Science Alliance 2008–2009 Annual Report

Science Alliance 2008–2009 Annual Report to the Tennessee Higher Education Commission

A glimpse at joint UT-ORNL science and engineering research receiving support from the Science Alliance

This report is a publication of the Science Alliance,
a Center of Excellence at the University of Tennessee

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Science Alliance Span of Operation
July 1984–2009

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Photo by David Luttrell

Science

sci·ence

(sī ‘ən[t]s)

(noun) The observation, identification, description, experimental investigation, and theoretical explanation of phenomena.

Alliance

al·li·ance

(ə-lī ‘ən[t]s)

(noun) A close association formed to advance common interests or causes.

Photo by Laura Buenning

Profile

Twenty-five years ago, in July 1984, the State of Tennessee pledged support to the Science Alliance as part of a new Centers of Excellence program. Centers of Excellence build upon and expand the research strengths of The University of Tennessee and other campuses across the state. The total budget of Tennessee's Centers of Excellence—$17.7 million—serves as "seed" money to attract external funding to the state.

Selected in 1984 through a statewide competition, the Science Alliance is one of 26 Centers of Excellence in the state. The center's programs follow a two-fold directive: to improve science and engineering research at UT Knoxville and to expand joint research ventures with Oak Ridge National Laboratory. Research and educational outreach at the center focus on areas of strategic interest to The University of Tennessee and Oak Ridge National Laboratory. ORNL, the largest Department of Energy multi-purpose national laboratory, is managed by UT-Battelle, a 50-50 limited liability partnership between The University of Tennessee and Battelle Memorial Institute.

Spotlight on Science

In the midst of concern about economic stability, 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 concern. Science Alliance programs help ensure the public's investment is well spent, building cross-disciplinary teams of chemists, physicists, biologists, mathematicians, computer scientists, and engineers addressing the most significant challenges of our time in a trio of converging fields: nanotechnology, information technology, and biotechnology.

This annual report highlights research sponsored by the Science Alliance during the fiscal year 2008–2009. In these pages we offer evidence of how to maximize the benefits of research funding by supporting the ideas and talents of our best scientists at the right time and in the right way. It is our pleasure to share this year of success and accomplishments with you.

Joint Directed Research and Development Projects initiated in 2008 and 2009

2008

1. Jeffrey Becker: Survey of fungal component of the gut microbiome; LDRD Project: Host genetic diversity as a variable selection environment for the gut microbiome, Elissa J. Chesler.

2. Qiang He: Linkage between soil microbial activities in the rhizosphere and functional characteristics of dissolved organic matter; LDRD project: Carbon drivers of the microbe-switchgrass rhizosphere interface, Christopher Warren Schadt.

3. Bin Hu: Development of highly efficient organic white electroluminescence for solid-state lighting; LDRD Project: Revolutionary method for increasing efficiency of white-light quantum-dot LEDs, Chad E. Duty.

4. Mike Langston: High-performance computational tools for systems genetic analysis; LDRD Project: Host genetic diversity as a variable selection environment for the gut microbiome, Elissa J. Chesler.

5. Norman Mannella: Doping control of epitaxial TiO_x and TiO_2 thin film hetero-structures for photo-electrochemical solar energy conservation; LDRD Project: Bandgap narrowing of oxide semiconductors using non-compensated n-p Co-doping for enhanced solar energy utilization, Zhenyu Zhang.

6. Janice Musfeldt: Investigating the physical properties of magnetic nanoparticles; LDRD Project: Neutron scattering study of magnetic and spin dynamic behavior in amine-stabilized transition metal and transition metal oxide nanoparticles, Andrew C. Christianson.

7. Jennifer Schweitzer: Plant-soil feedbacks impact carbon, nitrogen, and phosphorus cycling: impacts of biofuel crops?; LDRD Project: Carbon drivers of the microbe-switchgrass rhizosphere interface, Christopher Warren Schadt.

8. Liem Tran: Cross-scale interactions and ecological system dynamics: pattern-process relationships through space and time; LDRD Project: Scale-dependent metrics for bioenergy: land-nutrient-water interactions under future energy scenarios, Virginia H. Dale. (2008 only)

2009

1. Itamar Arel: A semi-supervised learning system using deep belief networks for multi-modal medical data analytics; LDRD Project: Data analytics for medicine using semi-supervised learning (DAMSEL), Barbara Beckerman.

2. Michael Best: Synthesis and assembly of geometrically defined building blocks for dynamic covalent synthesis of robust higher order organic frameworks; LDRD Project: Controlled hierarchical self-assembly of robust organic architectures, Benjamin Hay and Radu Custelcean.

3. Jon Camden: Rationally designed nanofabricated SERS substrates for ultra-sensitive detection: probing surface chemistry in mesoporous carbon electrodes; LDRD Project: Understanding interfacial electrochemical phenomena in advanced energy storage capacitors using spectroscopy and modeling, Kevin Shuford.

4. Aimée Classen and Nathan Sanders: Developing a systems biology approach for linking genetic and environmental constraints to primary productivity — can patterns scale to the field?; LDRD Project: Developing a systems biology approach for linking genetic and environmental constraints to primary productivity in model and nonmodel species, David Weston.

5. Michael Gilchrist: Integrating models of protein translation and gene fixation with experimental data in the archaeal system: *Ignicoccus-Nanoarchaeum*; LDRD Project: A systems biology approach to study metabolic and energetic interdependencies in the Ignicoccus-Nanoarchaeum system, Mircea Podar.

6. Arthur Ruggles: Molten salt cooled high temperature pebble bed reactor; LDRD Project: Investigation of molten salt thermal performance in pebble beds using unique heating techniques, Graydon Yoder.

7. Glenn Tootle: Adaptation of water resource systems to climate change through weather modification; LDRD Project: Uncertainty assessment and reduction for climate extremes and climate change impacts, Auroop Ganguly.

8. Zhili Zhang: Active control of surface plasmonics for nanoscale diagnostics; LDRD Project: Active control of surface plasmonics with ferroelectricity, Jian Shen.

UT-ORNL
Joint Directed Research and Development

Joint Directed Research and Development (JDRD) projects establish and build complementary areas of UT-ORNL research. The research is selected for its potential to simultaneously advance the university research agenda and make independent contributions to the scientific goals of a specific Laboratory Directed Research and Development (LDRD) project at ORNL. While both programs and projects are independent, as research results develop the two teams collaborate on publications and research proposals to national funding agencies. JDRD teams reported a total of six planned or submitted proposals to the National Science Foundation or the Department of Energy during FY09; three of these were funded.

Relatively small, JDRD grants concentrate on problems at critical developmental stages, where research results can provide strong arguments for increased awards and fruitful UT-ORNL connections. Proposed by some of UTK's most imaginative and able scientists, JDRD projects move the research on to the next, most optimal steps in finding solutions.

Proposals are solicited from the faculty following ORNL's fall LDRD awards announcement. UT Knoxville faculty members and LDRD team leaders interact and determine how the two projects are complementary. Proposals, including a letter of support from the LDRD team leader, are submitted to the Science Alliance in late fall. Selections are recommended by a review committee to the Science Alliance director, who makes the final decision. The awards are announced in January.

In 2009, the Science Alliance funded 15 JDRD projects; eight first-year and seven second-year projects.

Itamar Arel

UTK electrical engineering and computer science

The human brain is capable of some truly formidable tasks. One of those is the ability to assess images, text, and data all at the same time and, with substantial training and experience, to arrive at a very high level of comprehension in order to make critical judgments.

But humans also need to sleep, and so even if their working hours are focused and effective, they still need help to handle the amount of information required to provide effective health care to a large population.

Both cost and scale make it essential that health information technology assist in accurate, judicious, cost-effective diagnoses. But, mimicking the human capacity for studying high-dimensional inputs—such as large images and videos—and identifying particular medical content and patterns within such inputs present a challenge for the field of machine learning.

The JDRD research of Itamar Arel promises to deliver a breakthrough in the field of medical image analysis using a family of machine learning systems known as Deep Belief Networks (DBN). These are derived from recent neuroscience research that has discovered how the cortex, which is the seat of most cognitive functions of the brain including pattern recognition, captures spatial and temporal information in observed data by maintaining a hierarchical neural network. Through modeling these processes with DBN, computer-aided diagnosis can assist highly skilled medical practitioners in more efficiently determining patterns of interest and significance.

The corresponding LDRD research of Barbara Beckerman and her team in the ORNL Biomedical Science and Engineering Center (BSEC) is an alternative machine learning scheme known as DAMSEL, or Data Analytics for Medicine Using Semi-Supervised Learning. That research aims to provide a computational framework for both assessing and "mining" data in medical information systems by examining statistical properties and regularities within it.

The two learning schemes—DAMSEL and DBN—will allow for testing each against the other in order to both validate and support their respective approaches. Their test bed is mammography (breast cancer analytics) for which imaging, pathology data, and textual reports exist.

Itamar Arel (L)

Derek Rose (R), the doctoral student working on this project

Jeffrey Becker

UTK Microbiology

At this very second, trillions of microorganisms inhabit your mouth, gastrointestinal tract, and all other body cavities and surfaces. In fact, these bacteria, fungi, and other tiny life forms outnumber the cells of the human body ten to one, which means a substantial portion of "us" is not really us at all.

Scientists have always assumed that this diverse collection of microorganisms—termed the microbiome—intimately influences the health and well being of its mammalian host; but until just a few years ago, no one even knew how many different organisms shared our bodies, much less what they were doing there.

This is changing due to powerful new DNA sequencing technologies that analyze DNA from mixed population samples without the need to culture individual organisms—referred to as metagenomics.

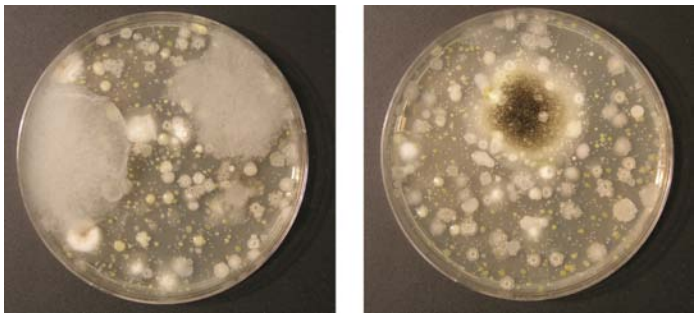
Using the mouse as a model system, JDRD team leader Jeff Becker and research professor Melinda Hauser take a metagenomic approach to cataloging the fungal diversity in a region of the large intestine known as the cecum, a site selected based on its role in gastrointestinal disease in humans.

Their work complements that of an LDRD team led by Elissa Chesler, which examines relationships between the bacterial residents of the cecum and the gene expression patterns in this region of the gut. Ultimately, Chesler's team will correlate what they learn with seven genetically defined strains of mice with predispositions to specific diseases, including obesity, hypertension, and various cancers.

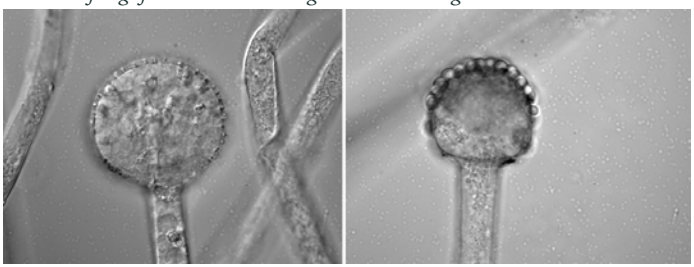
Since fungi represent a small fraction of the total microbiome, the JDRD team honed experimental skills in DNA extraction, to ensure that they sampled all of the organisms present in the gut material. Next, the trick was to find fungal DNA in this complex community mixture, making sure their samples were fungal specific, yet contained enough variation so all the fungi could be identified.

The team was, in fact, able to detect dozens of different fungal species in the cecum of all the mouse strains in the ORNL study; now they plan a more comprehensive study, using DNA sequencing technology at ORNL that produces over 400,000 sequencing reads in a single run.

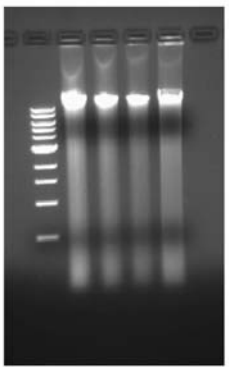
The National Institutes of Health Human Microbiome Project is devoting over $100 million in grants over five years to this effort. This study will serve as proof of concept in competitive grant applications for one of the first studies to examine the human fungal microbiome.



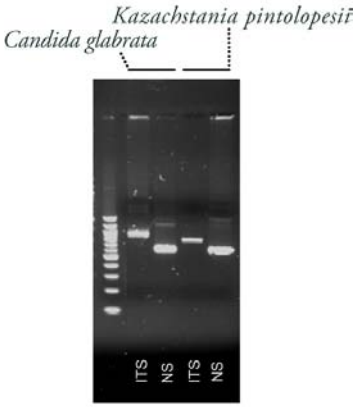
Cultured fungi from mouse cecum grown on solid agar medium



(above) Photomicrograph of sporulating structure of fungi cultured from the mouse cecum. (right) PCR, which stands for Polymerase chain reaction, enables researchers to produce millions of copies of a specific DNA sequence in approximately two hours.



Genomic DNA extracted from mouse cecum exudate



Ribosomal DNA products PCR amplified from cultured fungi

Michael Best

UTK chemistry

Did you know that nice crystals have nice properties?

Nice, that is, because they have stable and highly ordered structures; and they tend to offer beneficial properties for vital applications.

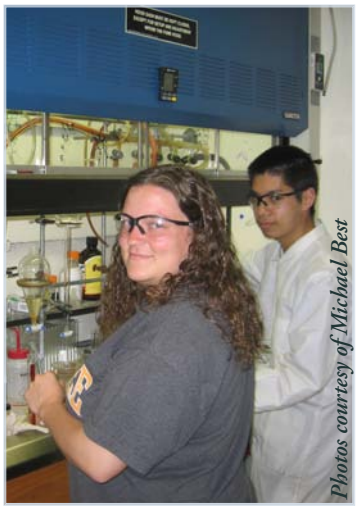
In order to develop new materials that exploit these desirable properties, scientists must be able to predict and control structure at the molecular level. Doing so is tough. Fortunately, JDRD scientist Michael Best's team excels at employing the very challenging tools and methods of synthetic organic chemistry required to create such materials.

These researchers are pursuing 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 retains the advantages of reversible self-assembly of materials, including adaptability and self healing, but generates materials with increased stability.

Best's initial step in designing appropriate molecular building blocks enlists the computer-aided design methods developed by LDRD team leader Benjamin Hay. Hay's computational methods identify building blocks that will self-assemble into predictable shapes. Following that, the chemists in Best's lab propose a method for synthesis. They then create the material and study their results to see if it satisfies the criteria for a robust, ordered crystalline framework. Working in parallel, the two teams are able to experiment with different approaches to maximize the scope of the new building blocks and the subsequent assemblies that will be generated from them.

Michael Best

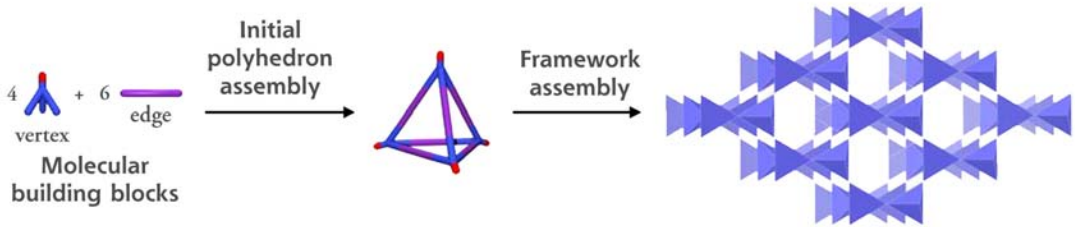
Because the synthetic phase involves a great deal of work, both in modeling and in combinatorial trials, the skilled organic synthetic chemists assisting in this project—graduate research assistants Chi-Linh Do-Thanh, Meng Rowland, Heidi Bostic and Matt Smith—are crucial for a successful and rapid outcome.



