Oak Ridge National Laboratory

REVIEW

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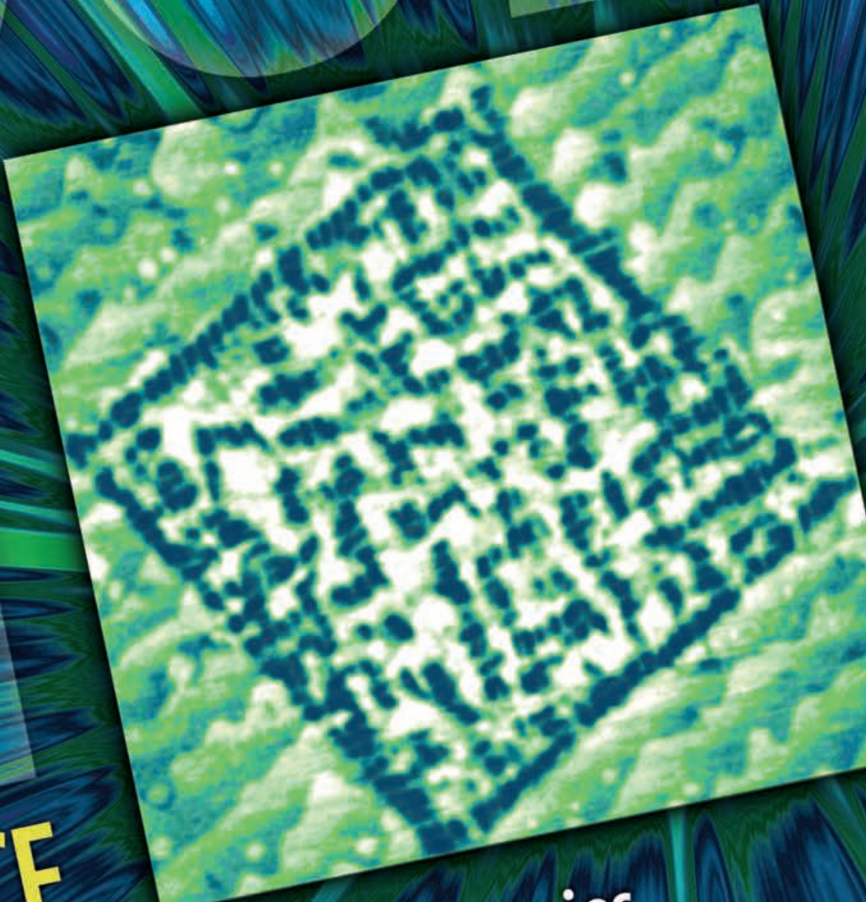
ZOOM IN on NANOSCIENCE



Better batteries
Probing nanopores
Molecular machinery

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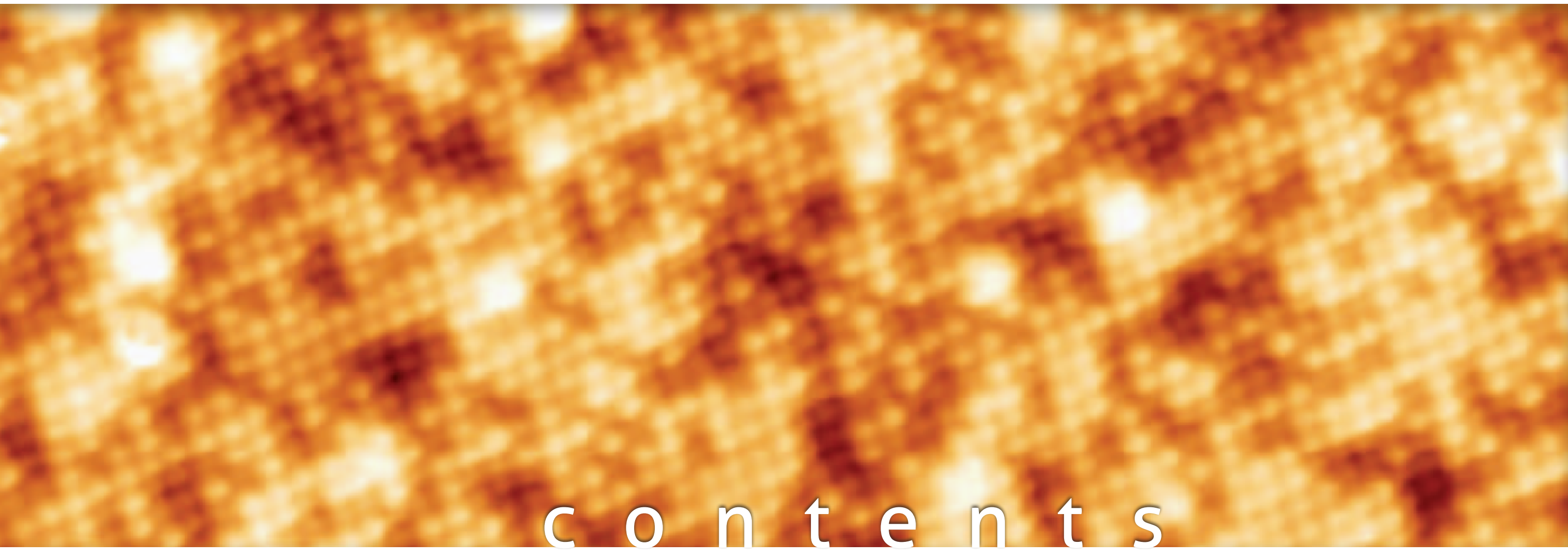

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A scanning probe micrograph of patterns written in a sample of bismuth ferrite. Research into this material by the Imaging Functionality Group at ORNL's Center for Nanophase Materials Sciences could have implications for future electronics and energy-harvesting materials.

