2008	08/31/2011	\$ 1,626,000	\$ 622,692
Egami	DOE-DE-FG02- 08ER46528	Neutron Scattering Research Network for Epscor States - Dept. Matching	09/01/2008	08/31/2011	\$ 997,839	\$ 210,099

## external funding

Principal Investigator	Project Name	Project Title	Project Title Start Date		Award Amount		Ex	FY 10 ependitures
Egami	DOE-FG02- 08ER46528	Neutron Scattering Research Network for Epscor States	09/01/2008	08/31/2011	\$	69,070		
Egami	ARRA-Washington Univ WU-HT-10-51	ARRA: Construction of the Parts for MRI-R2 Project	04/01/2010	03/31/2011	\$	146,046	\$	10,805
Guiochon	DOE-DE-SC0001014	Separation of Highly Complex Mixtures by Two- Dimension Liquid Chromatography	07/15/2009	07/14/2011	\$	240,000	\$	136,181
Hatcher	USGS-G09AC00126	Detailed Geologic Mapping, Central Georgia inner Piedmont and Tennessee Valley and Ridge	04/30/2009	10/30/2010	\$	42,700	\$	21,830
Hatcher	USGS-G10AC00001	Conversion of Detailed Geologic Maps to ArcMap-Compatible Geospatial Databases: Part 2	10/20/2009	10/19/2010	\$	25,000	\$	14,486
Joy	Electron Microscopy Facility	Unrestricted Research Support	04/11/1989	12/31/2047	\$	415,091		
Joy	Semicond. Res. Agency	Development of Analysis Software	03/01/2008	02/28/2011	\$	57,500	\$	16,043
Macek	DOE-DE-FG02- 02ER15283-MACEK	Theory of Fragmentation and Rearrangement Process in ion-Atom Collisions	02/29/2008	02/28/2011	\$	375,000	\$	141,758
Mays	Dow Chemical Co Jimmy Mays	Unrestricted Research Support	10/30/2002	12/31/2047	\$	35,000	\$	8,838
Mays	UT-B 4000076055	Plymer-Based Multicomponent Materials	11/20/2008	11/02/2010	\$	68,402	\$	30,394
Mays	NSF-DMR-0906893	Collaborative Research: Synthesis and Rheology of Strategically Designed Long-Chain-Branched Polymers	09/01/2009	08/31/2011	\$	80,000	\$	32,387
Mays	UT-B 400089712	Poly(cyclohexadiene)-Based Electrolytes for Batteries	01/26/2010	09/30/2010	\$	24,500	\$	1,984
Mays	UT Research Foundation- Hydrocarbon-Mays	Hydrocarbon Based Membranes as Alternatiives to Nafion	10/01/2009	06/30/2010	\$	67,224	\$	39,874
Mays	UT Research Foundation- Hydrocarbon-Mays	Hydrocarbon Based Membranes as Alternatiives to Nafion - Matching	10/01/2009	06/30/2010	\$	63,946		

Total External Funds	\$	623,117	\$ 1,606,746
	二		
Total Matching Funds ORNL	\$	992,119	\$ 1,148,634

All qualified applicants will receive equal consideration for employment and admissions without regard to race, color, national origin, religion, sex, pregnancy, marital status, sexual orientation, gender identity, age, physical or mental disability, or covered veteran status.

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Inquiries and charges of violation of Title VI (race, color, national origin), Title IX (sex), Section 504 (disability), ADA (disability), Age Discrimination in Employment Act (age), sexual orientation, or veteran status should be directed to the Office of Equity and Diversity (OED), 1840 Melrose Avenue, Knoxville, TN 37996-3560, telephone (865) 974-2498 (V/TTY available) or 974-2440. Requests for accommodation of a disability should be directed to the ADA Coordinator at the Office of Equity and Diversity.

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