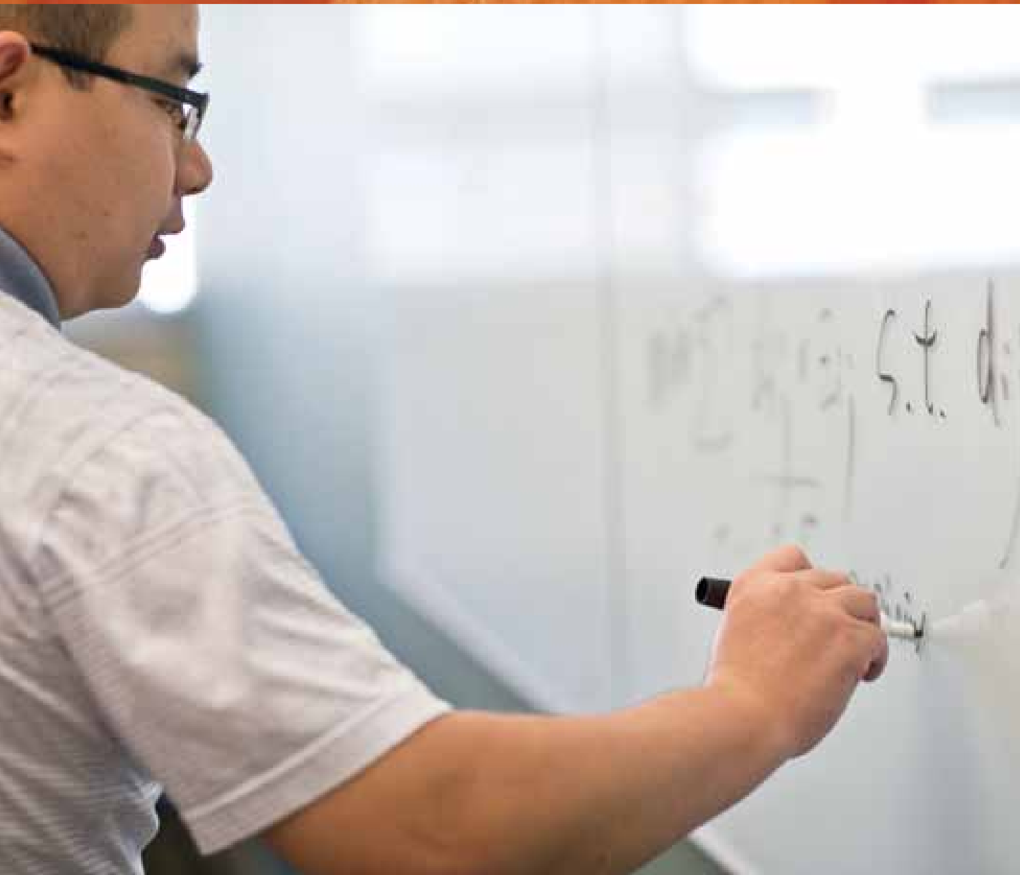
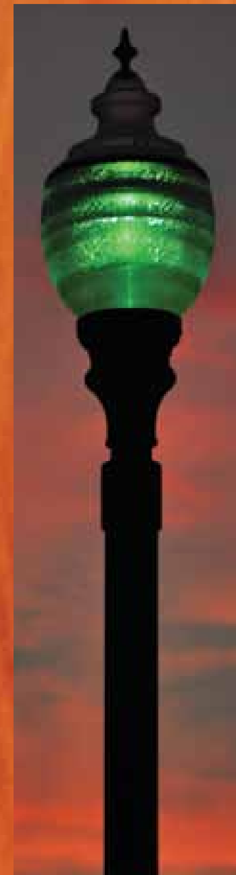
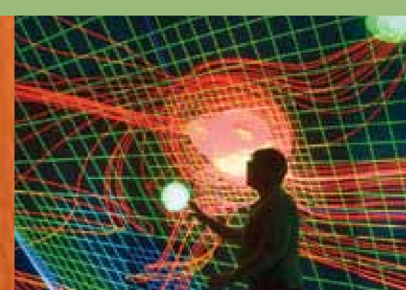



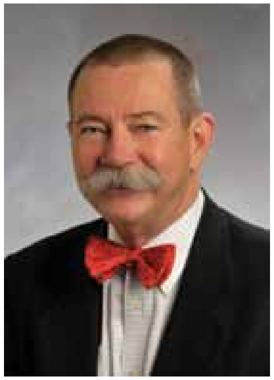
SCIENCE ALLIANCE 2011–2012

CREATING OPPORTUNITY

THE UNIVERSITY of TENNESSEE KNOXVILLE



In Memoriam: Jesse H. Poore

Jesse H. Poore, professor in the Department of Electrical Engineering and Computer Science, passed away at his home on April 25, 2012, after a career spanning forty years in leadership roles at Florida State University, Georgia Institute of Technology, UT, and other public and private organizations.

Jesse came to UT in 1986 as chair of the Department of Computer Science. During his tenure, he also served as co-director of the UT-ORNL Joint Institute for Computational Sciences, director of the Science Alliance, and vice president for information technology and chief information officer. His twenty-year research program at UT focused on the economical production of high-quality software.