NANOSCIENCE in the 21st century

A decade ago, in an address to the 2002 meeting of the American Association for the Advancement of Science, Presidential science advisor Jack Marburger declared that we were in the early stages of a revolution in science: "one in which the notion that everything is made of atoms finally becomes operational." According to Dr. Marburger, this revolution resulted from two developments: advances in instrumentation and the availability of powerful computing and information technology.

At Oak Ridge National Laboratory, we are at the forefront of this continuing revolution. The Department of Energy's investments in facilities and tools for nanoscale research—in particular, the Spallation Neutron Source, the Oak Ridge Leadership Computing Facility, and the Center for Nanophase Materials Sciences—provide us with remarkable opportunities for understanding, probing, and manipulating matter at the atomic and molecular level, where the fundamental properties of materials and systems are established and traditional boundaries between the scientific disciplines of physics, chemistry, and biology are blurred.

We take advantage of these resources by leveraging one of our distinctive characteristics as a national laboratory: the ability to focus multidisciplinary teams of scientists and engineers on large and complex challenges. This strategy is especially valuable at the CNMS, which is a critical ORNL asset for exploring nanoscale materials and phenomena. Teams working at the CNMS—many including university and industry partners—are developing a new understanding of the functionality and properties of nanoscale materials, systems, and architectures, with positive impacts for energy-related research, a primary focus for DOE, and for such areas as carbon sequestration, biomedicine, and quantum computing.

This issue of the *ORNL Review* highlights nanoscience research projects from areas across the laboratory's science and technology agenda, illustrating benefits of our multidisciplinary, multi-institutional approach. Already we can lay claim to a number of high-profile scientific publications, R&D 100 awards, and patents.

Our continuing role in the nanoscale revolution will build on another of our distinctive strengths: the translation of science to innovation. Our tradition of coupling basic to applied research and partnering with industry to license discoveries for commercial products provides a solid foundation for realizing the promise of nanoscale science, engineering, and technology.

Thomas Zacharia

Deputy Director for Science and Technology

Creative synergy

ORNL's Center for Nanophase Material Sciences delivers a one-two punch—providing both a cutting-edge research facility open to scientists around the globe *and* a world-class nanoscience program. "These two activities enhance each other," says CNMS director Sean Smith. "That's the effect we've been working toward during our first five years. Now that we've built up our user base, we receive consistently high-quality user proposals. As a result, both our users and the laboratory benefit from being involved in these projects; it really is a synergistic relationship."

One of five Department of Energy nanoscience centers, CNMS attracts users from both inside and outside ORNL for the same reasons: the center has specialized equipment researchers need and nanotech experts to boost the quality of users' research projects. Another huge bonus for CNMS users is the center's proximity to other materials research facilities. Just next door is the Spallation Neutron Source, the world's most powerful pulsed-neutron research facility; and the nation's most powerful research reactor, the High Flux Isotope Reactor, is just down the road. This unprecedented concentration of analytical capabilities, combined with ORNL's diverse R&D portfolio, is particularly attractive to users who want to analyze the material they work with in a number of different ways—without traveling all over the country.

A powerful tool

Research and development at the nanoscale is conducted across a range of disciplines at ORNL—from traditional nanotech fields like materials science to relative newcomers like nanobiology. Smith explains that the synergy created by scientists from different domains exchanging ideas is an extremely powerful tool for promoting scientific innovation. "That's why the CNMS is not tied to one specific project or scientific investigation area. We have a larger and more broadly user-encompassing mandate that allows us to encourage a host of different areas of investigation."

Batteries—In recent years the work of the center's Imaging Functionality group has been particularly successful in developing new scanning probe microscopy methodologies. The group has developed a suite of techniques for deciphering the structure and dynamic interactions of semiconductor metal-oxide films. These materials are a key component of energy storage devices, such as batteries, so understanding them in more detail paves the way for batteries that are more efficient, long-lasting and affordable.