Photos courtesy of Michael Best

Heidi Bostic (l), Chi-Linh Do-Thanh (r) and Matt Smith (above), graduate research assistants on this project.

The strategy for the assembly of ordered crystalline organic frameworks using dynamic covalent chemistry (DCC):



In this case, geometrically defined building blocks include tetrahedral vertex pieces as well as linear edges. The vertex contains two different reactive groups to be exploited for a two-step assembly process. Here, DCC will initially be used to couple identical moieties presented at three of the four vertices of the vertex, with edge pieces containing two complementary reactive groups. This results in the assembly of a pyramidal construct. The second reactive group on the vertex is then used to link the individual polyhedra, yielding higher order frameworks.

Jon Camden

UTK chemistry

Scientific investigation often proceeds very painstakingly. Sometimes discovery even comes at the rate of a single molecule at a time.

Only through exacting, fundamental laboratory research can we expect to improve high-performance materials suitable for all types of advanced applications, from advanced catalysis and portable power to high-efficiency solar cells.

Jon Camden

Jon Camden's JDRD team is involved in one essential part of the basic science required—the study of phenomena observed at the common boundary, or interface, between adjoining materials. The team uses Surface Enhanced Raman Spectroscopy (SERS), a powerful optical tool, to probe the chemistries of nanoparticles occurring at interfacial surfaces.

In order to use SERS for this purpose, though, Camden must first develop and fabricate material substrates with ultrahigh sensitivity, such that the interfacial structures can be targeted and probed, a single molecule at a time, to reveal geometries and dynamics.

SERS spectra provide detailed information describing the vibrating molecular structure and the orientation of chemicals adsorbed onto or located very near a nanostructured surface, ultimately arriving at something like a "movie" of what is going on at the molecular level.

While single molecule SERS (SMSERS) is not yet developed enough to be used routinely, this project combines Camden's considerable experience and skill in both nanofabrication and electron microscopy to enhance SERS measurements of the vibrational spectra emanating from the molecular structures. The results will reveal molecular bonds and their arrangements at the level of a single molecule.

The complementary LDRD team of Kevin Shuford and Robert Shaw uses modeling and fluorescence spectroscopy to study the interfacial electrochemical phenomena in advanced energy storage devices, such as supercapacitors.

From what is gained in basic understanding, a single molecule at a time, can come many joint proposals for future funding for applications as varied as studies of surface chemistries (related to energy) and ultrasensitive sensing (related to homeland security).

Aimée Classen & Nathan Sanders

UTK ecology and evolutionary biology

When humans get too warm, their internal thermostats bring blood to the skin to release body heat; they perspire, drink water, and move out of the sun to stay cool.

Plants have their own way of responding, says JDRD team leader Aimée Classen. Obviously they can't go to the tap for a drink, or pick up and move to the shade. But some plants have evolved elaborate genetic mechanisms to combat heat stress.

Classen, co-leader Nathan Sanders, and ORNL plant molecular ecologist David Weston have joined forces on companion JDRD/LDRD projects to compare genetic responses of plants in which the entire genome is known (model organisms) with non-model plants where the genome is not known.

"David is interested in heat shock," Classen says. "He works with gene networks and looks at how plants turn genes on and off to regulate their responses.

"You can measure plant reactions to heat through respiration and photosynthesis. Another way is to look at what the genes are doing."

Weston's team has been growing two model plants, Arabidopsis (small forage plants) and Populous (trees); Classen, Sanders, and crew are growing Solidago—the weedy plant we know as goldenrod that grows in ditches and across old fields. They will use Solidago species native to Tennessee's warm summer climate and those accustomed to cooler Connecticut summers.

Goldenrod is an excellent choice for a number of reasons, Classen says; "It has a huge geographic and thermal range—you see it from Mississippi to Canada; we know a lot about it; and it has a gigantic genome."

Ultimately, the two teams want to see whether heat stress causes the same genes to turn on or off in all three plants—a result that would suggest the genes were conserved (retained) through evolutionary time because they carry out vital tasks.

"What gets interesting," says Classen, "is discovering how much of a plant's innate ability to deal with temperature comes from genetic flexibility."

Though in its first summer, preliminary work is already proving useful in grant proposals and has sparked several side projects for undergraduate research.

Below top to bottom: 1. Lara Souza and Lauren Breza collecting Solidago altissima *genotypes in Tennessee. 2. Lauren Breza and Heather Tran processing Solidago genotypes in the laboratory. 3.* Solidago altissima *genotypes growing in the greenhouse at The University of Tennessee.*

Photos courtesy of Aimée Classen

Michael Gilchrist

UTK ecology and evolutionary biology

Protein translation[1] is a universal biological process that occurs in all living organisms.

The instructions a cell uses for making a particular protein are encoded within an organism's genome. The genome itself is made up of long strings of nucleotides, which join together to form double helix DNA molecules. The genes consist of long strings of nucleotides within a DNA molecule.

Somewhat surprisingly, only four different nucleotide molecules are used to encode the instructions held within a gene—adenine (A), guanine (G), cytosine (C), and thymine (T). As a result, genes encode their information in triplets of nucleotides called codons.

Since there are four types of nucleotides (A, T, G, or C) and three nucleotides in a codon, the genetic code consists of 64 different codons (4x4x4=64). However, 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 different codon choices.

Curiously, says JDRD team leader Michael Gilchrist, even though multiple codons can be translated into the same amino acid, they are not all used with the same frequency.

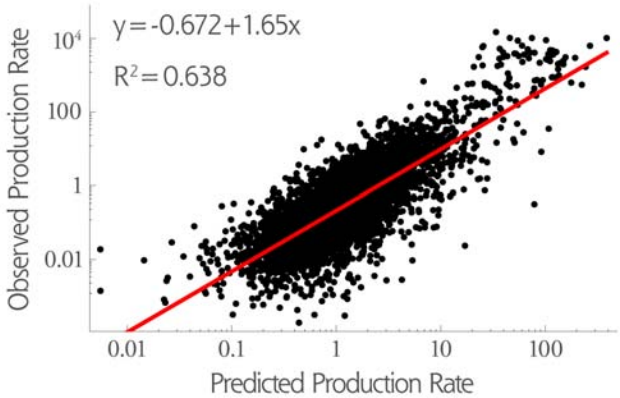
"Highly expressed genes seem to be quite picky (anthropomorphically speaking) about which codon they use to put an amino acid into the protein. In contrast, genes with low expression are not nearly so picky.

"People have seen this pattern for a long time and speculated about its cause. Our goal is 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 companion project leader, Mircea Podar, are developing computational tools to identify the subtle codon preferences within specific genes and to calculate how often, on average, each gene is expressed during an organism's life cycle.

Michael Gilchrist

"If you know the biological roles these genes play, then knowing how often they're expressed will tell you how important those different biochemical pathways are to the organism," says Gilchrist, "which should give you a clue about the organism's life cycle."



Predicted vs. observed gene expression rates in Brewer's yeast Saccharomyces cerevisiae. *Predictions are based on the bias or "pickiness" in codon usage of an individual gene and are generated by combining models of protein translation and sequence evolution.*

1 The synthesis of proteins directed by an mRNA template; the final step on the way from DNA to protein. [Sweden; http://nobelprize.org, "Texts & facts (basic level)," Josefin Lysell, Medical Student, Karolinska Institutet, Fredrik Eidhagen, Medical Student, Karolinska Institutet.]

Qiang He

UTK civil and environmental engineering

When we turn on our faucets here in the United States, we expect to get water that's safe to drink.

How long this will be true depends, in part, on research by JDRD team leader Qiang He and his LDRD partner project leader Christopher Schadt to determine what goes on between microbes and organic matter in our soils.

Research shows that microbes feeding on the secretions from nearby roots or dead plants alter the composition and characteristics of organic compounds dissolved in the soil. As a result dissolved nitrogen, phosphorous, sulfur, and other organic matter may be more or less likely to biodegrade, react with minerals in the soil, form carcinogenic byproducts during water-treatment disinfection, or become a food source for microbes and biofilms in water distribution systems, not to mention transporting contaminants to groundwater, lakes, and streams.

But exactly how microbial communities and dissolved organic material influence each other is unclear. To find some answers, Qiang He and doctoral graduate student Yan Zhang are studying the dissolved organic material and microbial communities in the soil surrounding decaying switchgrass roots, one of the crops being considered for renewable biofuel production.

The team's LDRD counterpart grows traceable, carbon-labeled switchgrass in the lab and uses it to study how the substances released into the soil by the roots influence surrounding microbial community structure and carbon cycling in the soil.

JDRD first-year results show that fermentative microorganisms increase during root decay and the dissolved organic compounds produced early in the process are predominantly acidic.

The JDRD team also found that dissolved organic carbon concentrations in runoff from the Beaver Creek watershed steadily increased during intense storms, but held to a near-constant rate in storms of less intensity, suggesting a different mechanism is at play in each. Runoff patterns are especially important because dissolved carbon can form compounds with toxic heavy metals, such as arsenic, cadmium, cobalt, and lead, and transport them into nearby lakes and streams.

Switchgrass grown in a UTK agricultural campus greenhouse. Insert: Qiang He

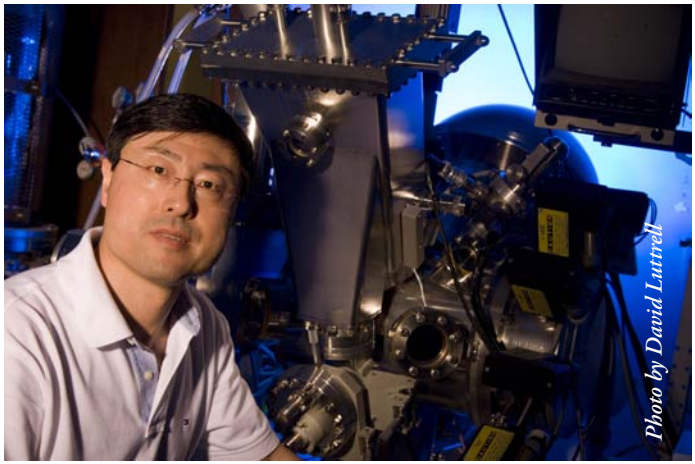
Information from this project served as key preliminary results for a successful National Science Foundation project beginning May 2009.

Bin Hu

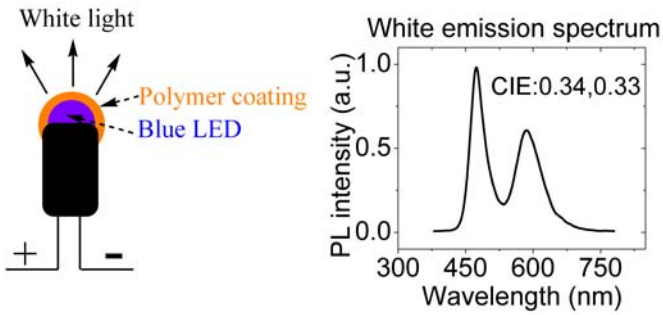
UTK materials science and engineering

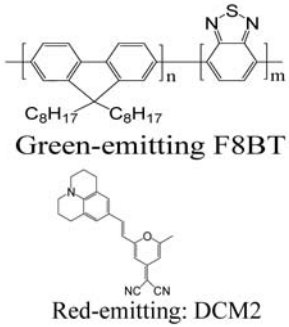
How difficult can it be to produce energy-saving white light? Difficult, to be sure! But also very worthwhile.

Solid-state LEDs (light emitting diodes) are now emerging as a cost-effective, energy-efficient alternative to conventional incandescent and fluorescent lighting. But efficiently producing a stable and reliable "white" light of the type and quality we are accustomed to has proven more complicated.



Bin Hu





White organic light-emitting diode with hybrid design, light-emitting spectrum, and chemical structures.

JDRD team leader Bin Hu has made considerable progress improving the quality and efficiency of white electroluminescence in concert with a new LDRD project headed by Chad Duty. The LDRD team concentrates on improving the efficiency of inorganic[2] white electroluminescence while, for their part, Hu and graduate student Ming Shao, along with exceptionally promising high school seniors Daniel Wentz and Nathan Cameron, focus on developing highly efficient organic white electroluminescence. In collaboration, both teams are well on their way to achieving superior hybrid light-emitting materials for advanced white electroluminescence.

In the course of his investigations, Hu has developed a unique experimental tool for studying the critical electroluminescent processes found in a hybrid design, achieving efficiencies of 100 percent (a vast improvement on the current level of 25 percent). The tool takes advantage of the "excitation" mechanism generated by magnetic fields.

Research discoveries in the first year of the project show promise that new control and manufacturing processes will make these materials even more attractive and competitive for lighting applications of all types.

The collaboration of basic science and advanced technology in this cooperative JDRD and LDRD enterprise has already resulted in two additional joint proposals for funding through the Department of Energy and two papers now in review.

2 A fundamental distinction in chemistry; organic molecules have hydrocarbon groups (carbon-based), inorganic molecules do not.

Mike Langston

UTK electrical engineering and computer science

Throw a lot of data anyone's way and the first thing they'll ask is whether you can help them visualize what it's all about. In the case of huge genome-scale data sets that is a thoroughly challenging job.

But Mike Langston and graduate research assistants Joshua New and Jordan Lefebvre are up to the task with novel algorithms, faster computational techniques, and web-based graphic tools such as the Ontological Discovery Environment that they've helped develop for biological scientists.

Langston's LDRD companion project leader Elissa Chesler generates large quantities of unique, high-quality laboratory data in the course of her experiments for characterizing the effects of host genetic diversity on gut microflora. In her team's LDRD work, researchers are faced with the task of integrating two massive and diverse data sets—one of intestinal gene expression in the tissue of mice and the other the genetic identity of gut microbiota. From such studies they hope to determine how susceptible an individual might be to intensely debilitating disorders such as Crohn's disease and irritable bowel disorder.

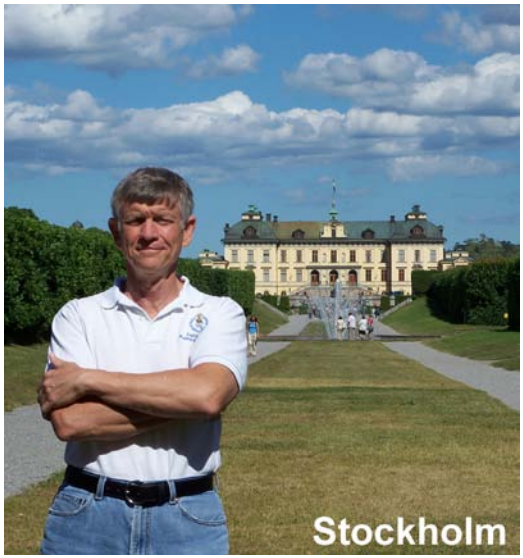
This is where Mike Langston and his research team come in.

"I view my role as a computational scientist as something of a middle man in the tool chain," Langston says.

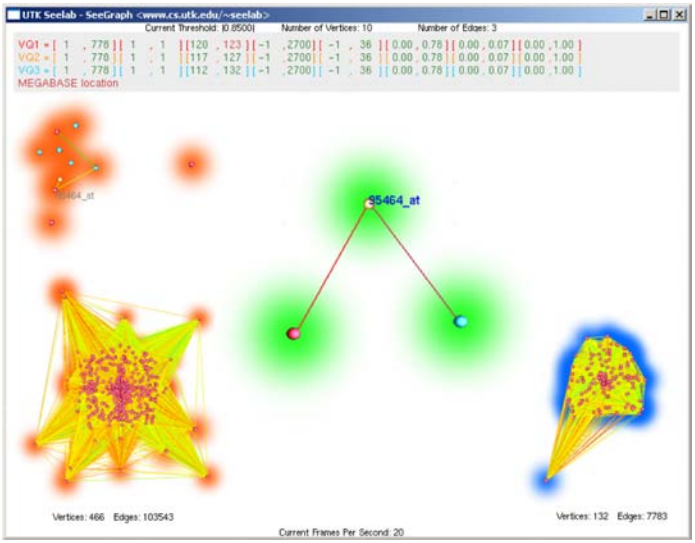
"The biological scientist produces data in huge supply. My team uses statistical and graph theoretical tools to eliminate noise and irrelevant data, reducing the problem to its core. We crack this core with our most efficient methods implemented on our fastest computing platforms."