Jesse was an esteemed colleague in the university community and a great friend in other circles related to fitness, health, art, food, and creative ventures. He was known among friends and colleagues as a person of vision, inspired leadership, and collegiality. Jesse was a generous mentor to students and staff, promoting independent thinking and learning and instilling individual confidence as he nurtured achievement. As director of the Science Alliance from 2000 to 2011, he was tireless in his attention to ways in which faculty and researchers at the state's historic land-grant university could engage in fruitful collaborations and advance their fields of study in service to the people of Tennessee. He will be greatly missed.

This report is dedicated to his memory.

From the Director

The Science Alliance was initiated in 1984 to foster collaboration between research groups at the University of Tennessee, Knoxville, and the scientific community at Oak Ridge National Laboratory. The twenty-eight years that followed witnessed unprecedented growth at both institutions and the development of many close collaborations between UT faculty and ORNL researchers.

Through the years, the State of Tennessee and UT have supported the creation of a number of joint institutes that parallel developments at the lab. These include the joint institutes for Neutron Sciences, Advanced Materials, Computational Sciences, Heavy Ion Research, and Biological Sciences.

One of the newest developments in thematic collaborations has been the establishment of the Bredesen Center for Interdisciplinary Research and Graduate Education. The Bredesen Center is a degree-granting academic unit within UT, which accepts students working on energy-related projects in the sciences, engineering, and energy policy between the university and ORNL.

The Science Alliance has initiated and supported many of the collaborative ties that UT and ORNL currently enjoy, including the Joint Directed Research and Development Program, which helps new, young faculty establish relationships with Oak Ridge researchers. Along with thematic programs of collaboration, both institutions have worked together to produce one of the finest shared scientific research communities in the nation, enticing some of the brightest minds from around the world to lead research programs at UT and ORNL. This history of collaboration has now produced one of the nation's premier university-national laboratory partnerships.

This year's annual report presents an overview of the history of collaborations and joint research programs, as well as a summary of the current efforts by the university through the Science Alliance to promote UT-ORNL collaborations.

Craig E Barnes

A History of Collaboration

Neighboring institutions with different histories

While the University of Tennessee and Oak Ridge National Laboratory have very different histories and goals, both are closely linked by the physical and biological sciences. The university's Knoxville campus can be traced back to the late 1700s; the national lab at Oak Ridge began as a secret facility to understand and purify uranium and plutonium during World War II.

As WWII approached, the state's flagship university was still known more for its literary and humanities faculty and agricultural studies than for research in the sciences. Even when the US Army located the Manhattan Project nearby, the university remained disconnected from the top-secret facility.

The end of the war changed all that.

OPPORTUNISTIC GROWTH

"The really strong interaction began right after World War II," explains Bill Bugg, who came to UT as a physics graduate student and later became head of the department. "All the GIs were coming home and seeking further education, and the Oak Ridge workers who had interrupted their graduate studies to work on the Manhattan Project were ready to resume their academic careers."

The university's board of trustees responded to this demand by offering newly minted PhD programs—in chemistry and physics, as well as in English.

"The university set up a program of teaching graduate courses wherever they needed to be taught—at UT or in Oak Ridge," Bugg says.

At this time, UT physicist Alvin Nielsen began to work a day a week at ORNL and George Schweitzer joined the chemistry faculty, specifically to start and oversee their graduate program at Oak Ridge.

"Many UT science faculty became one-day-per-week consultants and worked in the summers in Oak Ridge," Bugg says. "They were able to do research that would not have been possible on campus."

These earliest interactions were enhanced in 1964, when Nielsen, by then head of the physics department, won a grant from the Ford Foundation that allowed ORNL scientists to teach courses as adjunct faculty. That $500,000 allowed the lab and university to compensate ORNL scientists for time spent teaching at UT.

From the perspective of ORNL scientists and administrators, these early collaborations also held the promise of an invaluable commodity—cheap but highly enthusiastic labor in the form of graduate students.

Alex Zucker, who served in a variety of administrative roles at the laboratory, remembers feeling jealous of the arrangements other national labs had with nearby universities.

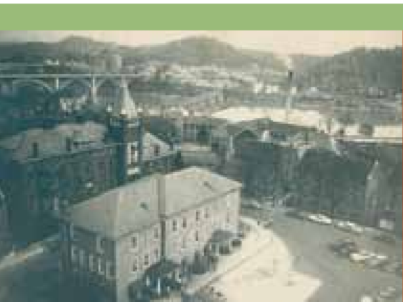
"I was envious of Berkeley," Zucker remembers. "They had free people. The people at the labs liked students—they take a lot of the work."

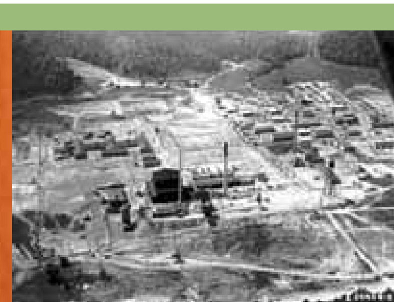
OPPORTUNITY BREEDS AMBITION

In 1982, the university began its most ambitious move to date toward melding UT's research interests with those of ORNL and strengthening the relationship between the two institutions.