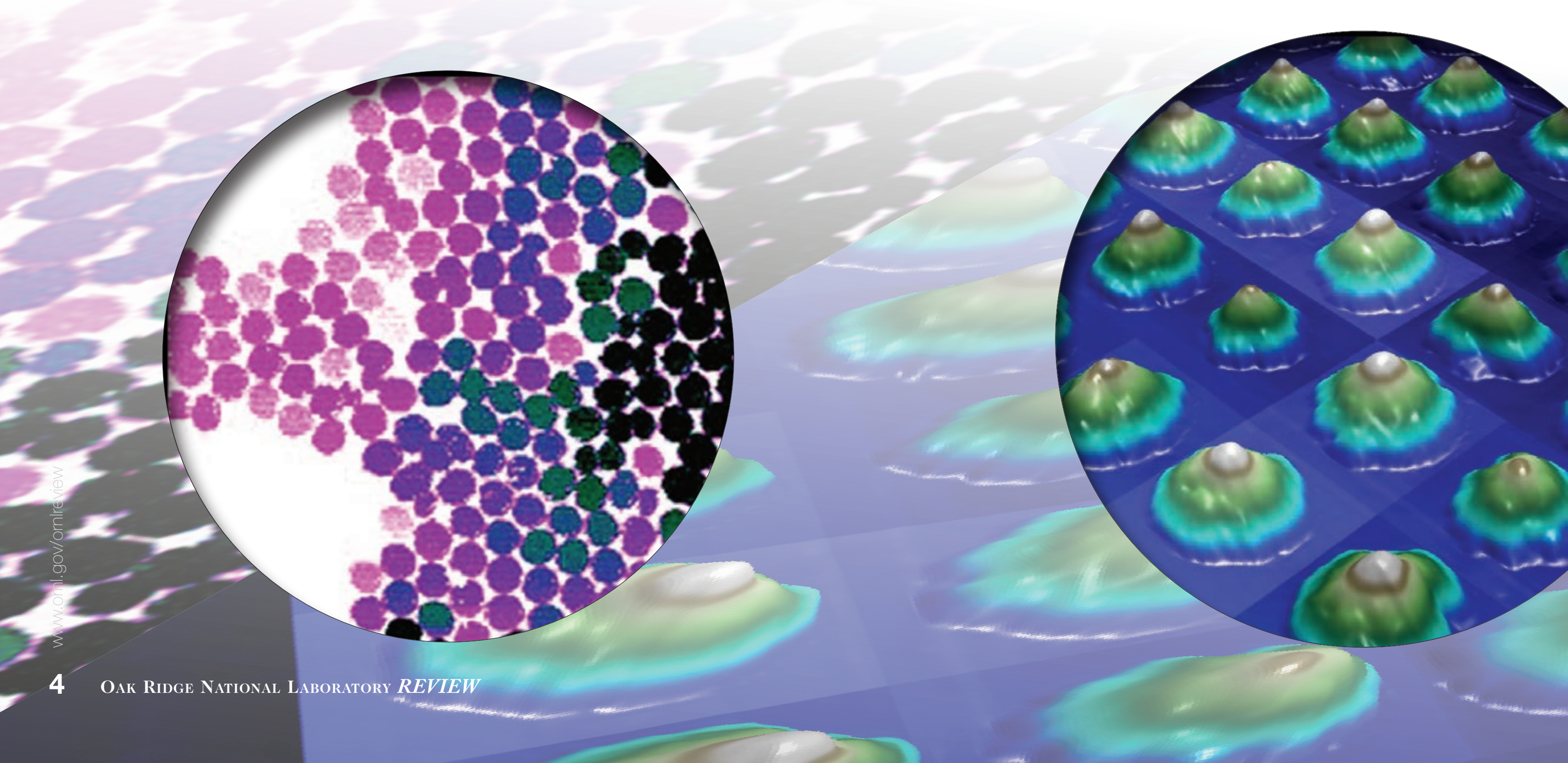
"If you look at the matrix of the lab's capabilities," Smith says, "the ability to characterize energy-related materials—to understand their structure at the nanoscale—will become increasingly important." At present, these capabilities are being put to use not only in research aimed at building better batteries, but also in solar energy research.

Solar cells—Researchers from both the CNMS and the SNS are focused on understanding and creating a new generation of devices that can convert light into electricity, such as the photovoltaic cells used in solar collectors. They are particularly interested in determining how the nanostructure of the materials used in solar cells is related to how the cells perform.

Without facilities like CNMS, we would have no way to learn what's going on at this level of detail.

To tease apart the intricacies of this relationship, researchers conduct detailed studies of photoelectric films using microscopic, x-ray and chemical techniques at the CNMS. Then they take their materials to the SNS to perform additional tests using neutron analysis. Smith explains that the center's three areas of specialty—synthesizing new materials, making hybrid materials from polymers and inorganic substances, and analyzing materials—provide CNMS with a multipronged way of determining the structure of a material and exploring the relationship between its structure and its performance.

Smith expects that the next generation of the center's work in the area of solar cells will capitalize on the ability to relate structure to performance. CNMS researchers will characterize the photoelectric film production process in real time, using neutron-scattering instruments at the SNS. "We'll examine the behavior of the materials throughout the process," Smith explains, "beginning with the three-dimensional fluid, depositing the fluid on the substrate, evaporating it, and creating the final thin-film device. We want to look at the dynamics of the process at each stage and understand their implications for the finished device."