The JDRD team returns relatively small and highly distilled solutions (sets of genes and proteins) back to the biological scientist, who then is able to verify novel results with more traditional "wet lab" techniques.

"This is a wonderful time to be a scientist," says Langston. "We're confronted by an amazing confluence of emerging technologies that challenge us to find new solutions for new problems, every day."



Mike Langston on one of his many overseas research trips; Sweden's Drottningholm Palace is in the background.



Langston and his colleagues devise novel combinatorial algorithms for high-performance computing platforms and use them to unravel subtle connections between genetic variations and gut microbial ecology. These techniques make it possible to pinpoint genetic polymorphisms that play key roles in gut microbial composition. The team then produces correlation graphs and other structures, and explores them using their clique-centric toolkit. They also apply new, tunable algorithms to visualize resultant clusters using tools from Jian Huang's SeeGraph laboratory (illustrated above).

Norman Mannella

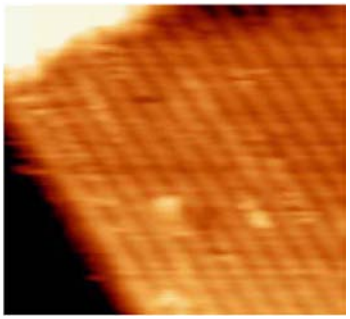
UTK physics and astronomy

As fossil fuels have dwindled in the modern age and their combustion has begun to adversely affect climate and the environment, the search for dramatically more efficient and less expensive solar energy conversion technologies has become a driving force behind research in nanomaterials.

As yet, no major breakthrough in the conversion efficiency of materials used in photo-electrochemical applications has been achieved, limiting photo-catalysis efficiency well below the ten percent target for commercial and industrial applications.

In a path-breaking step to address this challenge, JDRD team leader Norman Mannella partnered with the LDRD team headed by Zhenyu Zhang at ORNL. Combined expertise from the two teams integrates advanced materials synthesis with a fundamental understanding of materials properties for new high-efficiency solar energy applications—all guided by predictive theoretical modeling and simulations.

In the basic experimental approach chosen for this work, Mannella and graduate research assistant Amal Al Wahish use a technique known as molecular beam epitaxy (MBE) to grow high quality titanium oxide (TiO_2) thin films in a state-of-the-art chamber, where they can probe and characterize the structural, electronic, and chemical properties of the resulting films without removal (and so without the contamination that would result).

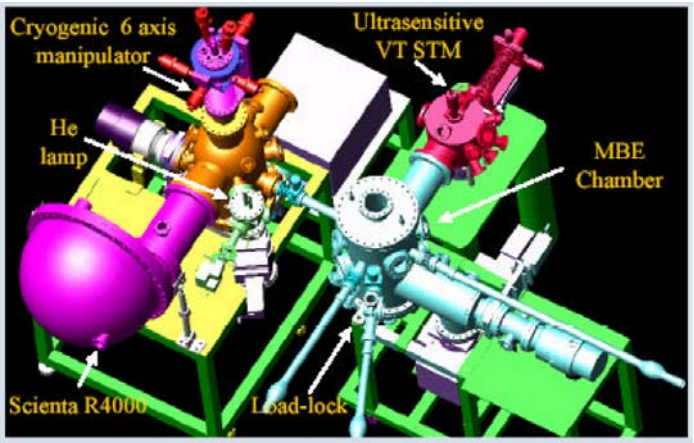


STM topography of Cr-N-TiO_2 nanocrystals showing atom rows (image size: 6 nm x 10 nm).

Norman Mannella

In a process known as "doping" the researchers intentionally add impurities to the transition metal oxide material, in an effort to "narrow the band gap." The team employs two novel doping schemes while leveraging the unique advantage of the MBE system to precisely control the structure and composition of the films.

In recognition of the potential in this line of inquiry, Mannella has recently been awarded his first National Science Foundation research grant in support of a major effort on growing thin film transition-metal oxides with MBE.



Schematic drawing of the MBE system in Mannella's Laboratory in UTK's Science and Engineering Facility. The MBE chamber is connected to a photoemission chamber with the ultrahigh resolution Scienta R4000 spectrometer and a variable temperature scanning transmission microscope (VTSTM).

Janice Musfeldt

UTK chemistry

Imagine yourself inside a manganese-oxide crystal; surrounded by a tiny jungle-gym-like lattice, you see manganese and oxygen atoms bonded at regularly spaced intervals. The atoms vibrate and the molecule hums with electromagnetic energy—which not only holds the system together, but is also responsible for atomic structure, chemical reactions, the attractive and repulsive forces associated with electrical charge and magnetism, and all other electromagnetic phenomena.[3]

Inside a three-dimensional material, the bonds reach in all directions, except, of course, at the edges.

But what if instead of three dimensions you confine the material to zero (a quantum dot), one (a straight line), or two dimensions (a plane)? Then, what happens to the charge and bonding, chemical reactivity, and magnetic structure?

These questions fascinate JDRD team leader Jan Musfeldt and LDRD companion-project leader Andrew Christianson. Both study the exotic physical properties of magnetic nanoparticles—especially how size and shape can be used to fine-tune desirable physical and chemical properties that are intimately tied to the electronic and magnetic structure.

When length-scales shrink to 30 nanometers or less, quantum confinement squeezes electrons into a space approaching the size of their wavelength, causing unusual (and even emergent) properties to occur.[4]

"Quantum confinement offers the opportunity to tune chemical bonding in nanomaterials," Musfeldt says, "yielding properties that, some day, may find application in novel devices."

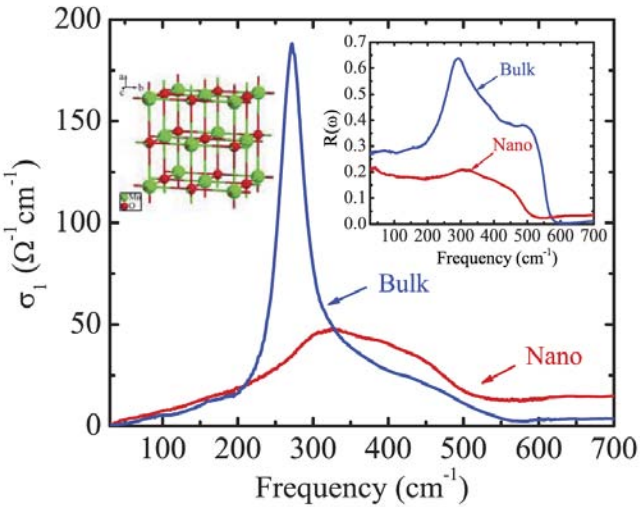
Her team is working with two model materials, manganese oxide (MnO) and molybdenum disulfide (MoS_2), to quantify the effects of strain and curvature on the chemical bonding. Their results should have wide future applicability, because each forms the chemical basis for a much wider class of materials, says Musfeldt.

3 The American Heritage® Dictionary of the English Language, Fourth Edition, Copyright © 2009 by Houghton Mifflin Company.

4 Nanophysics & Surfaces: Exploring Low Dimensional Structures, Des O'Mahony and Fran Pedreschi, Dublin Institute of Technology.

Two refereed publications, two presentations at international meetings, and a research grant from the Department of Energy have come from this work so far.

The Musfeldt research group: Henok, Jessica, Luciana, Ozge, Tanea, Xiaoshan, and Charles. Charles, Luciana, Ozge, and Xiaoshan contributed to this JDRD project.



Main panel: optical conductivity of bulk and nanoscale MnO at room temperature. Insets: rock salt crystal structure and measured reflectance of the two materials. Optical conductivity is calculated from the latter.

Arthur Ruggles

UTK nuclear engineering

For most of the last thirty years, little need or incentive existed for capturing as much of the heat as possible from power production systems. But now, for many obvious reasons—including renewed interest in efficient designs, more complete use of fuel, and reduction of wastes—this objective is becoming an important driver in energy research.

A significant part of improving efficiency is to increase the maximum temperatures possible in the thermodynamic power cycles that generate electricity. Fundamental research in thermal-fluid transport of this kind is once again a "hot topic," and UT's Department of Nuclear Engineering, with its longstanding expertise in this area, is poised to make use of work and partnerships in a number of applications, including high-temperature hydrogen production with the Department of Energy, and solar collecting systems with high-temperature energy storage in cooperation with Sandia Labs. In the latter application, storage becomes an important component for regulating energy supply.

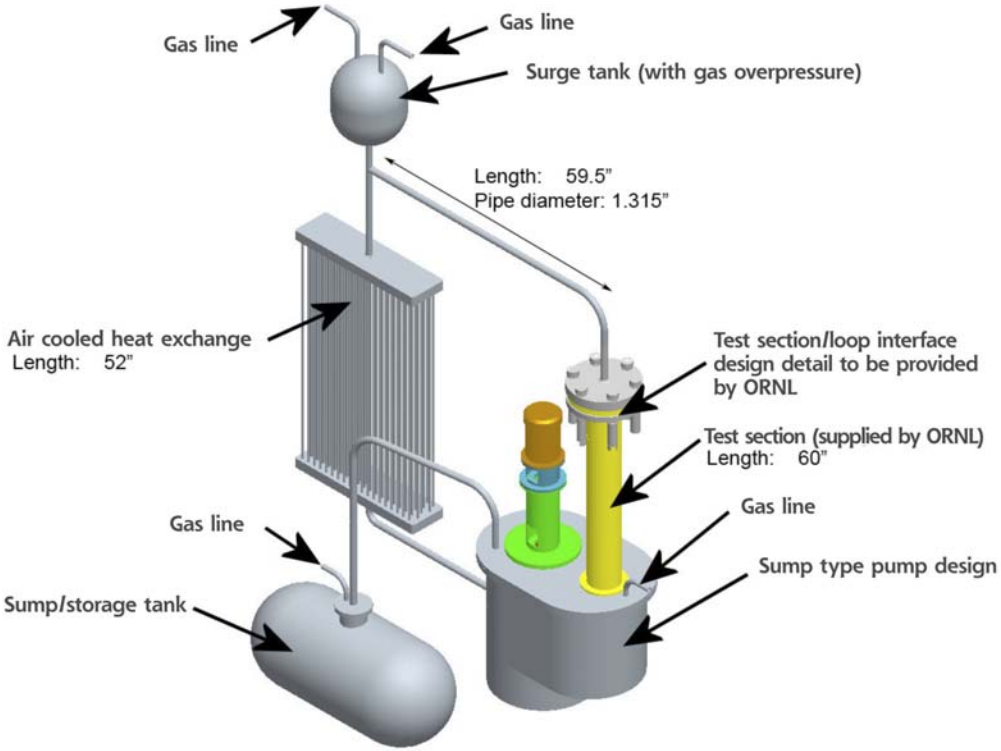
At ORNL an LDRD team headed by Graydon Yoder has put together a small molten salt loop system to reestablish and advance this much needed technology. Compared to older, conventional systems using gas or water, molten salts are receiving a lot of attention lately because they allow for transporting heat at higher temperatures and lower pressures.

In the companion JDRD research, Arthur Ruggles and his graduate research assistant John Ritchie will review, identify, design, test, and develop instrumentation that can operate at high temperatures both in experiments and for actual use in molten salt-based energy production systems.

Both ORNL's loop and UT's 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 for both the Electric Power Research Institute (EPRI) and Tennessee's new Solar Initiative.

John Ritchie with the molten salt pool. Ritchie is the graduate research assistant working with Ruggles on the project.

Below: the planned molten salt test loop



Jen Schweitzer

UTK ecology and evolutionary biology

"Just take a walk through a forest and it's easy to see that the soil underneath a pine tree looks different from soil under an oak, but we don't know very much about how individuals within a species alter their soils," says JDRD team leader Jen Schweitzer.

She and LDRD project team leader Christopher Schadt want to know more about this difference, most especially how plants change the soils and the microbial community feeding off roots and their secretions, or exudates, oozing into the soil and *vice versa*.

Jen Schweitzer

In recent years, many scientists have turned to genetics to expand what they know about living organisms, Schweitzer among them.

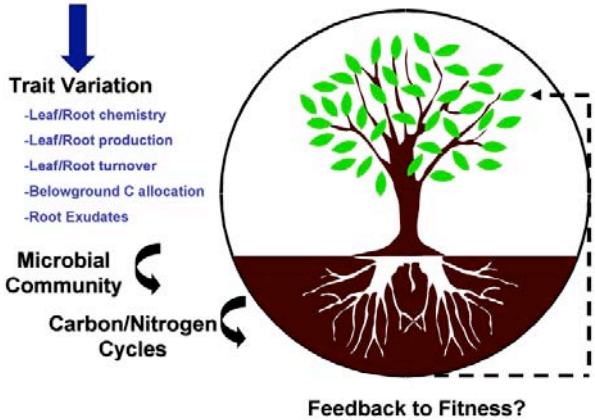
For their part, Schweitzer's team hopes to discover how much control plant genotypes have on the microbial communities responsible for degrading leaf litter and roots, a process which influences carbon (C) storage and nitrogen (N) and phosphorous (P) fertility of the soil.

This project addresses three important questions in microbial and ecosystem ecology, Schweitzer says.

How do varying plant traits, especially those of the roots, affect microbial community structure?

If the microbial communities vary, do ecosystem processes—in this case carbon storage and nitrogen turnover—vary as well?

Do changes in one mineral cycle (carbon) have similar effects in another (nitrogen and phosphorous)?



Conceptual framework for the proposed research, demonstrating the links between plant traits microbial communities, and nutrient cycles, as previously determined in several systems. The effects of these interactions across environments and the reciprocal fitness effects for the plant that produced those traits are little understood.

Schweitzer's team will test their ideas on specific genotypes of switchgrass, which have a wide range of root architectures and patterns of exudation, to examine the sustainability of switchgrass crops.

"Genetic based feedback between plants and soil processes is especially important in biofuel species because large areas of cropland are already being converted to biofuel crops and little is yet understood about their long-term effects on the soil," Schweitzer says.

The project supports two undergraduate students, teaching them the rudiments of ecosystem ecological research. In 2009, Schweitzer and her ORNL colleagues plan to use the data from this research in proposals to the National Science Foundation and Department of Energy.

Glen Tootle

UTK civil and environmental engineering

Cloud seeding, a close relative of rainmaking, has something of a "sleight of hand" reputation.

Still, with increasing populations in Utah, Arizona, Colorado, Wyoming, Idaho, and Nevada, not to mention California's ever-present agricultural demands, arid western states spend millions of dollars a year on cloud seeding projects.

"But, the question of the day," says JDRD team leader Glen Tootle, "is, does it work?"

In 2006, the state of Wyoming set out to find the answer through an $8.8 million cloud seeding project, targeting snowfall in the Sierra Madre and Wind River mountain ranges. Both feed the North Platte River basin and provide excellent locations for ground-seeding and experimental-control areas.

"The increase doesn't have to be huge to be significant," Tootle says. "Basically, cloud seeders will tell you the increase will fall within the general range of snow fall; maybe a 5, 10, or 15 percent increase."

Tootle says the project is unique. Unlike other seeding projects that put all the money into operations, Wyoming hired the National Center for Atmospheric Research (NCAR) to conduct an independent study to determine whether snowfall levels were the result of seeding or would have occurred anyway.