Union Carbide, which had managed ORNL since the war years, decided to relinquish its contract. The late Jack Reese, then-chancellor of the Knoxville campus, named a committee of physicists to determine whether UT could manage the facility.

"This was really the beginning of UT focusing on central issues, on big issues at Oak Ridge," according to Lee Riedinger, one of those committee members and UT's current interim vice chancellor for research. When the Department of Energy decided not to seek individual contracts for the three major components of its Oak Ridge operations, "that's when we dropped out. We were not ready as an institution, but it was good for us because it got us thinking of the big picture."






and cultures find ways to make “beautiful science” together.

BY WILLIAM DOCKERY AND LAURA BUENNING

Soon thereafter, then-governor Lamar Alexander called on Reese for projects to present to Howard Baker, the majority leader of the US Senate and senior senator from Tennessee.

“[Alexander] said he was going to ask Baker to see if they could write into the bid process some words that would require the next contractor to do something with UT,” Riedinger recalls.

Reese turned to members of the earlier study committee, and on a Sunday afternoon in October 1982, Riedinger, Paul Huray, and Ivan Sellin sat around Huray’s kitchen table and dreamed up the Distinguished Scientist Program. They decided that only by attracting researchers with international reputations could the university hope to improve its standing among national research institutions. With $10 million from the state legislature, the university initiated the Distinguished Scientist Program as a part of what came to be known as the Science Alliance, a formal organization that linked ORNL and UT science operations.

The Science Alliance was complemented by the creation of a number of joint institutes designed to exploit the strengths of both institutions and focus on collaborative efforts.

Soon thereafter, a Collaborating Scientist Program evolved from the Distinguished Scientist model. It allowed the university and ORNL to share the costs of hiring prominent research scientists at an early stage in their career to work for both institutions. An agreement between UT and ORNL was put in place in late 1991, and by 1993, eight collaborating scientists had been hired.

AMBITION NOURISHES CAPABILITY

This evolving process would bear fruit when, in 1998, rumors began to circulate that after fifteen years under Lockheed Martin, DOE would again put the management of its Oak Ridge operations in play.

“This time UT was ready,” Riedinger remembers. “DOE had split the contract so that it was only ORNL we were competing for and—because of the Science Alliance, because of the joint hires, because of the joint institutes—we were ready to demonstrate the capability to compete.”

“We had to have a partner, since we had no demonstrated ability to manage a reactor or a plant of that scope,” Riedinger explains.

The university identified Battelle, an international science and technology organization that already managed Pacific Northwest National Laboratory, as a potential partner, but Battelle remained aloof to UT’s overtures. It wasn’t until Battelle executive Bill Madia paid a visit to then-president Joe Johnson that the university found its partner.

“When Madia and Johnson met, it was clear within five minutes that this was a partnership we should sign,” Riedinger says. “Just before Thanksgiving 1998, we married Battelle.”

In 1999, Tennessee Governor Don Sundquist committed $26 million in state funds for creating additional joint institutes, and the university started hiring more collaborating scientists, which it then labeled joint faculty. The university and the lab modified the existing joint-faculty agreement, moving to a loaned-employee model to reflect the fact that ORNL scientists cannot be guaranteed permanent employment.

“The shared employee mechanism opened the floodgates,” Riedinger says. “That has led to the mass of people now working at both places. They come and go, but I think it works well.”

The Department of Energy awarded the management contract to UT-Battelle in 2000. In the succeeding years, the UT-Battelle partnership has flourished, state and national support has remade the ORNL campus, and UT has profited from a unique relationship with the largest US Department of Energy multipurpose national laboratory.

Cong Trinh's research advances biofuel production.