Nanobiology—In addition to lending its expertise to research efforts in established nanotech fields like materials science, CNMS hosts users who are investigating various aspects of nanobiology. These include research into how nanoparticles accumulate in living systems and investigations of the use of nanoparticles as delivery vehicles for genes and drugs for various kinds of therapy.

One particularly unusual nanobiology project employs microbes to produce nanoparticles for industry. This cross-disciplinary effort began several years ago when researchers in ORNL's Biosciences Division discovered that certain microbes, harvested from deep drilling operations, naturally produced nanoparticles in the form of metallic iron clusters on their cell membranes. "This observation was particularly interesting," Smith says, "because nanoparticles are widely used in industry, but their synthesis is generally costly and less easily scaled to large quantities than would, in principle, be possible using the microbe route." Scientists at ORNL are studying the potential for using similar microbes as a source of low-cost nanoparticles for applications such as creating photovoltaic thin films. In addition, the CNMS is using its analytical resources to get a better understanding of the nature of nanoparticles produced by biological processes and how they might be used in alternative energy applications and in materials that imitate biological materials. "Without facilities like CNMS," Smith observes, "we would have no way to learn what's going on in these biological systems at this level of detail."

Unique perspective

The value of CNMS is rooted not only in its unique research facilities but also in its expertise in producing and characterizing materials at the nanoscale. Smith notes that the center brings a unique perspective to addressing research problems. "For example," he says, "in the microbe study I mentioned earlier, the researchers knew that the microbes were making nanoparticles on their membranes, but problems arose when they tried to harvest the particles, which were sticking together and forming clumps. At the suggestion of one of our staff members, the researchers introduced small quantities of dispersant into the process. That didn't seem to bother the microbes, but it prevented the clumping and allowed the scientists to control the size and distribution of the particles."

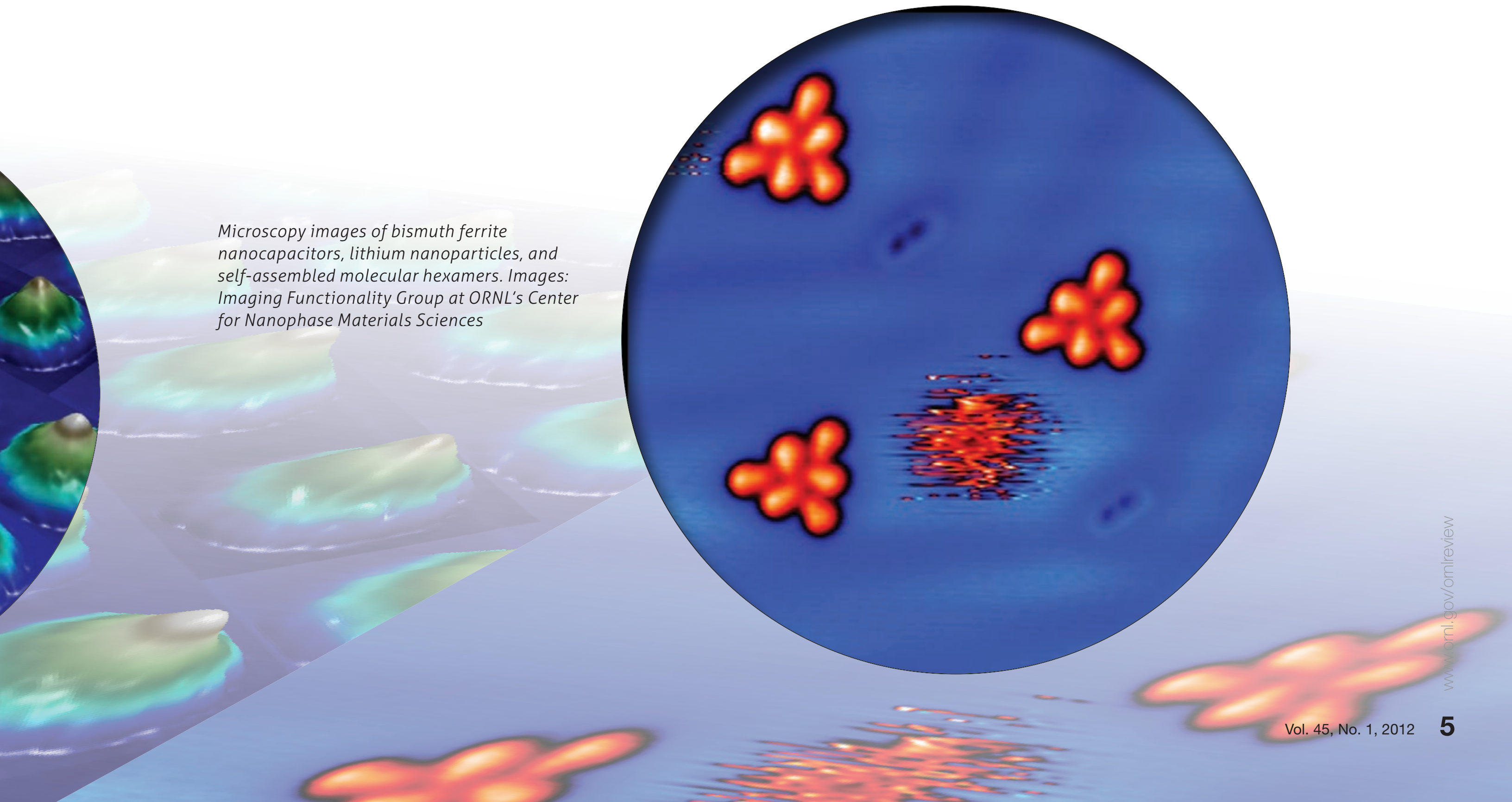
This illustrates the ability of CNMS to find effective, if unexpected, solutions. "Nanoscience is an incredibly broad area which impacts technology in health, medicine and many other fields," Smith says. "We don't do research in all of these areas, but we can facilitate interactions among researchers and help move the research forward."