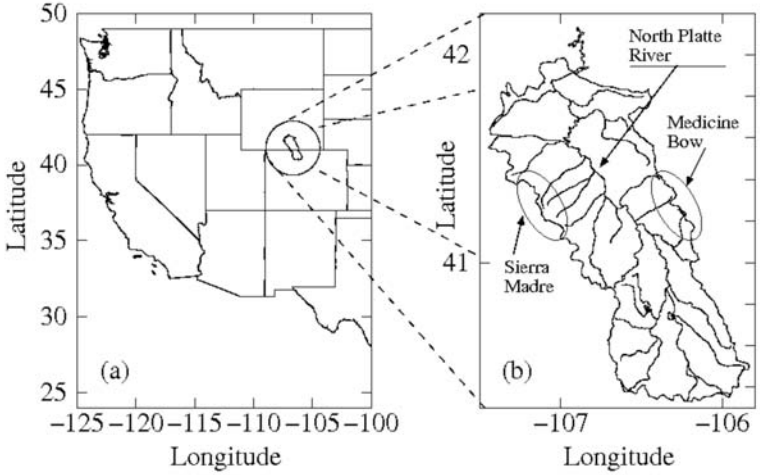
Tootle and companion LDRD project leader Aroop Ganguly have joined forces to help NCAR determine if an increase in snow will actually make any difference to the ranchers, farmers, or anyone else in the watershed who goes to the tap for a drink of water.

"Especially given the consensus in the scientific community that temperatures are on the rise," Tootle says.

It will be some time before data are available from the Wyoming project. In the meantime, Tootle and the team are running preliminary computer scenarios "to see how a one-half degree Celsius rise in temperature every 10 years and a 2 percent, 5 percent, or 10 percent increase in snow pack might affect stream flow.

"Many people have played the game of increasing or decreasing temperatures or precipitation to see what happens to stream flow, but what makes this a nice scientific contribution is adding weather modification to our scenarios," Toole says.

Tootle says the project also has far-reaching potential in the Tennessee Valley, where increasing temperatures and flat-line precipitation could alter water supplies and hydroelectric power.



The Study Area: The North Platte river is a 680 miles long tributary of [the] Platte river that collects water from the North Platte Headwaters watershed in Colorado and Upper North Platte watershed in Wyoming. North Platte Headwaters watershed is surrounded by Elkhead, Rabbit Ears, and Laramie mountain ranges whereas Upper North Platte watershed has Sierra Madre and Medicine Bow mountains in the west and the east, respectively . . . . [The] North Platte river feeds lake Simona located north of the basin.

[In figure above:] (a) Western United States show location of North Platte basin. (b) North Platte basin . . . showing tributaries and snow augmentation mountain ranges.

Graphic and text[5] from: "Weather Modification and Climate Variability Impacts on Streamflow" by Haroon Stephen, Glenn Tootle, Cody Moser, and Oubeid Aziz: AWRA[5] 2009 Spring Specialty Conference, Anchorage, Alaska, May 4-6, 2009.

5 Permission to reprint granted on September 9, 2009 by the American Water Resources Association.

Zhili Zhang

UTK mechanical, aerospace, and biomedical engineering

Fundamental discoveries in science and engineering rarely get the press they deserve.

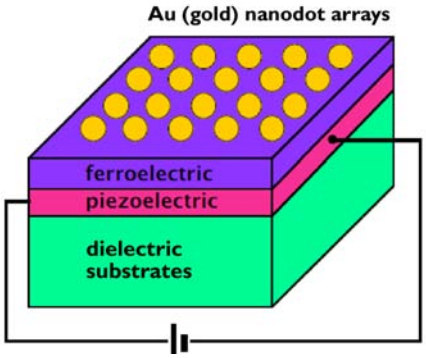
One such discovery occurred in the last decade when scientists succeeded in "squeezing" spectral light into sub-wavelengths and thus revolutionized conventional optics for the purpose of studying nanoparticles.

This breakthrough enables close examination of surfaces at the metal/dielectric (insulating) interface and, if current experimentation is successful, promises dramatic innovations in renewable energy, single molecule spectroscopy, and signal transmission.

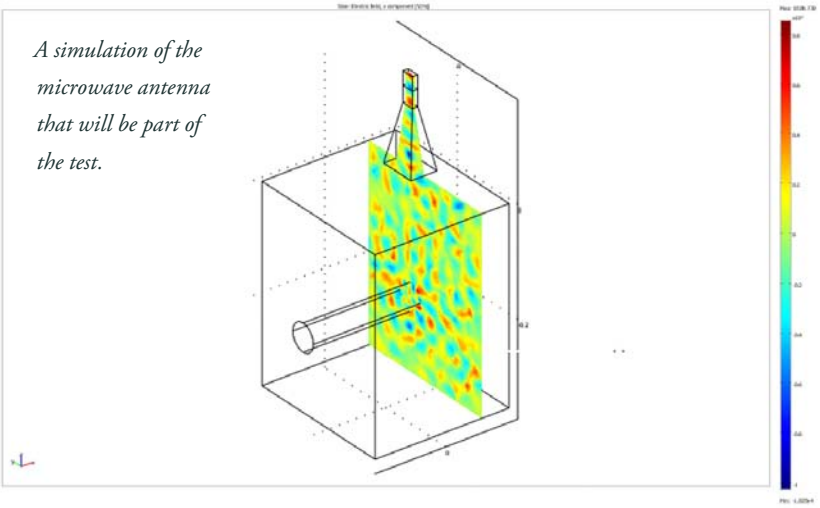
Basically, nanoparticles are inserted into an impressive new material ($LuFe_2O_4$) recently engineered and fabricated at ORNL; then small amounts of voltage are applied, in a sense "tuning" the surface spectral response. In this way the specially-engineered surfaces can adapt to different environments 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 control and discernment of nanoparticles, both in changing environments and in diagnoses of the special, dynamic characteristics of flow. For instance, the technique could potentially be critically important in aerospace engineering for diagnosing hypersonic flow around and about external surfaces of vehicles in flight.

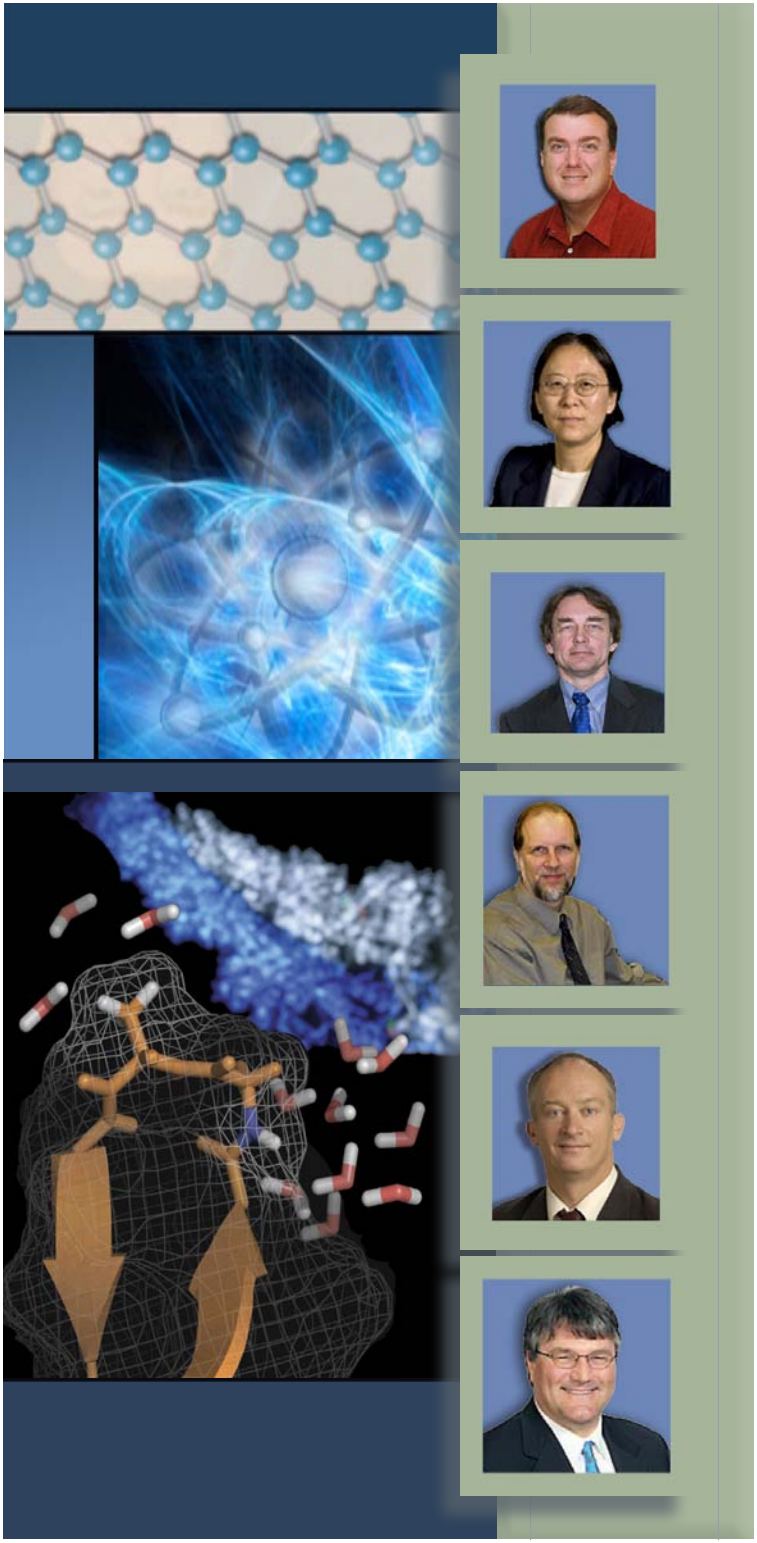
JDRD researcher Zhili Zhang, undergraduate research assistant Jeremy Petersen, and the rest of the team, will use Surface Enhanced Raman Scattering (SERS) spectroscopy and a new fiber optic laser purchased specifically in support of this project to validate both experimentally and by computer modeling the properties of the new material fabricated by ORNL. Their results will provide feedback and a comprehensive analysis to the LDRD team led by Jian Shen.



Above: 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.



A simulation of the microwave antenna that will be part of the test.



UT-ORNL Governor's Chairs

The new Governor's Chair Program, directed by the UT Office of the Executive Vice President, now has six appointments. Governor's Chairs offer competitive salaries, annual research funds, and start-up support for additional resources, such as related faculty appointments, research staff, and instrumentation. The Science Alliance helps to administer the program. Governor's Chair appointees are pictured on the left (from top to bottom).

Howard Hall, a nuclear chemist, is an expert in preventing and responding to nuclear terrorism. He holds a joint appointment in UTK nuclear engineering and ORNL global nuclear security.

Yilu Liu is an expert in the technologies used to monitor power grids. Her work will help to create the next-generation "smart grid." Liu holds appointments in UTK electrical engineering and computer science and ORNL energy and transportation science.

Alexei Sokolov uses a variety of tools, including powerful lasers and neutrons, to understand and control the properties of unique polymer materials. His joint appointment is in UTK chemistry and ORNL chemical sciences.

Robert Williams studies the genetics of central nervous system diseases and addictions. He holds appointments in UT Health Science Center anatomy and neurobiology and collaborates with ORNL biosciences.

Jeremy Smith applies neutron science and high-performance computational simulation to studies of bioenergetics and structural change in proteins. He holds appointments in UTK biochemistry and cellular and molecular biology and ORNL life sciences.

Thomas Zawodzinski, a physical chemist, studies electrochemistry and transport in energy conversion and storage devices. His joint appointment is in UTK chemical and biomolecular engineering and ORNL materials science and technology.

As originally conceived, the Governor's Chair Program might ultimately support 40 appointments.

UT-ORNL

Distinguished Scientists

The Distinguished Scientist Program backs high-profile leadership appointments in science and engineering; all are internationally recognized leaders in their respective fields. In cases where appointees are directly affiliated with an ORNL division, individuals hold joint UT-ORNL posts as tenured, distinguished UTK professors and ORNL senior scientists; both institutions contribute to the salary and research funds that support these positions.

This program anchored the Science Alliance in its partnership-building role in its early years and beyond. No new appointments have been made since the advent of the Governor's Chair Program, and none are planned.

But I am not afraid to consider the final question as to whether, ultimately—in the great future—we can arrange the atoms the way we want; the very atoms, all the way down! . . . (within reason, of course; you can't put them so that they are chemically unstable. . .).

– Richard Feynman, from "There's Plenty of Room at the Bottom," 1959

Elbio Dagotto *UTK physics and astronomy; ORNL materials science and technology*

Nanoscale dimensions and correlated electronic behavior

Scientists have speculated in earnest about the behavior and properties of materials with nanoscale dimensions, at least since Richard Feynman's famous 1959 talk suggesting that devices and materials could someday be fabricated to atomic specifications. Even earlier in the century, 1932 Nobel Laureate Irving Langmuir and Katharine Blodgett introduced the concept of one-molecule-thick films and the two-dimensional physics to describe such a surface.

A nano-length object behaves differently from its larger-scaled counterpart. For one thing, more surface area in relation to volume creates a different dynamic inside the material. Atoms and molecules in one-dimensional materials are next to each other in a line; in two dimensions, they form a one-atom/molecule-thick plane. Electronic and atomic movement is confined (restrained) to the interior of the nanoscale object—a fact that changes the material's mechanical, thermal, and catalytic characteristics. At nanoscales the movement of every atom and electron is influenced by its neighbors—hence physicists use the phrase "strongly correlated electronic behavior" to describe what happens with these materials.

Theoretical physicist Elbio Dagotto develops computational techniques and models to predict how strongly correlated electronic materials respond in the presence or absence of an electronic or magnetic field. His group studies a family of materials called transition metal oxides, which

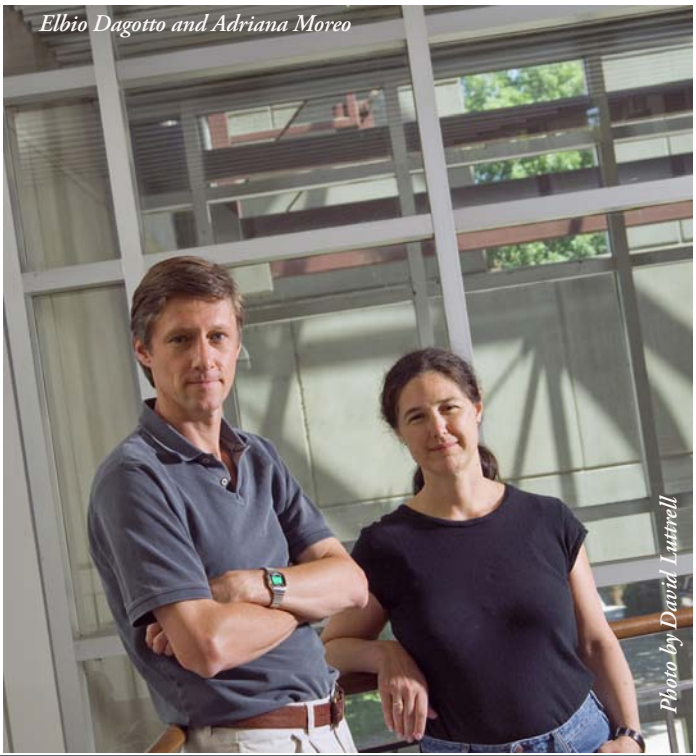

Elbio Dagotto and Adriana Moreo

Photo by David Luttrell

have enormous promise for improving memory devices and energy saving electronics. Taking advantage of new scientific ability to prepare multilayered materials with atomically perfect interfaces between alternating layers of oxides, they use their models to explore how differences in chemical composition might be exploited to transfer charge from one material layer to another.

Recently Dagotto's group also successfully implemented and applied a technique called the Time-Dependent Density Matrix Renormalization Group. This technique allows the study of dynamical properties of electrons, as opposed to studies that calculate averages over time. The calculation of time-dependent quantities allows studies of non-equilibrium situations, which are often found in real materials.

Takeshi Egami *UTK materials science and engineering and physics and astronomy; ORNL materials science and technology*

High-temperature superconductivity

Superconductors allow current to flow without resistance in low temperatures.

How low? Well, the first observed superconductivity in 1911 by Dutch physicist Heike Kamerlingh Onnes took place at a chilly 4 Kelvins above absolute zero, theoretically the coldest temperature possible. For comparison, ice melts at 273.15 Kelvin; water boils at 373.15.


Takeshi Egami

Photo by Jack Parker

Seventy-five years later, 1987 Nobel Laureates K. Alexander Müller and J. Georg Bednorz created a brittle copper oxide (cuprate) compound that superconducted at a breakthrough 30 Kelvins.