Cong Trinh

Profitable metabolic detours

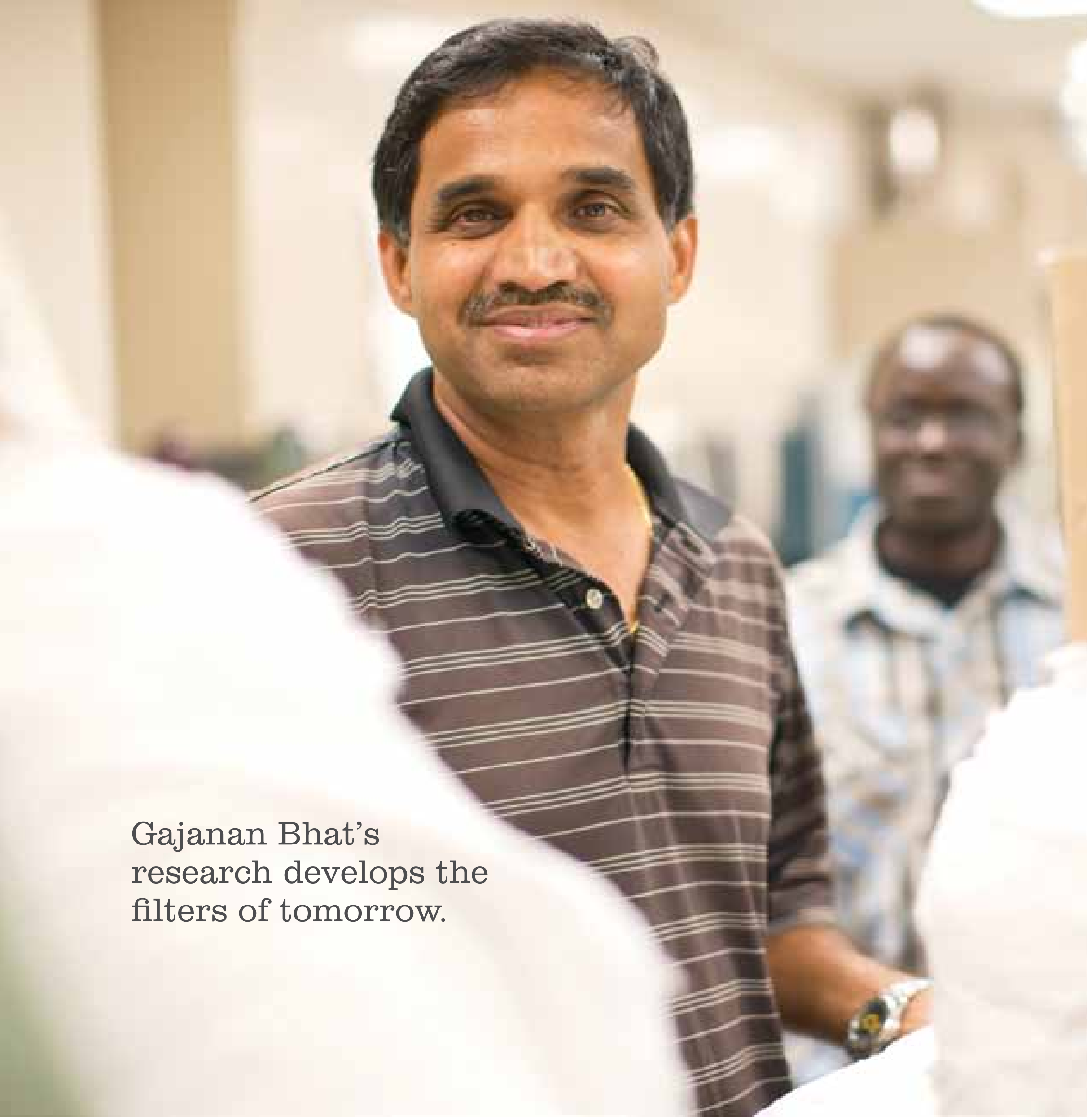
BY LAURA BUENNING

Most of us understand metabolism as the process living organisms go through to consume nourishment and survive. The series of steps taken from food consumption to growth to reproduction are called metabolic pathways.

Nature creates a network of these pathways, Cong Trinh says, and organisms have multiple routes from which to choose.

"On their own they won't expend energy taking a more difficult pathway, but they can be redesigned to use atypical pathways and, as a result, yield valuable end products."

Trinh and ORNL's Adam Guss are re-engineering two separate microorganisms to use pathways that will convert biomass into an array of biofuels and other biochemicals.



Gajanan Bhat's research develops the filters of tomorrow.

Gajanan Bhat

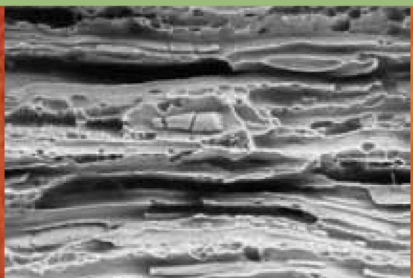
Keeping filters clean

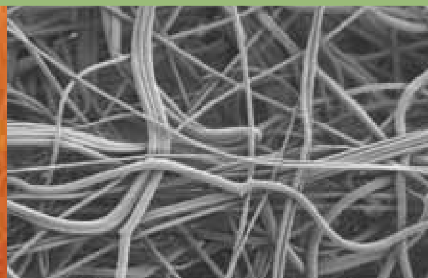
BY LAURA BUENNING

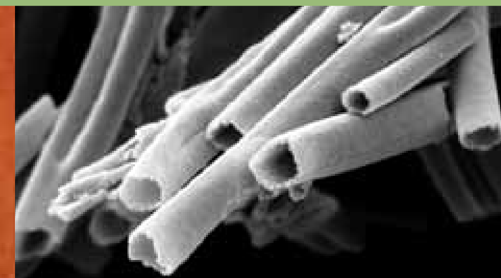
In the bioenergy arena, harsh conditions affect the pretreatment (filtering) of biomass. ORNL's Ramesh Bhave has an idea for a filter that would make biomass more immediately available to biochemical conversion and, in the process, increase the yield of sugars and other chemicals of value.

Gajanan Bhat's team is developing a protective coating for the new filtration membrane—one that will prevent deposits from fouling the membrane with material that can only be removed by expensive chemical cleansing.

"Our challenge," Bhat says, "is to make a coating that keeps the filter's surface free of debris and the nanopores open."