Tremendous facilitator

Despite the broad applicability of the center's findings and facilities, Smith expects two areas of nanoscience to dominate its activities over the next few years. "First," he predicts," "research into energy materials is going to be huge. We are already heavily engaged in designing new materials to support and advance energy technologies, such as batteries, supercapacitors and solar panels, and we will continue to be."

Smith also expects nanomedicine and nanobiology to become increasingly important. He notes that these are areas in which CNMS works even more frequently than usual with partners across ORNL. "Our mission is basic energy sciences," he explains, "but by collaborating with research groups who are engaged with things like gene therapy and emulating biological systems, we can help them make progress in those areas as well. Nanoscience plays an enormous role in these fields, and we will be pushing hard to help them reach their goals.

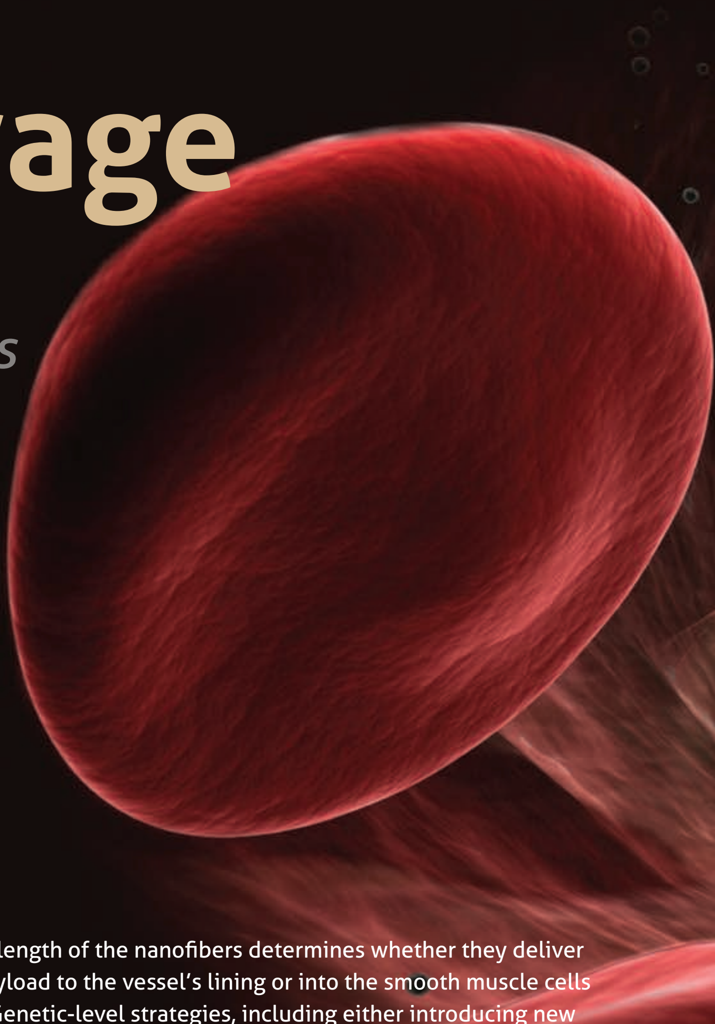
"This kind of cross-disciplinary research is what I'm talking about when I say that CNMS can be a tremendous facilitator," Smith says. "Helping people in diverse areas to better understand their materials or processes, or to understand how to work more effectively at the nanoscale, allows them to move their research forward in their own domains, and that benefits all of us." Ⓡ — *Jim Pearce*



Microscopy images of bismuth ferrite nanocapacitors, lithium nanoparticles, and self-assembled molecular hexamers. Images: Imaging Functionality Group at ORNL's Center for Nanophase Materials Sciences

Vascular voyage

Nano platforms deliver drugs, genes and more to individual cells



In the 1960s blockbuster film *Fantastic Voyage*, miniaturized rescuers, injected along with their submarine into the bloodstream of an intelligence agent, rush to destroy a blood clot in his brain. Surprisingly, that's the sort of problem-solving adventure Tim McKnight and his research team launch every day—without the secret agent and the submarine.