A widely accepted theory for the superconductivity in elements and simple alloys at near absolute zero temperatures came in 1957, but proved inadequate to explain the phenomenon in more complex compounds at higher temperatures. In spite of all the work since then, and the variety of compounds found to exhibit this phenomenon, the microscopic mechanisms propelling high-temperature superconductivity remain a puzzle.

Takeshi Egami uses neutron scattering and other experimental techniques and theoretical modeling to study the local structure and dynamics of the complex compounds that exhibit high-temperature superconducting behavior.

This year his work with a new family of superconductors, iron (Fe) pnictides (compounds in the nitrogen group on the periodic table), led to a new idea explaining why superconductivity in these particular compounds is unusually strong. Egami says this exciting class of superconducting compounds, first reported by a Japanese group led by Hideo Hosono in 2008, appears both electronically and structurally simpler than their cuprate counterparts, and thus might be easier to understand.

Atomic-scale dynamics of liquids and glasses

The viscosity of liquids can change by as much as 15 orders of magnitude (10^{15}) over a temperature range of a few hundred degrees, while the structure remains nearly the same. The atomic origin of this dramatic behavior is unknown.

Phonons,[6] or lattice waves, that give us a basic understanding of how atoms vibrate in crystals, cannot help scientists resolve questions about the structure and dynamics of liquid and glass. Liquid structures lack the distinct regularity found in crystals.

6 The quantum unit of acoustic or vibrational energy, phonons are wavelike and particle-like properties and are transmitted through vibrating material at the speed of sound.

Consequently the phonons are scattered haphazardly throughout the fluid and only have a lifetime of 10^{-12} seconds.

For some time, Egami has pursued the idea that the dynamics of local atomic-level stresses—a stress each atom experiences due to interaction with neighboring atoms—might play a similar role to that of crystalline phonons. Indeed his group's computer simulations verified that they play an equivalent role as phonons in crystals. They also demonstrated that the relationships among atomic-level stresses develop correlations in both space and time, as the liquid cools, explaining the rapid rise in viscosity.

Egami says a fully developed theory explaining the correlations among atomic-level stresses should bring the solution of this long-standing problem in liquid physics within reach.

Georges Guiochon *UTK chemistry*

Separation science – separating substances in chemical compounds

Single-celled algae are a promising alternative biofuel resource, but not all species produce the oils (lipids) used in biodiesels equally well. Just understanding the complex, metabolic processes of living organisms challenges current scientific knowledge and technology, let alone identifying the metabolites specific to increased lipid production.

An expert in the art of separating chemical compounds Georges Guiochon joined forces with others searching for better biodiesel resources. He turned his team's extensive expertise with multidimensional chromatography to the study of four different species of blue-green algae that appear on a Department of Energy list of species with potentially high-yield.

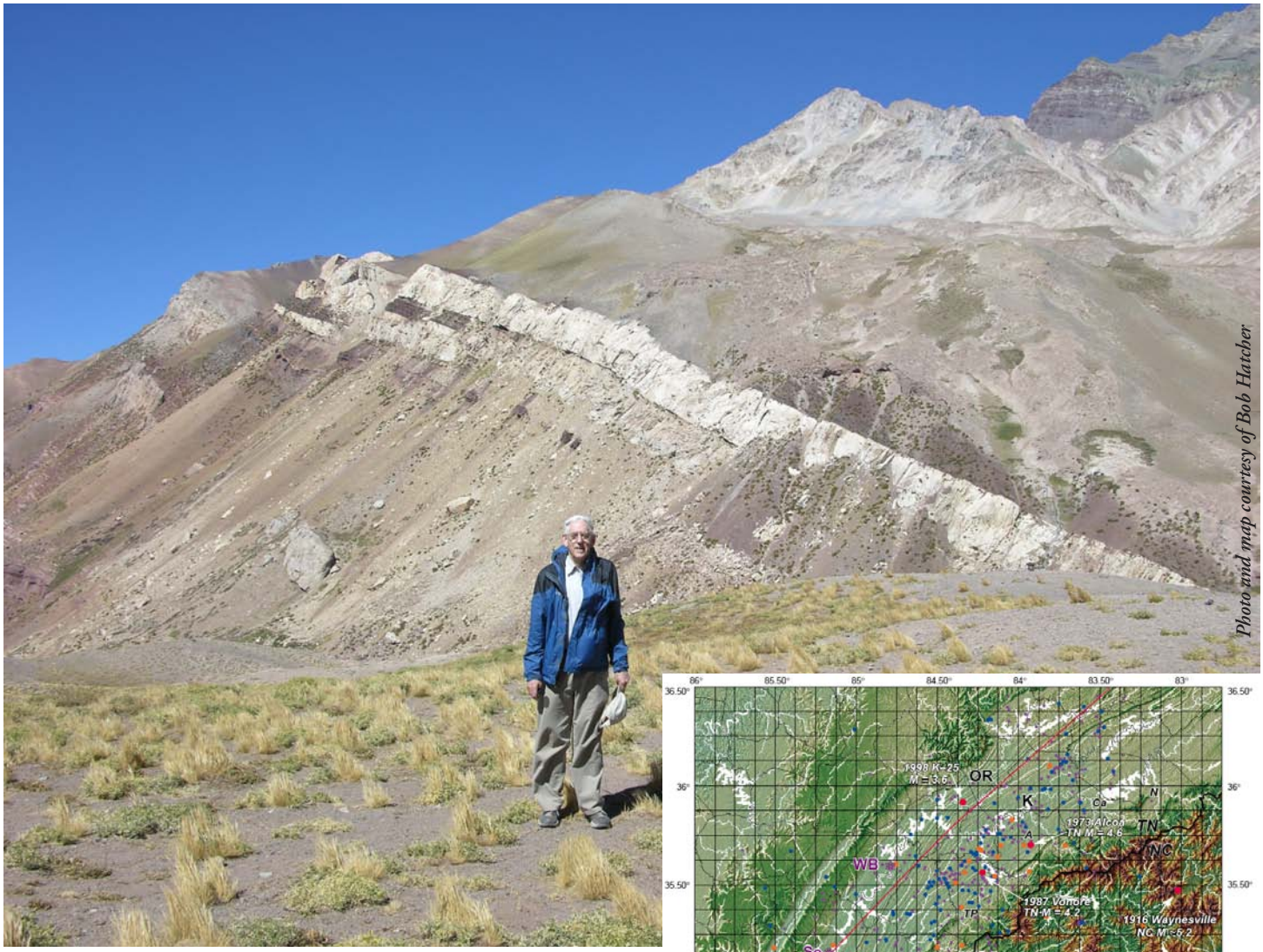
Unraveling the thousands of metabolic compounds involved in lipid production requires separation methods far more powerful than any individual technique currently available. Such complexity even defies the most powerful analytical methods—liquid chromatography (HPLC), which separates chemicals but is limited to a few hundred per column; mass spectrometry (MS), which identifies molecular structure but only on relatively simple mixtures of up to a dozen compounds; and nuclear magnetic resonance (NMR), which identifies spatial arrangements, but only if the sample is pure or nearly so.

To address the problem, Guiochon says, the burden to separate the highly concentrated metabolite mixtures falls to a two-dimensional, or two-step, HPLC technique, where the hundreds of compounds collected at the exit of one column are sorted by a second column, which separates them according to different characteristics. These simpler mixtures can then be analyzed using mass spectrometry.

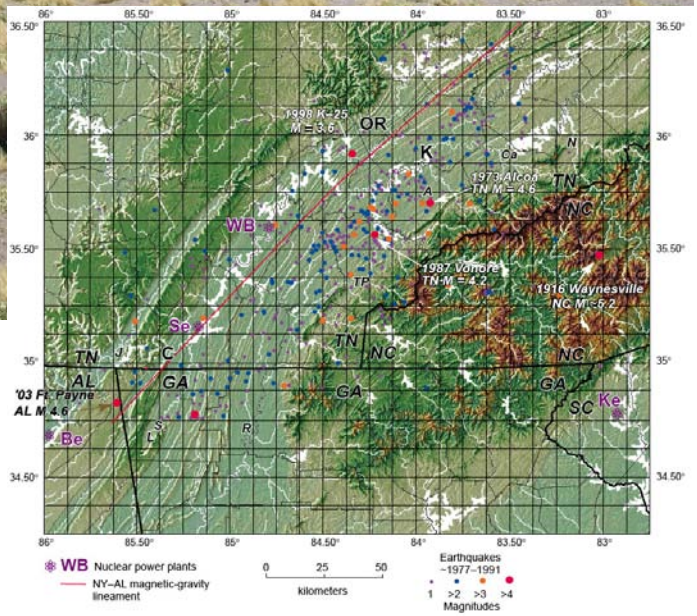
Significant information on the behavior and physiology along with limited, but promising, data about lipid metabolism in the chosen algal species is already available. These organisms produce long linear alkyl alcohols or carboxylic acids with properties similar to the hydrocarbons used to power diesel engines. Once Guiochon's group has identified the lipid producing metabolites, they can use their results to identify those algae with the greatest diesel-fuel-like lipid production. This research will help identify renewable resources that use solar energy to convert carbon dioxide into diesel fuel.

Guiochon received the Csaba Horvath Memorial Award of the Connecticut Chromatography Council in April 2009. This medal is given to a person in the field of separation science whose work has exemplified, and will continue to enhance the advancement of, separation science.

Georges Guiochon



Bob Hatcher below a large inactive fault in the Argentine Andes west of Mendoza.



Digital elevation model of parts of East Tennessee and nearby states showing the distribution of earthquakes in the ETSZ, locations of the largest historical earthquakes in the region, and the locations of nearby TVA and Duke Power Company nuclear plants. Smaller letters are localities of interest in the project.

Robert Hatcher *UTK earth and planetary sciences*

Structural geology and tectonics of continental crust

Continental crust forms when new material is added to older pieces of crust through buildup of oceanic and continental volcanic arcs, such as the Aleutians and the Andes, and when colliding continents separate and leave fragments behind. Both processes produce mountain chains, which then erode as the new continental

crust evolves into part of the stable continental land mass. Confirmation of this process resides in the ancient interiors of continents—"shields"—made up of the roots of ancient mountain chains that have been added to the continents over billions of years.

This process is reasonably well understood, as are those that produce earthquakes and volcanic activity at crustal boundaries where plates are destroyed (as off the coast of Washington and Oregon) or formed (as along the Mid-Atlantic Ridge).

Bob Hatcher, a structural and tectonics geologist who studies the processes that generate and change the Earth's continental crust, has long been fascinated by one of the great unsolved mysteries in crustal tectonics: Why do major earthquakes occur in the "stable" interiors of continents?

Historically, large earthquakes have occurred in the southeastern United States—in the Mississippi Valley (1811–1812; New Madrid seismic zone: magnitude[7] 3; 7½ to 8 quakes in 3 months) and near Charleston, South Carolina (1886; magnitude 7). Neotechtonic[8] studies have shown that major earthquakes recur about every 400 to 600 years in the New Madrid and about every 600 years in Charleston. Understanding this phenomenon has a direct bearing on the stability of the infrastructure of our civilization.

The East Tennessee seismic zone (ETSZ), which extends from just north of Knoxville southward into northwestern Georgia and northeastern Alabama, is the second most active in the eastern U.S. behind the New Madrid seismic zone. The U.S. Geological Survey has estimated the ETSZ is capable of producing a magnitude 7.5 earthquake. But because no earthquakes of a magnitude greater than 5 have been recorded, little incentive has existed to conduct prehistoric studies that detail maximum magnitude or frequency.

In 2009, Hatcher and others received funds from the Nuclear Regulatory Commission to conduct a neotectonics study of the ETSZ. Primarily a field study, the team is especially interested in finding layers of sandy material overlain by nearly impermeable clay; where the sand could be saturated with water and, during an earthquake, rupture through the clay layer, spreading light-colored "sand blows" onto the surface. Many similar features have been recognized in west Tennessee and in the Charleston area.

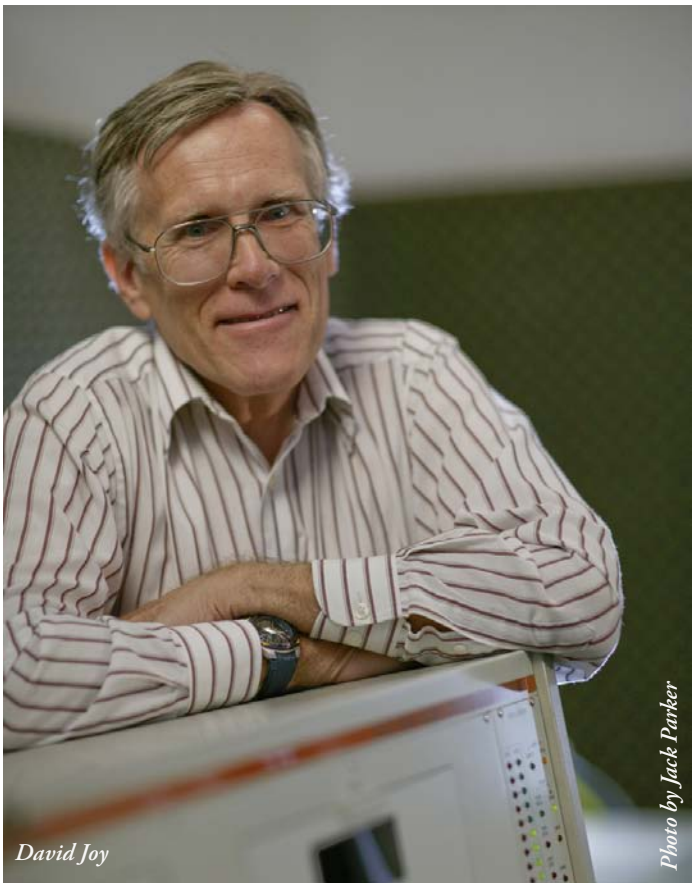
7 Earthquake magnitude is a measure of the amount of energy released by the quake inside the Earth, based on seismograph records. This is not a linear scale, so a magnitude 6 earthquake releases 30 times the amount of energy of a magnitude 5, and a magnitude 7 releases 900 times the energy of a magnitude 5 quake.

8 A term used to describe faulting, plate motion, volcanism, and other processes occurring during the past 5 million years of Earth history.

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

Nanomanufacturing with electron and ion beam imaging technology

It's hard to imagine machinery a thousand times smaller than the width of a human hair. Still, scientists are optimistic that the technology for building useful nanodevices will lead to an array of new materials and products, all the way from longer-lasting batteries to "smart pills" that deliver the right drug dose at the right time. But, coming up with precise calibrations for



David Joy

Photo by Jack Parker

nanotechnology's equivalent of "tool-and-die" production will be tricky because the scales are smaller than most of today's instruments can measure.

David Joy specializes in electron and ion beam imaging, electron optical analysis, and the precise measuring techniques needed to solve this difficult problem. His group searches for techniques that will provide absolute nanoscale calibrations.

Recently, Joy created a series of innovative tests to gauge the accuracy and performance of electron and ion-beam imaging tools. The tests were inspired by British physicist Lord Rayleigh's nineteenth century insight that Moiré patterns, or fringes, could be used to test the perfection of diffraction gratings—a series of light-splitting, parallel lines or grooves on a transparent or reflective surface. Often seen as rippling waves across a computer screen, Moiré fringes are interference patterns visible when two similar but slightly different grating patterns overlap.[9]

Joy says the improved precision has already proven useful in an unexpected quarter. He and entomology graduate student Andrew Haddow are measuring the three-dimensional size and shape of mosquito eggs, less than one micrometer in width, to determine whether they come from one of the species that carry the West Nile virus. If identified as suspect, the eggs can be destroyed before they hatch and become a threat to public health.

Joy's group is also part of a National Institutes of Health and Department of Energy sponsored project studying the effect that cerium oxide (CeO) nanoparticles have on living tissue, in this case *E. coli*. Thought of as the material of choice for next generation catalytic converters, CeO particles can assume a long, sharp, needle-shaped form, potentially capable of penetrating cell walls. Scanning transmission and electron microscopies revealed that the CeO rarely penetrated *E. coli* cell walls. So, while they did stop growth, the microbes remained alive to resume growing once the CeO was removed. Interestingly, Joy's group also found that their focused ion beam tool was an excellent scalpel, capable of cutting *E. coli* in half without any mechanical damage or distortion.