Qiang He

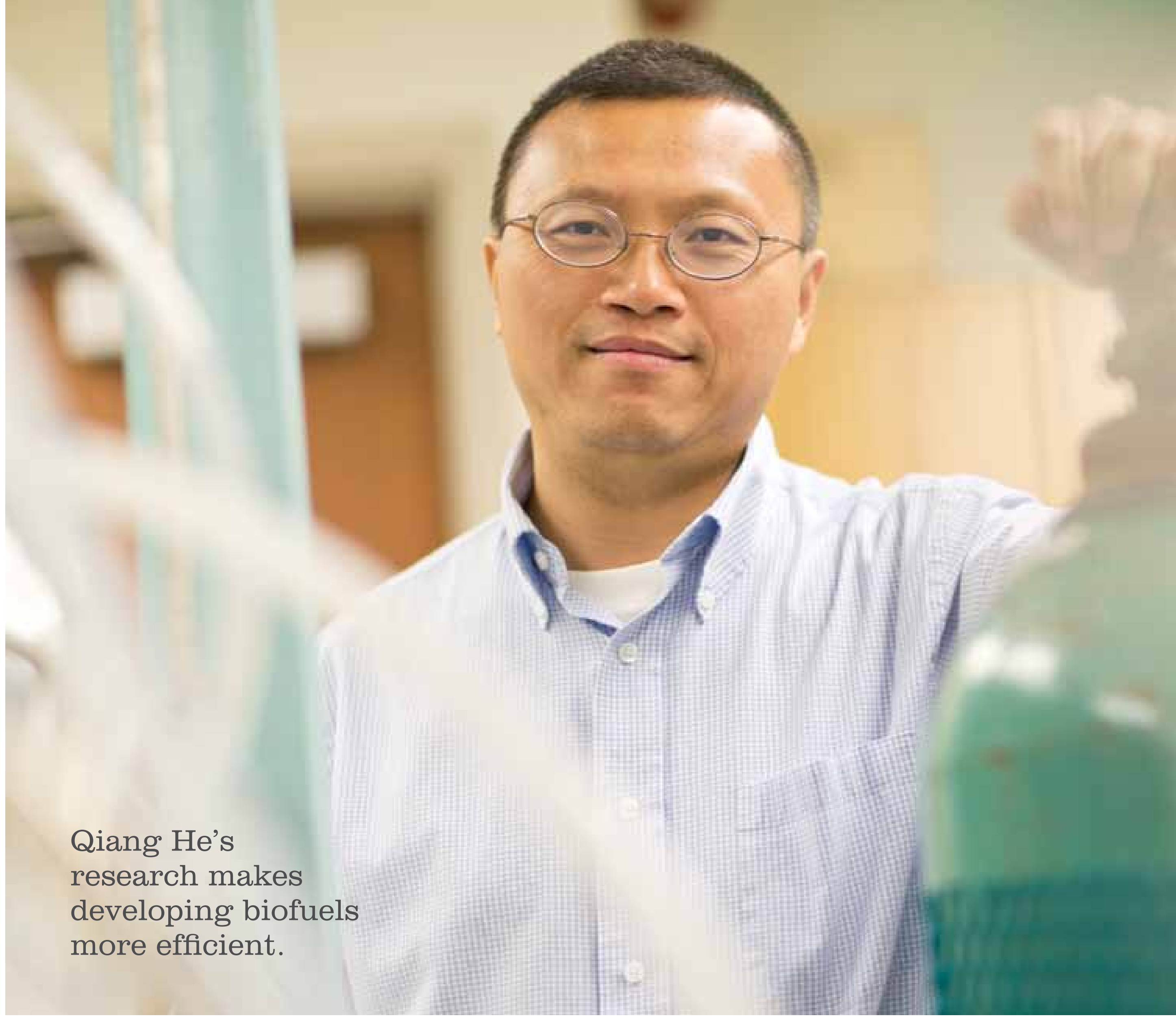
Biomass digesters

BY LAURA BUENNING

Researchers get ideas from all sorts of places. For Qiang He, the inspiration began inside the stomach of a cow. Where better to look for microbes capable of decomposing switchgrass for biofuel production than in the gut of grazing ruminants?

The problem of identifying effective decomposing microorganisms remains key to developing efficient cellulosic biofuel processing techniques. But mimicking the natural host-microbe relationships in industrial settings is too complex to be realistic.

So, rather than looking inside the cow, He studies the anaerobic digestion of cow manure as a source of unexplored microbial communities capable of decomposing residual plant material.



Qiang He's research makes developing biofuels more efficient.

David Keffer

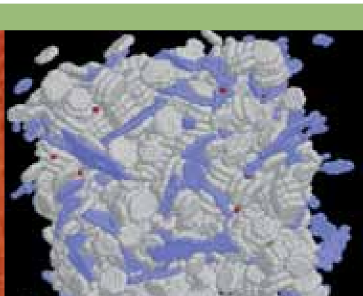
I experiment, therefore I compute

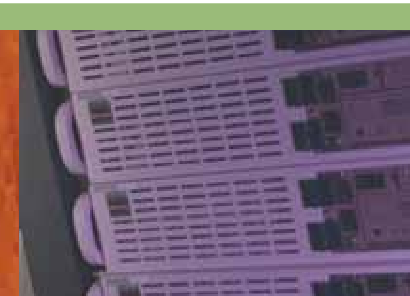
BY THERESA PEPIN

In the brave new world of scientific computation and simulation, it can often seem as though the experiment never ends. Experiments feed data to computation, which, in turn, offers back structure and analysis. The results are models that can be compared with laboratory findings to validate and fine-tune continuing experimentation—all toward the goal of rapidly optimizing performance and accelerating progress.