McKnight, a scientist in ORNL's Microelectronic Systems Research Group, heads a team of researchers who are developing tools designed to deliver therapeutic agents to localized regions of tissue. These agents include genes that are introduced into the tissue to elicit certain responses, as well as other genetic material designed to "silence," or suppress, the actions of existing genes. One of the most promising applications of this technology is its ability to treat tissue inside blood vessels before and after various surgical procedures.

Surgeons' efforts to widen narrowed vessels, remove clots, and insert stents to keep vessels open often result in post-surgical inflammation and a buildup of vascular smooth muscle cells—the kind that make up the walls of blood vessels—around the affected area. This buildup can restrict blood flow and may require follow-up surgery.

McKnight notes that stents coated with drugs to minimize the inflammatory response of blood vessels produce mixed results. Problems sometimes arise from the fact that blood vessels are composed of two kinds of cells: a thin lining of endothelial cells and a thick, underlying layer of smooth muscle cells. The latter often reacts to surgery by rapidly reproducing in an effort to isolate the foreign body (in this case, the stent) from the rest of the body. Unfortunately, drugs that prevent this overgrowth of muscle cells can also inhibit the healing of the endothelial layer of cells, which is necessary to fully repair the blood vessel.

Genetic back door

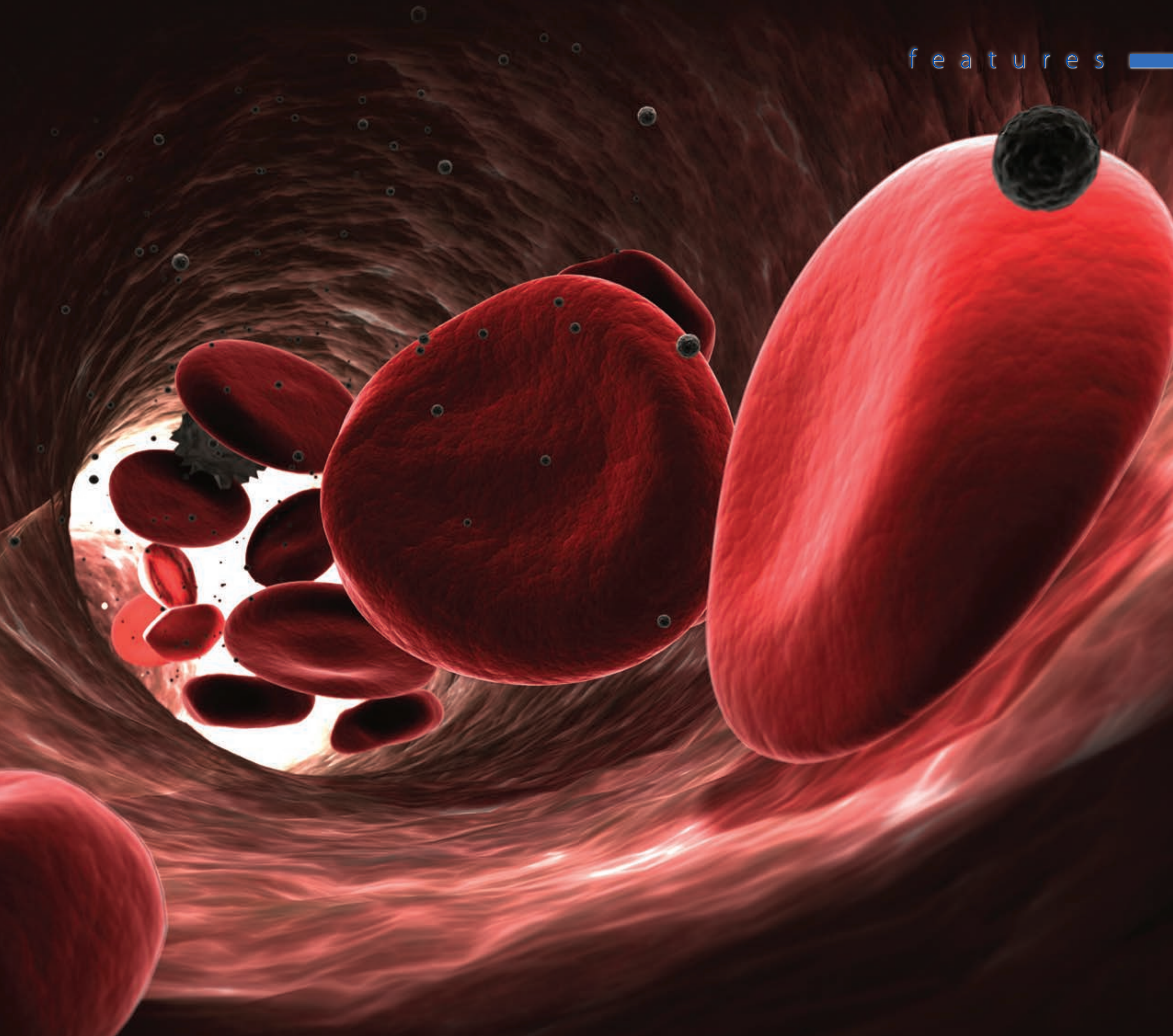
To reduce unwanted cell growth, McKnight and his colleagues are developing genetic techniques that can be applied during surgery. The key to their approach is a very small device that is inserted into a blood vessel the way an angioplasty balloon is inserted into a narrowed artery. One side of the device is covered in vertically aligned carbon nanofibers (VACNF). An array of these closely spaced fibers extends from the device like bristles on a hairbrush. When the array is pressed into the interior surface of the blood vessel, the individual nanofibers deliver genetic material or drugs to a large number of cells in the vessel wall.