9 Encyclopedia Americana, 2008; and "Irving John Good: Science in the Flesh," In Cybernetics, Art and Ideas, Jasia Reichardt (ed.), London: Sudio Vista, 1971, pp 104-106.

Joseph Macek *UTK physics and astronomy; ORNL physics*

Atomic-scale systems

Since the early days of quantum mechanics, physicists have speculated about whether external forces might cause swirling electron vortices to appear inside simple atomic systems.

In 2007, theoretical physicist Joseph Macek discovered vortices could indeed be observed in the measurements of electrons ejected during impacts of charged particles or photoabsorption (a situation in which all of the energy of a photon is transferred to an atom, molecule, or nucleus).

Imagine the spinning, snaking vortex of a tornado. According to Macek's three-dimensional representations, something like this happens when a proton punches its way into atomic hydrogen. A vortex forms as electrons move in response to the collision, leaving evidence of the original proton-hydrogen impact in their wake.

A search for experimental corroboration led the group to some unusual features observed in 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, molecule, or even a solid, and two electrons eject


Joseph Macek

simultaneously. Observed both in computer simulation and experiments, these features have eluded explanation.

Macek says the atomic-scale vortices provide a likely explanation for these interesting structures. Detecting atomic-scale vortices in this context holds wide implications for the group's discovery, since electron correlations are central to atomic, molecular, and condensed matter (solids) phenomena.

Experimental results support the group's vortex theory. Studies probing electron correlations show circumstances where two electrons are completely absent from the atomic system; a situation which, in Macek's calculations, corresponds to instances where there are zero measurable quantities.

Jimmy Mays *UTK chemistry; ORNL chemical sciences*

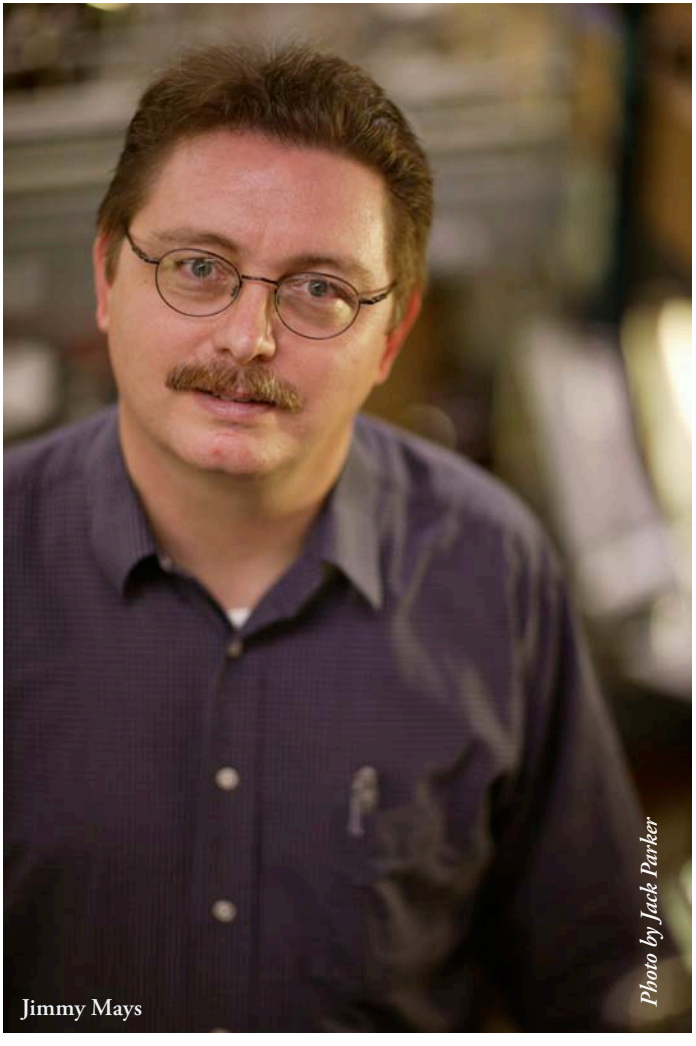
Polymer fuel cell membranes

The hydrogen fuel cell has potential as a lightweight, green energy resource for automobiles and other applications. Simple in concept, the cell strips positively charged protons from pure hydrogen entering the cell on the anode side. These are drawn through a semipermeable membrane by an oxygen-rich cathode on the other side of the cell. Meanwhile, the electrons enter an external circuit, supply electrical power for motors and other equipment, and reenter the cell on the cathode side, where it and hydrogen protons unite with oxygen and become water.

The polyelectrolyte or proton exchange membrane separating the anode and cathode is key to a fuel cell's operation. Developing inexpensive, robust, highly conductive membranes that will stand up to the elevated temperatures and low relative humidity inside fuel cells is one of the details standing in the way of success.

Under Department of Energy sponsorship, Jimmy Mays's team, (notably Suxiang Deng, UTK postdoctoral fellow in chemistry), synthesized and patented membranes based on an inexpensive hydrocarbon polymer base. Tests show the membranes are thermally and chemically stable and conduct protons better than Nafion at a fraction of the cost. Nafion, an expensive DuPont product, is the membrane-of-choice used in most fuel cells today.

Mays's group is exploring other potential uses for their membrane, including for water desalination and inside batteries.



Jimmy Mays

Improving polymer synthesis

In work for the National Science Foundation, Mays's group is working with a team of rheologists[10] and theorists to improve synthesis methods for specific well-defined branched polymers. Branched polymers are macromolecules with side chains dangling from a backbone.

Long branches dramatically affect how a polymer flows, a critical point because many products are manufactured from melted material under high shear conditions—for example the polymer films that become kitchen wrap or polymer fibers used in disposable diapers.

10 Scientists and engineers who study the deformation and flow of matter.

Polymer chemists learned long ago that branched polymers can be processed more easily and at higher rates than linear polymers (those with chains that go on and on) Mays says. But, too much branching, and you compromise polymer strength and solvent resistance.

The discovery, some ten years ago, of metallocene catalysts for making polyolefins, such as polyethylene and polypropylene, made it possible for scientists to synthesize polymers with a small number of exceptionally long branches. This process takes advantage of the benefits of branching without compromising strength; but the exact nature of the branching remains unknown. Mays and his team will study these molecular structures to discover how particular branched architectures affect the flow of the material. Their results will help to develop less expensive plastics with better performance.

Mays received the 2008 Distinguished Service Award from the American Chemical Society Division of Polymer Chemistry and was the 2009 Bayer Lecturer at Cornell University. This lecture series focusing on polymer chemistry began in 1987.

UT-ORNL Joint Institutes

Joint UT-ORNL institutes link distinct, complementary resources in select, high-priority scientific and engineering fields at UTK and ORNL. The institutes open the doors to leadership-class research instrumentation and computing facilities for university faculty world-wide. Equally important, joint institutes bring laboratory scientists within reach of rewarding teaching and mentoring experiences, less available at a national laboratory.

The Science Alliance support for UT-ORNL joint institutes began with the Joint Institute for Heavy Ion Research (JIHIR). Organized in 1982, JIHIR opened joint facilities on the ORNL campus in 1984. In 2000, UT-Battelle used the JIHIR model to organize additional joint institutes in computational, biological, advanced materials, and neutron sciences. During FY09, the Science Alliance provided leadership and administrative support to the joint institutes for Advanced Materials (JIAM) and Neutron Sciences (JINS). As in previous years the center handled JIAM administrative services, including accounting and clerical assistance, and contributed leadership and funds through the Distinguished Scientist appointments of interim director Ward Plummer, Elbio Dagotto, Takeshi Egami, David Joy, and Jimmy Mays. JINS received similar leadership and funds through Director Takeshi Egami's Distinguished Scientist appointment. The Science Alliance also contributed partial funding to JIAM, JIHIR, and the Joint Institute for Computational Sciences (JICS).

Detailed information about each program, including a 2010 budget proposal can be found on the university's Organized Research Unit Proposals web page (http://research.utk.edu/orus/).

Joint Institute for Advanced Materials

The Joint Institute for Advanced Materials fosters interdisciplinary research and educational opportunities related to developing new materials with superior properties (such as the greater toughness and high-temperature strength required for airplane skins) or those that can be tailored to support new technologies (such as pocket-sized supercomputers or medical implants that alter their shape in response to temperature).

In FY09, JIAM support brought three new graduate fellows to UTK, bringing the total to nine—five in physics, two in materials science and engineering and two in civil and environmental engineering. The fellowships add $10,000 to student stipends, bringing them up to the more competitive $28,000 to $35,000 range. The joint institute also contributed matching funds to three successful research proposals, among them a Department of Defense EPSCoR[11] project led by Veerle Keppens, UTK materials science and engineering, and the NSF IGERT,[12] Sustainable Technology through Advanced Interdisciplinary Research project[13] (STAIR) led by David Keffer, UTK chemical and bimolecular engineering. Pengcheng Dai, UTK physics and astronomy, was awarded a JIAM Chair-of-Excellence appointment, joining Hanno Weitering, UTK physics and astronomy, and Dayakar Penumadu, civil and environmental engineering. Dai's work on a new class of high-temperature superconducting materials recently received significant scientific acclaim.

JIAM began operation in FY07, following a five-year incubation period as the state-funded Tennessee Advanced Materials Laboratory (TAML) center of excellence. Both JIAM and TAML were directed by Distinguished Scientist Ward Plummer, who resigned his UTK appointment at the end of 2008. Deputy director George Pharr assumed this leadership role in February, 2009. Pharr will guide the design of a planned $30 million facility to be built at UT's Cherokee Farm campus and has plans for a "seed money" program to attract outside grants to the joint institute.

Joint Institute for Biological Sciences

The Joint Institute for Biological Sciences focuses on biology, energy, and health. UT's new 35,000-ft^2 JIBS building with 18 laboratories equipped for high-throughput genomic, transcriptomic, proteomic, and metabolomic research, and 35 offices and conference rooms opened for occupancy in January 2008. JIBS manages full access to these facilities and encourages UT faculty, students, staff, and administrators to participate and collaborate in their use.

The $125 million DOE BioEnergy Science Center (BESC) is headquartered in the JIBS facility. This ORNL-led project focuses on new methods for producing large volumes of ethanol from grassy and woody plant material at a price that is competitive with gasoline. The energy crops under consideration, such as switchgrass and hybrid poplars,

UT's JIBS building located on the Oak Ridge National Laboratory campus.

11 Experimental Program to Stimulate Competitive Research.

12 Integrative Graduate Education and Research Traineeship, the National Science Foundation flagship interdisciplinary training program.

13 See page 37 for more information on the STAIR IGERT.

have resistant cell walls, hardened to withstand weather, insects, and disease. Bioprocessing using a single or a single group of microorganisms to move the plant material from biomass to biofuel would reduce costs, as would genetic modification of the plants to make them less resistant to breakdown. Both are on the BSEC research agenda.

Gary Sayler, UTK microbiology and the Center for Environmental Biotechnology, directs the JIBS research and development program; JIBS biophysicist, Jeremy Smith holds the state's first Governor's Chair appointment. Smith uses neutron scattering and computer simulation techniques to learn more about biological proteins. The joint institute continues recruitment of Governor's Chair candidates to fill critical gaps at UTK and ORNL in plant sciences, microbiology, climate change and biogeochemistry.

Joint Institute for Computational Sciences

Research to design new materials, investigate protein development in living organisms, or simulate a core-collapse supernova requires heavy-duty computing power—the kind of power available in UT's $65 million supercomputer in the National Institute for Computational Sciences, headquartered at the Joint Institute for Computational Sciences. The NSF award included a contribution of $30 million for computer hardware and $35 million for operating expenses over five years.

Named Kraken after the mythical Norse sea monster, the supercomputer ran at full capacity for the first time early in 2009. On the latest Top500 list this June—the globally recognized rankings for supercomputers—Kraken was ranked the fastest university-managed supercomputer in the world and sixth fastest overall. Another upgrade in October 2009 will boost Kraken to become the first academic petaflops system.

But good as it is to claim a high ranking, JICS is more concerned with the science these computers can facilitate. Kraken fulfills one-third of the joint institute's goals. The remaining two-thirds involve developing programs to take full advantage of petascale and beyond computing power and training researchers to use supercomputing power in their own disciplines.

In FY09, JICS support for Igor Jouline, UT-ORNL joint faculty member in bioinformatics and genomics, resulted in a new software tool, HSP-HMMER, which was 100 times faster than the standard tool used for domain identification of huge and ever increasing protein databases. What previously took two months to run can now be executed in 24 hours.

JICS is directed by Jeff Nichols, ORNL associate laboratory director, computing and computational sciences.

Joint Institute for Heavy Ion Research

Stable atomic nuclei maintain specific neutron-to-proton ratios; if they do not, the nuclei experience some level of instability. Slightly less than 300 proton-neutron combinations are stable enough to exist permanently in nature. Thousands more can be synthesized by scientists or created in the stars. But these heavy, exotic nuclei, with too many neutrons or protons to be stable, quickly give off electrons or positrons until they reach more stable arrangements.

Scientists create the new, superheavy elements by fusing lighter nuclei. But their existence is brief. The new nuclei heat up and must find a way to cool back down to a stable state. Often, to do so, they simply break apart through fission.

NSF's largest supercomputer is up and running in full production mode. Kraken is the world's fastest academic supercomputer. The petascale system is managed by The University of Tennessee.

Graphic by Danny Wilson

The Joint Institute for Heavy Ion Research supports work in this fascinating area of physics. Their programs supply critical research assistance and manage dormitory facilities for scientists visiting the ORNL Holifield Radioactive Ion Beam Facility.

UT's JIHIR building located on the ORNL campus sports a new addition, dedicated in February 2009.

JINS is under construction at the SNS site and is scheduled for completion in April 2010. The state of Tennessee provided the $7.6 million for its construction. You can see the completed Center for Nanophase Materials Sciences in the background. Photo and caption from http://neutrons.ornl.gov/jins.

In spite of recent progress, it's still a challenge to find the optimal combination of beam and target as well as other conditions to maintain the structural integrity of superheavy nuclei long enough to fuse into new elements at rates that can be measured experimentally. This is due in part to the relationship between the barriers to fission, which stabilize the nucleus, and excitation energy, i.e. the energy difference between the excited state produced by fusion and the ground (stable) state.

Groundbreaking calculations by JIHIR scientists J.C. Pei, Witek Nazarewicz, J.A. Sheikh and A.K. Kerman show that even superheavy nuclei receive a little protection from the electric field produced by the nucleus. The results, consistent with recent experimental data, offer clues to the conditions for creating new elements and provide a wider context for understanding other types of fission, such as that used in reactors to supply energy. Their work should help to establish the mass and charge limits in producing and studying atomic nuclei.

Carrol Bingham serves as JIHIR director; Witek Nazarewicz is the Holifield Facility's scientific director. Both are professors in UTK physics and astronomy. A $500,000 addition to the JIHIR building was dedicated in February 2009 during the Japan-U.S. Theory Institute for Physics with Exotic Nuclei (JUSTIPEN) workshop.

Joint Institute for Neutron Sciences

Scientists use various imaging techniques to magnify what is happening to individual atoms and molecules. For the lighter atoms, like the hydrogen found in abundance in biological materials, neutrons hold the key.

Neutrons can penetrate material far better than charged particles. For them, because they interact with nuclear rather than electrical forces, it's almost as if the material isn't there at all—that is, until by chance a neutron slams into the nucleus of an atom. Typically, an atomic nucleus is 100,000 times smaller than the distance between it and another nuclear center. Scientists use the scattering patterns from those occasional collisions to tell them about material structure.[14]

To use neutrons, though, you need an accelerator or a reactor capable of hurling huge quantities of them into a material so hard that some will bounce off atomic nuclei; and following that, you need expensive instruments to interpret the data.