David Keffer has become well versed in this multiscale modeling process. And now, his team applies their high-performance tool kit to understand the fundamental relationship between nanostructure and lithium-ion conductivity in lignin-based carbon fiber anodes.

David Keffer's research helps scientists optimize their experiments.





David Jenkins

Dry cleaning flue gas

BY LAURA BUENNING

Carbon dioxide ranks high on the list of problematic ingredients in flue gas. Wet scrubbers that combine water and organic compounds deliver the most effective method available to date. But you pay a high-energy penalty to regenerate the solution for reuse, David Jenkins says, not to mention their volatile nature and long-term instability.

Jenkins and a team led by ORNL's Radu Custelcean are pursuing a promising alternative approach using scrubbers filled with porous, crystalline powders to attract and hold the CO_2 until it is released where it will not enter the atmosphere.

David Jenkins' research keeps carbon dioxide from entering our atmosphere.

Aimée Classen

Carbon bandits

BY LAURA BUENNING

Plants and fungi share an ancient symbiotic bond. Soil fungi living in and among root structures receive carbon from the plant, which they use to grow and multiply. In return, they supply the plant with soil nutrients and moisture.

Recent studies, however, show mycorrhizal fungi will sometimes cheat the plant, stealing its carbon without giving back adequate nutrients. Sometimes they even scavenge carbon from the soil, says Aimée Classen. The project's PhD student, Jessica Bryant, is trying to determine if this switch from symbiont to free-living—from carbon sink to carbon source—might significantly affect atmospheric carbon levels.

Aimée Classen's research identifies how fungi affect the atmosphere.

Steven Wilhelm

Troubled waters

BY THERESA PEPIN

In the long list of worries that life entails, the availability of clean fresh water should be right up there. And yet, although we may vaguely suspect that our waters are "troubled" from time to time, it seems to be natural for us to assume that nature will somehow take care of them for us, no matter what. Wrong.

Steven Wilhelm and his team add High-Throughput Transcriptomics to the arsenal of tools that tells us more about algal blooms, why there has been such an alarming increase in degradation of fresh waters in recent decades, and what we can do about it.

Steven Wilhelm's research protects freshwater resources.

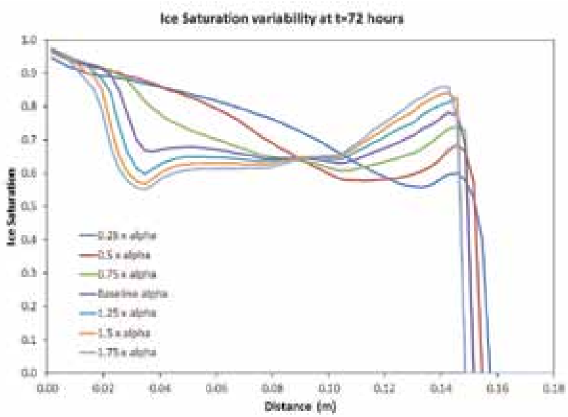
Edmund Perfect

Deep thaw

BY THERESA PEPIN

Vast expanses of Arctic permafrost hold the key to projecting future warming scenarios as our climate changes. What will befall our world as these great, hulking masses of permafrost thaw? How do we learn enough on such a grand scale to really understand what may happen?

The collaboration led by Ed Perfect and ORNL's Richard Mills pairs a deeper knowledge of the physical processes involved in ground freezing and thawing with massively parallel computation on leadership-class supercomputers to model the impact of global warming.



Edmund Perfect's research hones predictions about future climate change.

Veerle Keppens

Thermo-shifts

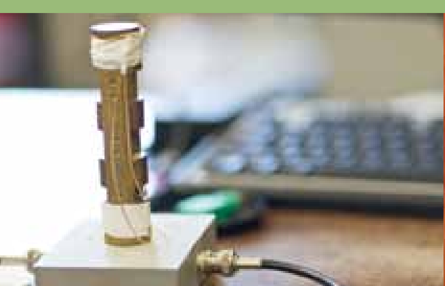
BY LAURA BUENNING

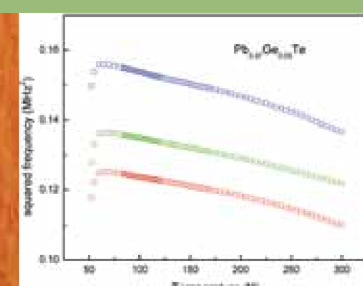
Imagine being able to generate thermoelectric power from minute changes in temperature.

As promising as this sounds, efficient thermoelectric materials—those that impede the transfer of heat from one side of the material to the other, while allowing electrons to pass—are hard to come by.

Working in tandem, Veerle Keppens and ORNL's Olivier Delaire search for microscopic clues to the origins of suppressed thermal conductivity, in hopes of uncovering beneficial thermoelectrical materials.

Veerle Keppens' research turns temperature shifts into electricity.