The length of the nanofibers determines whether they deliver their payload to the vessel's lining or into the smooth muscle cells below. Genetic-level strategies, including either introducing new genes or silencing the expression of existing genes, can then be used to influence the response of the surrounding tissue. "The purely mechanical nature of this approach provides flexibility with respect to what can be delivered to the cells, and may circumvent some of the existing limitations of viral- or chemical-mediated gene delivery methods," McKnight explains. "This strategy can be used to address many medical conditions where highly localized effects are desired, such as dampening the inflammatory response after coronary artery surgery or the removal of blood clots in cases of ischemic stroke. It might also be used to limit the reactive response that tends to occur in tissue surrounding some biomedical implants."

In addition to introducing genetic material into tissues, McKnight and his team have tested methods of "immobilizing" DNA on nanofibers in the array. Under this scenario, the investigators hope to provide a measure of control over genetic-level manipulation. For example, suppose a nanofiber carries a small segment of DNA containing the genetic instructions for producing a particular protein. When the nanofiber is inserted into the nucleus of a cell, the cell is able to produce that protein. However, when the fiber and its attached DNA are removed, the cell loses the ability because it no longer has access to the necessary genetic information.

Neural interface

In addition to blood-vessel-related applications, nanofiber arrays have shown promise for use in implants in the central nervous



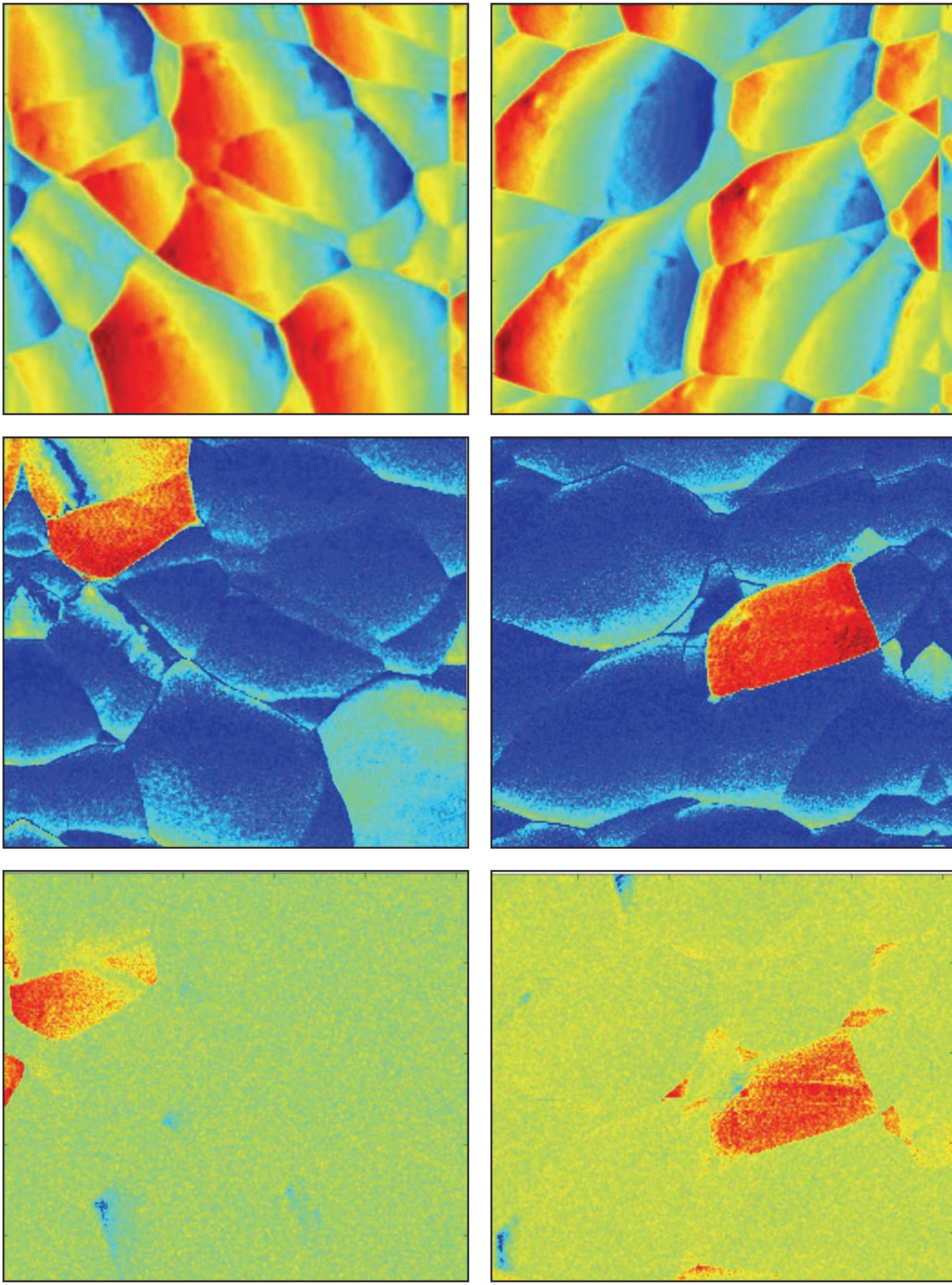
system, such as deep brain stimulators used to treat Parkinson's disease and other neurological conditions. Working through ORNL's Laboratory Directed Research and Development program, microelectronics researcher Nance Ericson and his team have taken the first steps in this direction with their research into electrically-addressable nanofiber electrode arrays.