The Spallation Neutron Source (SNS) and nearby High Flux Isotope Reactor (HFIR) at ORNL do just that. An accelerator-based source, the SNS can generate the most intense pulsed neutron beams in the world. HFIR, with its steady

14 Neutron scattering: a primer, Roger Pynn, Los Alamos Science, Summer 1990.

neutron-rich stream, produces different and complementary results. Together, they combine to make ORNL the world's foremost center for neutron science.

The Joint Institute for Neutron Sciences helps scientists get the most out of the two facilities. Construction of a $7.6 million, 28,000-ft^2 building to house the joint institute began in October 2008; completion is expected early in 2010.

In FY08, JINS won a competitive three-year Department of Energy EPSCoR Implementation Award to build a collaborative Neutron Scattering Research Network among UTK, the SNS, and HIFR and the EPSCoR states.[15] JINS and participants in the network share postdoctoral fellows with the SNS and HFIR and collaborate on biology, polymer science, condensed matter physics, and other cross-cutting interdisciplinary fields.

In FY09 JINS awarded nine $12,000 neutron fellowships and sponsored four workshops. JINS is directed by Distinguished Scientist Takeshi Egami.

15 Eligibility for EPSCoR participation is restricted to states that historically received less federal R&D funding and have demonstrated a commitment to developing their research base and improving the quality of science, mathematics, and engineering research conducted at their university or college. It is a family of federal-state science and technology programs administered within seven federal agencies.

Other Ventures

Each year the Science Alliance contributes seed and matching funds to new research ideas and instrumentation, annual programs for students, and conferences that fall within the scope of its mission.

Proposal Development and Grant Writing Support

In FY08 the Science Alliance began to focus on providing institutional funding and support for ever larger multi-institutional and interdisciplinary-team research projects. In 2009, that strategic shift proved timely and the center made especially impressive strides in response to the calls for funding made possible by the American Recovery and Reinvestment Act (ARRA). Altogether, Science Alliance proposal development and grant writing teams provided support for grant applications valued at nearly $130 million. The chart on page 34 details a number of these.

Proposal development funded by the Science Alliance was accomplished with the assistance of Carmen Trammell, Charles Senn, Theresa Pepin, Darlene Casey, Lisa Carroll, Dorsey Bottoms, and Laura Buenning.

Particularly noteworthy was the Science Alliance's leadership role in Tennessee's Recovery Act Management Team (TRAM) in connection with the Broadband Technology Opportunities Program (BTOP). As a representative of UT, Tennessee's land grant university, the Science Alliance worked with ORNL, multiple state agencies, and private-public partnerships for six months to prepare a package of proposals for extending affordable broadband to the large rural areas of the state. If funded, the $85 million federal investment in the tightly-coupled package of proposed state projects will give many more citizens in every distant corner of Tennessee access to: university training and content; governmental services; e-commerce; and telehealth; not to mention the skills and connections to learn and compete in every arena worldwide.

Given that broadband infrastructure is such a critical foundation for research and dissemination of information, it can be argued that the ARRA BTOP proposals make possible a far greater return on

Science Alliance proposal development and grant writing team support for grant applications valued at nearly $130 mllion

Proposal Title	Principal Applicant	Grant Agency	Amount
The impact of political conflict on youth: assessing long-term well-being via an event history - a resource model	Brian Barber	Jacobs Foundation	$750K
Tennessee digitization newspaper project	Joanne Deeken	National Endowment for the Humanities	$460K
ARRA: Our stories will save us	Becky Fields	National Institutes of Health	$970K
ARRA: Healthy beginnings: coordinated preschool health	Nan Gaylord	National Institutes of Health	$1.3M
ARRA: Community partnering against health disparities: surviving TN fly ash	Joanne M. Hall	National Institutes of Health	$1.07M
ARRA: The role of sleep in predicting adherence to diabetic management	Ken Phillips	National Institutes of Health	$857K
ARRA: Efficacy of group acupuncture for cancer symptoms	Ken Phillips	National Institutes of Health	$965K
The Pharos expansion of the Global Ring Network for advance applications development	Greg Cole	National Science Foundation	$6M
Acquisition of a cryo transmission electron microscope with tomography	Gerg Duscher	National Science Foundation	$3.6M
Acquisition of a molecular beam epitaxy apparatus with *in-situ* analytical capabilities	Ramki Kalyanaraman	National Science Foundation	$1.9M
Center for extreme-scale computational astrophysics	Anthony Mezzacappa	National Science Foundation	$23.7M
Development of a versatile scanning probe microscope for broadband investigations	Hanno Weitering	National Science Foundation	$2.7M
ARRA: Broadband technology opportunities program	Executive Office of the Governor of the State of Tennessee	National Telecommunications and Information Administration	$85M

investment for all other research funded by the economic stimulus in the state. As of August 2009, UT applications for ARRA research funding amounted to over $546 million, including the following broad categories: approximately $145 million for health care; $75 million for basic and applied science with an additional $210 million for energy and climate change; and $49 million for STEM education and research. Clearly, UT researchers are rising to the challenge of these extraordinary times and opportunities.

From the most basic research on alternative energy resources to health care alternatives; from preparing children to succeed in science, technology, engineering, and mathematics to using supercomputers to understand genetic diseases, UT education and research can improve the lives and make the most of the talents of all Tennesseans—but only if their schools, libraries, hospitals, and homes have access to the information. A notable case in point is the preproposal survey of central Appalachia for the recently completed, $10.6-million, NSF-funded ACCLAIM project (Appalachian Collaborative Center for Learning, Assessment, and Instruction in Mathematics) that turned up more than 100 rural mathematics teachers looking for, but lacking access to, the means to pursue advanced degrees. Results such as this compel us to think beyond initial funding ideas to those who should ultimately benefit from the research. Broadband reaching into the most remote areas of the state will help bridge the gap between distressed rural areas and UT's educational resources.

UT-ORNL Joint Seed Money

In FY08, John Biggerstaff, UTK Center for Environmental Biotechnology, and Michael Zemel, UTK nutrition, received Science Alliance funds to expand the work of an ORNL Seed Money project led by Christopher Mann. The two teams are combining fluorescent and holographic microscopy in the same instrument. Their new techniques will eliminate the multiple, time-consuming, and expensive scans now needed to acquire three-dimensional images of biological specimens.

Mann designed the microscope in FY09; Biggerstaff and Zemel will support a graduate research assistant hired to design and test an incubator platform, so scientists can examine live, flowing cells and living mitochondria under conditions similar to those found in nature.

Affymetrix Core Lab

Researchers use DNA microarrays, such as the Affymetrix microarray system, to study the role that genes play in disease, the effectiveness and safety of therapies, and many other biological factors that affect human well-being. Using UTK's Affymetrix Gene Expression GeneChips, investigators are able to examine distinctions among gene expression in a wide variety of cell types and tissues.

UTK's Affymetrix Core Facility caters to in-house and local users, but the work is expensive and funds are often limited. In FY09 the Science Alliance and the Office of Research matched funds in an effort to make full use of this valuable, but costly, technology. Pooled with support from various biological departments and colleges, the funds finance an Affymetrix Core Lab Awards Program for proof-of-principle research designed to strengthen grant applications. In FY09, $56,000 was awarded to nine investigators.

Julia Gouffon directs the Affymetrix Core Facility.

Sustainable Energy Education and Research

The pressure to find renewable energy resources at a price we can afford remains high in the wake of the economic downturn of July 2007. Energy experts[16] predict a 32 percent increase in world energy consumption between 2010 and 2030; 13 percent of this is U.S. demand. On the positive side, U.S. carbon dioxide emissions are predicted to drop nine percent. But, we have no reason to relax; the United States remains one of the "grand gas guzzlers" of the world.

Confronted by an economic crisis, not to mention our increasing energy costs and demand, shrinking petroleum resources, the acidification[17] of our oceans, and threat to the Earth's ozone from carbon dioxide emissions, Congress enacted the 2009 American Recovery and Reinvestment Act (ARRA), on February 17, 2009. The bill provides $787 billion to stimulate the economy and create a more sustainable future. Of that

16 Department of Energy, Energy Information Administration (http://www.eia.doe.gov/oiaf/forecasting.html).

17 http://www.ocean-acidification.net/.

total, $43 billion targets energy issues, $111 billion goes to infrastructure and science, and $53 billion to education and training.[18]

Fortunately, The University of Tennessee and Science Alliance are in a position to take advantage of the opportunity presented by the ARRA and help the nation deal with its energy problem. For two years the Science Alliance has contributed to UTK Sustainable Energy Education Research Center (SEERC) projects. Science Alliance support for the STAIR project also falls into this category (more about STAIR on page 37).

Polymeric Photovoltaic Devices

The largest share of U.S. CO_2 emissions come from generating electricity[19] (EIA figure 81). So, a solar cell filled with polymer photovoltaic devices could become an attractive "green" source of electricity, if scientists can master the technology to make it both efficient and inexpensive.

A team of five UTK researchers led by Bamin Kohmami, UTK chemical and biomolecular engineering, joined together to study a special class of easily processed, soluble polymers whose properties make them excellent candidates for photovoltaic devices. Called conjugated polymers, the carbon-based semiconductors have unique advantages because they are both good at absorbing sunlight and at assuming the conditions needed to convert light into electricity. They are limited, however, in their ability to actually convert the light to charge and move it along.

The team—also including Barry Bruce, UTK biochemistry, cellular and molecular biology; Mark Dadmun, UTK chemistry; Bin Hu, UTK materials science and engineering; and Jimmy Mays, UTK polymer chemistry—created and analyzed materials with three different nanocomposite structures. Two incorporate highly conductive carbon nanostructures (nanotubes or fullerenes); a third employs chlorophyll-containing biological molecules as tiny photosynthetic reaction centers.

UT Zero Energy House

We know it intuitively. Our households burn plenty of energy, what with heating and cooling, washing machines and dryers, refrigerators, and dehumidifiers; and then we have our toys—video games and DVD players, not to mention the plasma televisions and computers that draw power even when they are "off." Energy Information Administration statistics for 2008 show residential consumption in the U.S. to be 3.77 billion kilowatt-hours per day—that's 36 percent of total U.S. consumption.

Only recently, though, as electric bills began to soar, have we given this the attention it deserves.

UT Zero[20] is aimed at satisfying our energy-hungry households without endangering the environment or resources of future generations. The Science Alliance contributed to this project.

The UT Zero Energy House and the Solar Platform for Excellence in Energy Design (S.P.E.E.D.) projects combine Tennessee architects, scientists, and engineers from UTK and ORNL in a venture targeting the rigorous DOE-sponsored 2011 Solar Decathlon. Every two years the Solar Decathlon enlists 20 winning college and university teams in a competition to design, build, and operate the most attractive and energy-efficient solar powered house. These are exhibited for a week on the National Mall in Washington, D.C., where they are open to the public and judged for first, second, and third place in the competition.

This summer (2009), the UT Zero team, led by Edgar Stach, UTK architecture, and graduate student Neil Parrish, moved construction of their prototype house

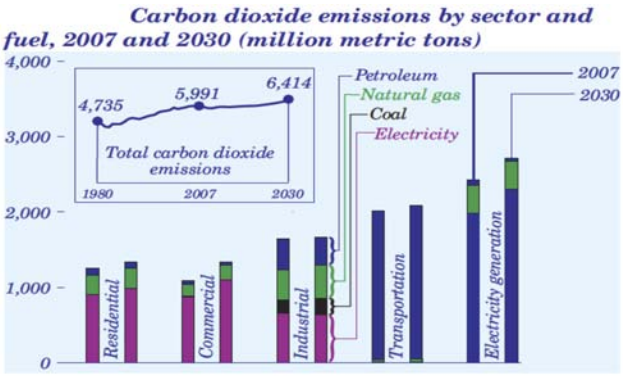


Figure 81 in the "Annual Energy Outlook 2009 with Projections to 2030," Energy Information Administration, Official Energy Statistics from the U.S. Government. Release date March 2009.

18 http://www.recovery.gov/?q=content/investments.

19 Energy Information Administration, Annual Energy Outlook 2009 with Projections to 2030, http://www.eia.doe.gov/oiaf/aeo/emission.html.

20 http://utzero.utk.edu/.

outside, where, when finished, it will use power from the sun for all its basic functions.

The companion S.P.E.E.D. project team has constructed a 375 kW solar array above a green roof on the UTK Art and Architecture building. The new array is expected to offset 16.8 million pounds of CO_2, an amount equivalent to 2,300 acres of trees—and produce near $100,000 per year of clean energy. The project tests the performance of this green technology, a vital step in fulfilling UTK's goal to become carbon neutral.

Support for Students

Integrative Graduate Education and Research Traineeship

IGERT is the National Science Foundation's flagship interdisciplinary training program, designed to improve graduate education and research in science, mathematics, engineering, and technology. IGERT funding establishes innovative model programs, introducing graduate students to a research environment that transcends traditional disciplinary boundaries. Students accepted in an IGERT program receive a $30,000 per year stipend for two years.

The Science Alliance contributes to two UTK IGERT projects, one of which explores the use of hydrogen as a sustainable energy resource; the other trains future biologists to make the most of a seamless computing and experimental environment. Respectively, professors David Keffer, UTK chemical and biomolicular engineering, and Cynthia Peterson, UTK biochemistry, cellular and molecular biology, are principal investigators on the projects. A description of each follows.

STAIR

Sustainable Technology through Advanced Interdisciplinary Research

While STAIR research specifically deals with the hydrogen fuel cycle, the skills being developed in the classroom and in the laboratory will find application in a broad range of alternative energy sources. The STAIR project's interdisciplinary curriculum combines faculty from molecular biology, chemistry and three engineering departments. STAIR graduate students earn a PhD in one of three areas of sustainable energy: hydrogen production through biological pathways; nanoporous materials for hydrogen storage; and structure/property relationships in hydrogen-based fuel cells.

Claudia Rawn, a UTK joint faculty member and senior research member in ORNL's materials science and technology, co-directs the project. The program currently has 12 graduate students.

SCALE-IT

Scalable Computing and Leadership Edge Innovative Technologies for Biology

For decades scientists typically gave little thought to collaborating with researchers outside their immediate fields. Over time, UT Knoxville has become a leader in the effort to change that mentality. And the payoff has been tremendous, says SCALE-IT's leader Cynthia Peterson.

Graduate students in the SCALE-IT project integrate advanced computer science and mathematical tools into molecular biophysics and systems biology research. Trainees can use UTK and ORNL resources to attack the most challenging problems in biology, from atoms to ecosystems. Their projects integrate UTK faculty from genome science and technology, chemistry, molecular biology, ecology and evolutionary biology, computer science and others as well as researchers at Oak Ridge National Laboratory and the NSF-sponsored National Institute for Mathematical and Biological Synthesis (NIMBioS) at UTK.

SCALE-IT had one graduate trainee in FY09 and has recruited seven students for FY10. Also, two new graduate trainee projects are confirmed for FY10. The first will process large data sets from the Spallation Neutron Source (SNS) to create images of protein-to-protein interaction. The results are aimed at the engineering of biodetoxification enzymes for bioremediation. The second will create a computer model of enzymatic reactions.

Harry Richards directs the SCALE-IT IGERT.

Summer Fellows: Research Experiences for Undergraduates in Mathematics, Chemistry, and Physics

The Science Alliance co-sponsors an NSF summer program to provide Research Experiences for Undergraduates (REU). It attracts top-performing students in mathematics, physics, and chemistry from around the country and is highly competitive. (In 2009 there were an astonishing 100 applicants for the 12 positions available in mathematics alone.) Many of these students come from high-quality 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. One of the best students from the 2008 program recently accepted an assistantship in the mathematics department beginning fall 2009.

In one highly popular Math REU exercise, undergraduates work through two famous papers with graduate students. Going beyond the basics, the student-scholars come to appreciate how understanding deepens and expands with multiple readings and discussion. Without this program, these talented undergraduates would not have the opportunity to study and conquer such challenging mathematical papers in a classroom until graduate school. The road to professional research in mathematics is a long one, and so the students' intensive engagement with graduate teaching assistants also helps them understand and welcome the demands of life as a math graduate student.