Husheng Li

Power flows

BY THERESA PEPIN

Controlling how power flows is as important as producing it in the first place.

Husheng Li and his team are designing a wireless communication network to add “nerves” to “muscles” for controlling distributed energy resources in the smart grid. Planned to be flexible, reliable, “plug-and-play,” and self-healing, the design of the communication network will be field tested in the Distributed Equipment Communication and Control laboratory at ORNL. Li’s goal is to render microgrid power flow controls more robust and efficient.

Husheng Li’s research moves electricity more smartly across the grid.

Lee Han

Faster than real time

BY THERESA PEPIN

People say you can't predict the future. But the fact of the matter is that we must, or we can't keep up with the present.

When disaster strikes or chaos threatens, when we need to get emergency personnel in while getting evacuees out, we need to know a great deal ahead of "real" time in order to make decisions quickly enough.

Lee Han and his team have built the foundation for a faster-than-real-time traffic simulation system—some 1,000 times faster than the state-of-the-practice.

Lee Han's research helps first responders reach emergency scenes faster.

Qing Cao

Sensors and smarts

BY THERESA PEPIN

Every day, everywhere, mobile devices quietly gather all kinds of information in quantities previously unimaginable. While some of the data reflects what individuals actively do with a particular device, other data comes from sensor-detected context, such as location and time.

If the various streams of data can be accurately characterized and analyzed in real time and full context—as is the ambitious aim of Qing Cao's work—their "fusion" would allow us to infer patterns of activity that enable even smarter applications.

Qing Cao's research makes our smart phones even smarter.




Distinguished Scientists

The Distinguished Scientist Program supports high-profile, internationally recognized leadership appointments in science and engineering. The program anchored the Science Alliance partnership-building role during the center's early years. Appointees were recruited to joint UT-ORNL positions as tenured distinguished UT professors and senior ORNL research staff. Since 2005, joint appointments at this level have been made through the Governor's Chair Program.

Learn more at **scialli.utk.edu**.

Elbio Dagotto
Nanoscale dimensions and correlated electronic behavior
UT Department of Physics & Astronomy; ORNL Division of Materials Science & Technology

Elbio Dagotto studies transition metal oxides and the recently discovered iron arsenide materials, which become superconductors at temperatures as high as 55 Kelvin. These materials and others studied by Dagotto show promise for improved memory devices, solid-state batteries, and other energy-saving electronics.

Takeshi Egami
Atomic-scale dynamics of liquids and gasses; High-temperature superconductivity
UT departments of Materials Science & Engineering and Physics & Astronomy; ORNL Division of Materials Science & Technology

The physics of liquids is much less developed than the physics of solids. Takeshi Egami explores new science of liquids and gasses using computer simulation (including quantum mechanical calculations) and neutron and synchrotron x-ray scattering experiments.

Georges Guiochon
Separation science
UT Department of Chemistry

Georges Guiochon is an expert in using multidimensional chromatography to separate the components of complex samples. His research improves the efficiency of chromatographic columns, optimizes conditions for maximum production rate of safe and effective pharmaceuticals, and examines the complex fundamentals of supercritical fluid chromatography.

Robert Hatcher
Structural geology and tectonics of continental crust
UT Department of Earth & Planetary Sciences

A structural and tectonics geologist, Bob Hatcher studies the processes that create and evolve Earth's continental crust. His team conducts detailed field and laboratory studies of the southern Appalachian Mountains, comparing them with other ancient and modern mountain chains around the world.

David Joy
Accurate microscopic and nanoscale imaging
UT departments of Biochemistry & Cellular & Molecular Biology and Materials Science & Engineering; ORNL Division of Materials Science & Technology

David Joy develops precise measuring techniques for electron- and ion-beam imaging, which is essential to improve production of nanoscale materials.

Joseph Macek
Electron vortices in simple atomic systems
UT Department of Physics & Astronomy

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

Jimmy Mays
Synthesizing new polymer membranes for fuel cells
UT Department of Chemistry; ORNL Division of Chemical Sciences

Jimmy Mays synthesizes new, precisely tailored polymers and examines their molecular architecture, composition, and blending capability to discover how form and structure, including their nanostructural order, might be manipulated to create useful materials.

UT-ORNL Joint Institutes

Five UT-ORNL joint institutes link distinct, complementary resources in select, high-priority scientific and engineering fields at the University of Tennessee, Knoxville, and Oak Ridge National Laboratory. Each opens doors to leadership-class research instrumentation and computing facilities; offers an environment conducive to collaboration; and provides the physical space where scientists and engineers can exchange ideas and work collectively to answer complex research questions.

Learn more at **scialli.utk.edu**.

UT-ORNL Joint Institute for Advanced Materials
The Joint Institute for Advanced Materials (JIAM) promotes interdisciplinary research and education related to developing new materials with superior properties (such as greater toughness and high-temperature strength) or those that can be tailored to support new technologies (such as pocket-sized supercomputers).

UT-ORNL Joint Institute for Biological Sciences
The Joint Institute for Biological Sciences (JIBS) supports interdisciplinary, crosscutting research that accelerates progress in complex bioenergy and bioenvironmental systems. It also aids access by UT-ORNL faculty, staff, and students to state-of-the-art capability in genomic, transcriptomic, proteomic, and metabolomic analysis of biological and environmental systems.