The 2009 summer Math REU projects are listed with their mentor-professors and described in detail at http://web.utk.edu/~utkreu/2009projects.html.

Lest one worry that such gifted students were confined to work, they also went on several excursions, including hikes (a first for many) and mild/wild rafting trips (a first for even more). We expect that many will be back at UTK—sooner or later—for both the science and the scenery.

Wanzhen Lu

Courtesy of the UTK Mathematics REU

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). 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.

On March 28, 2009, UT was host to 34 middle school and high school Olympiad teams with approximately 800 participants. Held at the Knoxville

Elton Banks (r) and Lan Tran (l) from Memphis Central High School working on the Tennessee Science Olympiad Disease Detectives event.

campus since 1994, this state tournament brings winners from six regional Olympiads to compete for trophies and medals. The winning teams in each division also receive travel support to advance on to the national competition. Not unlike the Summer 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 Oak Ridge High School and Bearden Middle School of Knoxville. Both teams went on to perform well in the stiff competition of the 2009 National Science Olympiad at Augusta State University in Georgia. The Bearden team won the gold medal in the "Write It—Do It" event and was the first place team in the exploratory "Bottle Rocket" event.

The Tennessee Junior Science and Humanities Symposium (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 at the state level are invited to present their papers at the national symposium, where they may win scholarship awards.

Tennessee's 44th Annual TJSHS was held on the Knoxville campus March 5-6, 2009, with 68 students and 18 teachers representing 16 Tennessee high schools. Twenty five young scholars submitted original research papers, spanning a variety of topics and scientific disciplines. Students 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.

Headed up by TJSHS award-winning teacher Kristin Baksa, the winning delegation of top five students from the Knoxville round traveled to the 47th National Junior Science and Humanities Symposium, held April 29-May 3, 2009, in Colorado Springs, Colorado. First place Knoxville winner Chris King won first place in the engineering competition. For this outstanding accomplishment, he received a $16,000 scholarship for college and will be representing the United States at the London International Youth Science Forum scheduled for July 29-August 12, 2009, at Imperial College, London, UK.

Conference Support

UT-ORNL-KBRIN Bioinformatics Summit

The 8th Annual Bioinformatics Summit was held at Fall Creek Falls State Park in Pikeville, Tennessee, March 20-22, 2009. The regional summit has acquired a well-deserved reputation for enhancing

Harrison Emery of Ross N. Robinson Middle School in the Tennessee Science Olympiad "Wright Stuff" event.

collaborative links and integrating multidisciplinary research efforts—resulting in numerous new, cooperative projects in bioinformatics research and education. A total of 202 researchers, educators, and students attended the conference, jointly sponsored by the UT Health Science Center for Integrative and Translational Genomics, the UT Molecular Resource Center, and the Science Alliance.

In addition to Geospiza/Digital World Biology workshops, scientific presentations were organized in three plenary sessions under the headings of medical and translational informatics; systems biology; and next-generation sequencing and epigenetics. Proceedings can be found at www.biomedcentral.com/1471-2105/10/S7/I1.

In a final review of educational opportunities, Cynthia Peterson, director of the UT-ORNL Graduate School of Genome Science and Technology updated participants on 1) the SCALE-IT[21] program and 2) the new National Institute for Mathematical and Biological Synthesis (NIMBioS), a one-of-a-kind institute at UTK. NIMBioS is the result of a $16 million NSF award that will draw more than 600 national and international researchers each year to participate in working groups, workshops, and conferences. See www.nimbios.org.

The 2010 Bioinformatics Summit will rotate back to Lake Barkley State Park in western Kentucky in the spring. Areas of interest are expected to focus on the use of next-generation sequencing technologies in research laboratories, clinical informatics, and integrative systems biology.

21 More about SCALE-IT on page 37.

Plans for Fiscal Years 2010—2012

The Science Alliance Enters a Period of Transition

In 2005, Tennessee's new Governor's Chair Program began to change the course of the Science Alliance UT-ORNL partnership-building agenda. Prior to this time, the UT-ORNL Distinguished Scientist Program had been the focal point for the center. Following a transformational strategy, the Governor's Chair Program, under the guidance of the UT Office of the Executive Vice President, was charged with recruiting high-profile appointments to joint UT-ORNL appointments; this gave the Science Alliance the opportunity to explore other avenues for UT-ORNL support. The UT-ORNL Joint Directed Research and Development Program was the first of these. Beginning in earnest in 2006, JDRD research now supports 15 to 16 projects each year.

Our success increased in FY07 and FY08. The Science Alliance provided institutional funding for two approximately $1.2 million Integrative Graduate and Research Traineeship (IGERT) proposals. NSF funding for each began in July and August of 2008. The Science Alliance has plans to maintain this momentum, offering short-term, "encouragement" funds in such strategic areas as sustainable energy—including bioenergy—computational sciences, and materials sciences.

What's next?

Today, again, we have the opportunity to refocus—to apply our resources to help the university crest the next hill. The hard work to establish joint programs must be transformed into measures that will get the most out of joint appointments and institutes and our UT-Battelle connections.

Science Alliance support for UT-ORNL joint institutes, long on the center's research agenda, is less important as the institutes acquire their own funding from competitive resources. On their way to becoming independent, the joint institutes have established resources in computational sciences, advanced materials, neutron sciences, biological sciences, and nuclear physics. In 2008, the Joint Institute for Computational Sciences received the first installment of the $65 million NSF award to build and operate a petascale computing system in the National Institute for Computational Sciences. The Joint Institute for Neutron Sciences under the leadership of Distinguished Scientist Takeshi Egami also received a $1.9 million DOE EPSCoR award to build a collaborative research network.

With this and other funding on its way, the Science Alliance will phase out joint institute support to focus on current needs, most especially on 1) expanding the UTK-ORNL research base by increasing competitive external grants and contracts; and 2) stimulating the growth of jointly operated UTK-ORNL graduate education programs, such as the Graduate School of Genome Science and Technology. Expansion of graduate programs of this type will be most beneficial to both institutions at this point in the UT-Battelle partnership.

Grant and contract support

In FY08 the center began contributing institutional funding and preoposal-development assistance for large interdisciplinary-team research projects. In FY09, Science Alliance proposal development and grant writing teams provided support for grant applications valued at nearly $130 million. Particularly noteworthy is the center's leadership role in the State of Tennessee's Recovery Act Management Team (TRAM) in connection with the Broadband Technology Opportunities Program (BTOP). As a representative of UT, Tennessee's land grant university, the Science Alliance worked with ORNL, multiple state agencies, and private-public partnerships for six months to prepare a package of proposals for extending affordable broadband to the large rural areas of the state.

Graduate education

Graduate research and education is another important part of the center's outreach. At this point, however, it is time to change the formula for distributing Science Alliance funds, making it more competitive. In the future the Science Alliance will establish a program that focuses graduate support on strategic themes at the university and ORNL.

Funding the Future

The Science Alliance has an exceptional record of success bringing senior leadership, increased external funding, strategic new research, and remarkable graduate and postdoctoral research to UT and ORNL. As a proven Tennessee investment the Science Alliance should be funded to the greatest extent possible. New income will be used to target and encourage research in strategic areas important to Tennessee and the nation.

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Courtesy of ORNL

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

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Courtesy of UT Zero research team

UT-ORNL joint faculty

UT-ORNL joint faculty

Name	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
Plummer, Ward	ORNL/MSTD	UTK/Physics	Materials	Distinguished Scientist/Professor
Hall, Howard	ORNL/GNSD	UTK/Nuclear Engr	Nuclear	Governor's Chair
Liu, Yilu	ORNL/ETSD	UTK/EECS	Electrical	Governor's Chair
Smith, Jeremy	ORNL/Biosciences	UTK/BCMB	Molecular Biophysics	Governor's Chair
Sokolov, Alexei	ORNL/CSD	UTK/Chemistry	Materials	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
Banks, David	ORNL/NCCS	UTK/EECS	Ricky Kendall	Computing
Barnes, Ted	UTK/Physics	ORNL/PD	Glenn Young	Nuclear Physics
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
Efremenko, Yuri	ORNL/PD	UTK/Physics	Glenn Young	Neutrons
Eguiluz, Adolfo	ORNL/MSTD	UTK/Physics	Steven Zinkle	Materials
Ericson, M. Nance	UTK/EECE	ORNL/ESTD	Ted Fox	Electrical Engineering
Gao, Yanfei	ORNL/CSMD	UTK/MSE	Thomas Schulthess	Materials
George, Easo	UTK/MSE	ORNL/MSTD	Steven Zinkle	Materials
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	
Jin, Rongying	UTK/Physics	ORNL/MSDT	James Rushton	
Jouline, Igor	UTK/Biology	ORNL/CSMD	Jeff Nichols	Comp. Biology

UT-ORNL Joint Faculty (continued)

Name	Joint Appointment at	Based at	ORNL Contact	Field
Kilbey, S. Michael	UTK/Chemistry	ORNL/CNMS	Linda Horton	
Larese, John	ORNL/CSD	UTK/Chemistry	Phillip Britt	Neutrons
Mahfouz, Mohamed	ORNL/CSED	UTK/MABE	Brian Worley	Computing
Maldonado, Ivan	ORNL/NSTD	UTK/Nuclear	James Rushton	
Moreo, Adriana	ORNL/MSTD	UTK/Physics	Peter Tortorelli	Materials
Morris, Jamie	UTK/MSE	ORNL/MSTD	Steven Zinkle	Materials
Papenbrock, Thomas	ORNL/PD	UTK/Physics	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
Sayler, Gary	ORNL/Biology Sci	UTK	Berry Berven	
Simpson, Michael	UTK/MSE	ORNL/CNMS	Linda Horton	Materials
Weitering, Hanno	ORNL/MSTD	UTK/Physics	John Wendelken	Materials
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
UTHC--University of Tennessee Health Sciences
UTK--University of Tennessee Knoxville

external funding

Photo by Laura Buenning

External Research Funds Brought in During FY09

The table that follows lists the research funds 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 projects, including large research grants to ORNL. In FY09, Distinguished Scientist participation was important to several research teams that brought funding to ORNL.

Elbio Dagotto

- ORNL field work proposal (FWP) funded at $1.2 million; renewal proposal to be submitted in the summer of 2009.

Takeshi Egami

- Atomistic study of bulk metallic glasses funded by DOE Basic Energy Sciences; 2008 budget more than $1 million.
- Atomistic mechanisms of metal-assisted hydrogen storage in nanostructured carbons funded by DOE Basic Energy Sciences; 2008 budget of $730 thousand.

David Joy

- DOE stimulus grant of $1.5 million for new microscopes.
- SEM imaging in liquids (LDRD project) funded at $340 thousand.

Jimmy Mays

- Polymer based multicomponent materials funded by DOE Basic Energy Sciences; ongoing at $1.7 million per year.
- Synthesis, assembly, and nanoscale characterization of confined, conjugated, and charged polymer brushes for advanced energy systems (LDRD project) funded two years at $550 thousand.

Principal Investigator	Project Name	Project Title	Start Date	End Date	Award Amount	FY 09 Expenditures
Egami	UT-B 4000039517	Atomistic Study of Bulk Metallic Glasses	03/01/2005	12/31/2009	$ 470,430	$ 65,757
Egami	UT-B 4000080940	Summer Assistantship	05/05/2009	08/04/2009	$ 5,036	$ 4,410
Egami	UT-Battelle 4000039718	Atomistic Study of Bulk Metallic Glasses	03/14/2005	03/14/2009	$ 377,173	$ 47,838
Egami	NSF DMR-0404781	Complex Electronic Oxides	08/01/2004	07/31/2008	$ 501,950	$ 21,958
Egami	UT-Battelle 4000071951	Atomistic Structure of Gold Nano-Particles	07/31/2008	07/30/2009	$ 33,760	$ 28,132
Egami	NSF DMR-0602876	Materials Research Network: Structure and Dynamics of Complex Ferroelectrics	07/01/2006	06/30/2010	$ 264,000	$ 70,987
Egami	DOE-DE-FG02-	Neutron Scattering Research Network for Epscor States	09/01/2008	08/31/2011	$1,561,000	$ 214,184
Guiochon	NSF CHE 0608659	Fundamental Studies in Non-linear Chromatography	07/15/2006	06/30/2010	$ 479,979	$ 222,325
Guiochon	DOE DE-FG05-88ER13859	Separation of Highly Complex Mixtures by Two-Dimension Liquid Chromatography	07/15/2007	07/14/2009	$ 220,000	$ 80,543

Principal Investigator	Project Name	Project Title	Start Date	End Date	Award Amount	FY 09 Expenditures
Hatcher	USGS-08HQGR-0098	Conversion of Detailed Geologic Maps to ArcMap-Compatible Geospatial Databases	05/30/2008	05/29/2009	$ 25,000	$ 23,301
Hatcher	US Nuclear Regulatory Commission	Large Earthquake Seismology in the East Tennessee Seismic Zone	02/18/2009	02/17/2010	$ 35,000	$ 25,914
Hatcher	USGS-G09AC00126	Detailed Geologic Mapping, Central Georgia Inner Piedmont and Tennessee Valley and Ridge	04/30/2009	04/29/2010	$ 42,700	$ 7,412
Joy	Electron Microscopy Facility	Unrestricted Research Support	04/11/1989	12/31/2047	$ 415,091	$ 1,541
Joy	NASA JPL	CheMin - A Martian Science Probe	06/08/2005	11/01/2009	$ 65,300	$ 3,916
Joy	JEOL, Inc.	Neural Network Analytical System for the Analysis of Secondary Electron Spectra	07/01/2007	09/30/2008	$ 25,000	$ 1,956
Joy	Semicond. Res. Agency	Development of Analysis Software	03/01/2008	02/28/2010	$ 57,500	$ 38,959
Macek	DOE-DE-FG02-02ER15283-MACEK	Theory of Fragmentation and Rearrangement Process in Ion-Atom Collisions	02/29/2008	02/28/2010	$ 250,000	$ 132,865
Mays	Dow Chemical Co. - Jimmy Mays	Unrestricted Research Support	10/30/2002	12/31/2047	$ 35,000	$ 7,580
Mays	DOE DE-FG36 06G016037	Poly(cyclohexadiene) Based Polymer Electrolyte Membranes for Fuel Cell Applications	04/01/2006	09/30/2009	$ 893,749	$ 176,722
Mays	VA TECH - MAT'L WORLD NET	Materials World Network: Molecular Engineering of Polymers for Processing Performance Properties	05/01/2006	05/31/2009	$ 212,950	$ 38,089
Mays	Univ. of Michigan	Advamced Tube Theories	11/01/2007	08/31/2008	$ 32,017	$ 15,489
Mays	UT-B 4000068198	Characterization of Confined, Conjugated, and Charged Polymer	04/18/2008	10/18/2008	$ 48,274	$ 33,758
Mays	UT-B 4000071101	Development of New Copolymer Architectures for Next Generation Plastic Neutron Scintillators	07/09/2008	09/30/2008	$ 22,000	$ 22,000

Principal Investigator	Project Name	Project Title	Start Date	End Date	Award Amount	FY 09 Expenditures
Mays	UT-B 4000076055	Polymer-Based Multicomponent Materials	11/20/2008	11/02/2009	$ 31,805	$ 21,559
Mays	NSF-DMR-0906893	Collaborative Research: Synthesis and Rheology of Strategically Designed Long-Chain-Branched Polymers	09/01/2009	08/31/2010	$ 40,000	$ -
Plummer	NSF DMR-0451163	Enhanced Electron-Phonon Coupling at Metal Surfaces	09/01/2005	08/31/2009	$ 480,000	$ 86,676
Plummer	NSF DMR-0451163 (Match)	Enhanced Electron-Phonon Coupling at Metal Surfaces	09/01/2005	09/31/2009	$ 28,000	$ 13,440
Plummer	UT-B 4000064130	Growth and Characterization of Magnetic Nanostructures	10/10/2007	09/23/2009	$ 47,838	$ 27,656
		Total External Funds			$ 6,652,714	$ 1,407,311
		Total Matching Funds ORNL			$ 982,195	$ 1,104,264

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