UT-ORNL Joint Institute for Computational Sciences
The Joint Institute for Computational Sciences (JICS) advances scientific discovery and state-of-the-art engineering and computational modeling and simulation. JICS takes full advantage of the petascale and beyond computers in the Department of Energy National Center for Computational Sciences (NCCS) and UT's National Institute for Computational Sciences (NICS).

UT-ORNL Joint Institute for Heavy Ion Research
The Joint Institute for Heavy Ion Research (JIHIR) links UT, ORNL, and Vanderbilt University research that explores the structure of atomic nuclei, via several types of experimental programs and an extensive UT-ORNL theoretical nuclear physics initiative.

UT-ORNL Joint Institute for Neutron Sciences
The Joint Institute for Neutron Sciences (JINS) promotes worldwide neutron scattering collaboration among researchers in biological and life sciences, energy sciences, polymer science, condensed matter physics, and computational sciences.




Governor's Chairs

The Governor's Chair program attracts exceptionally talented, internationally recognized research scientists and engineers to joint appointments as tenured UT professors and ORNL distinguished research staff. Initiated by former Tennessee Governor Phil Bredesen, the program takes advantage of the synergy between the state's flagship campus and the nation's leading multipurpose national lab. The program is managed through the UT Office of the Executive Vice President.

Learn more at **scialli.utk.edu**.

Howard Hall

Global nuclear security

UT Department of Nuclear Engineering; ORNL Division of Global Nuclear Security Technology

Howard Hall applies his background in nuclear chemistry to the nearly overwhelming challenges in nuclear security. His research addresses questions of proliferation, counterproliferation, detection of and response to radiological or nuclear threats, radiochemistry, and nuclear forensics.

Brian Wirth

Computational nuclear engineering

UT Department of Nuclear Engineering; ORNL Consortium for Advanced Simulation of Light Water Reactors

Brian Wirth investigates the performance of nuclear fuels and structural materials in nuclear environments. His research improves predictions about the longevity of nuclear reactor components.

William Weber

Materials' response to radiation

UT Department of Materials Science & Engineering; ORNL Division of Materials Science & Technology

William (Bill) Weber's team uses direct measurements of materials irradiated with high-energy ions in UT's new particle accelerator and powerful computational simulation to predict the long-term resilience of materials in nuclear environments.

Jeremy Smith

Molecular biophysics simulation

UT Department of Biochemistry & Cellular & Molecular Biology; ORNL Division of Biosciences

Jeremy Smith and the Center for Molecular Biophysics team of UT professors and ORNL staff scientists combine experimental neutron scattering and large-scale computational simulation and modeling techniques to describe molecular structure and motion.

Alexei Sokolov

Dynamics of soft materials

UT departments of Chemistry and Physics & Astronomy; ORNL Division of Chemical Sciences

Alexei Sokolov studies molecular motion as the key to macroscopic properties of materials. His primary interest is in the fundamental properties of soft materials—or by definition, materials that can change.

Frank Loeffler

Environmental systems microbiology

UT departments of Microbiology and Civil & Environmental Engineering; ORNL Division of Biosciences

Frank Loeffler's research team characterizes the intricate microbial processes that enable naturally occurring bacteria to break down toxic contaminants, immobilize radioactive wastes, reduce greenhouse gas emissions, and control the biogeochemical cycling of carbon and nitrogen in soils, sediments, and freshwater bodies, including groundwater.

Terry Hazen

Environmental microbiologists; Bioremediation and bioenergy

UT departments of Civil & Environmental Engineering, Microbiology, and Earth & Planetary Sciences; ORNL Division of Biosciences

Terry Hazen studies what happens as naturally occurring bacteria break down and detoxify hazardous materials, such as metals/radionuclides, petroleum, and chlorinated solvents. His group explores environmental biogeochemical stress-response pathways, from the molecular to the ecosystem level.

Yilu Liu

Power systems and smart-grid technology

UT Department of Electrical Engineering & Computer Science; ORNL Division of Energy & Transportation Science

Yilu Liu develops new and better ways to monitor and understand flow of electricity through the nation's power grid. Her group is working to devise a smarter electric grid that automatically resolves minor disruptions before they escalate to major blackouts.

Thomas Zawodzinski

Electrical energy storage

UT Department of Chemical & Biomolecular Engineering; ORNL Division of Materials Science & Technology

Thomas (Tom) Zawodzinski explores basic mechanisms of chemical processes occurring in materials found in electrochemical systems, such as batteries and fuel cells. His team characterizes and improves the rates of those all-important chemical reactions at the heart of fuel cell and battery technology.

Robert W. Williams

Genetics and human health

UT Health Science Center, Department of Anatomy & Neurobiology

Robert (Rob) Williams studies genetic and environmental causes of human diseases using novel mouse populations and massive human genetic data sets. His group's research ranges from metabolic to neuropsychiatric diseases.



Science Alliance
218 Claxton Complex
1122 Volunteer Boulevard
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SCIENCE ALLIANCE 2011–2012

CREATING OPPORTUNITY

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