"These arrays may have critical advantages over traditional neural implants," McKnight says. "The performance of these central nervous system implants is often compromised by formation of scar tissue. Nanofiber arrays may address this problem by providing genetic-level strategies to reduce the inflammation of the surrounding tissue. This should allow implants to remain effective longer."

It may also be possible to develop implants that vary the amount of stimulus the electrode arrays deliver in response to the reaction of the surrounding tissue. McKnight notes that his team has developed techniques to fabricate nanofiber electrode systems on flexible films. These electrodes can be used either to inject current through the nanofibers to stimulate the neural tissue, or to record the bioelectrical activity of the nerve cells. "We have shown we can use these electrodes to measure the levels of neurotransmitters—the chemicals that enable nerve cells to communicate with one another—in the surrounding tissue," McKnight says. "This may allow us to vary the stimulus required to ensure that the tissue responds at optimal levels."

Rapid response

McKnight and his team foresee a wide range of applications for this suite of nanofiber-based tools. "We can stimulate excitable tissues, such as nerve cells," he says. "We can monitor their response to stimulation, and we have a genetic-level interface which enables us to reprogram localized cells to do things we want them to do—or stop them from doing things we don't want them to do. The VACNF platform is extremely versatile." *—Jim Pearce*



Better Batteries from the Ground Up

ORNL microscopy explores the "room at the bottom" in lithium-ion batteries

Today, people talk about their electronic devices almost as if they were living, breathing beings. We wake our computers up, our cell-phones die and we have longer conversations with our GPS devices than with many of our friends.

As new wireless technologies appear in devices from tablet computers to electric cars, efforts to improve these life forms focus on a common organ: the heart-like battery. Yet despite an accelerating demand for battery-powered devices, the pulse of the electronics world is not as well understood as you might think.

"In some sense, we think of batteries are ideal devices, but from a chemical viewpoint, they are very complicated," says ORNL senior scientist Sergei Kalinin. "Batteries look ideal only when they're inside a package, and you don't care what's inside."

Kalinin is among a team of scientists at ORNL's Center for Nano-phase Materials Sciences that is developing new microscopic methods to analyze and understand nanoscale complexities inside electrochemical systems such as lithium-ion batteries. "Richard Feynman famously noted that there is plenty of room at the bottom," Kalinin says, referring to the physicist's 1959 talk on the potential of nanoscience. "This room does not do us much good if we cannot explore it."

It's like we're trying to understand the individual properties of a brick in a house while we're flying by in an airplane.

At first glance, batteries seem simplistic because they consist of only three major components—negative anode, positive cathode and electrolyte. But each part is itself a complex matrix of different materials that interact as ions and electrons flow through the battery in charging and discharging cycles. To top it off, batteries come in all shapes, sizes, materials and configurations, leaving scientists with myriad factors to consider when studying battery performance.

"The bottom line is that these systems are very complicated," Kalinin says. "Batteries are made of pieces that are tens of nano-meters to microns in size. Unless you study them on these length scales, you cannot learn much about their structure and how they operate. They are defined at this scale. Beyond that, you're looking at the assemblies."

"It's like we're trying to understand the individual properties of a brick in a house while we're flying by in an airplane. We only see the house; we don't see the bricks," he says.

Fellow CNMS scientist Nina Balke explains that the operation of lithium-ion batteries at the nanoscale has been largely unexplored because few techniques operate at the appropriate resolution.

"Batteries are well characterized on the device level, but most characterization techniques don't tell you what's going on at the nanoscale," Balke says. "Very few techniques allow you to look at ionic transport on a scale that shows grains, grain boundaries and defects—which, in sum, make up the battery."

Studying the nanoscale puzzle pieces that make up a battery is not an easy task for microscopists because of the dynamic nature of batteries. Electron microscopes, for instance, can produce images of individual atoms in a material, but only if the atoms remain motion-less for several seconds. The flow of electrons and ions through batteries can easily disturb this atomically perfect picture and muddy the view that electron microscopes provide.

To tackle the challenge of analyzing battery dynamics at the proper resolution, Balke and Kalinin turned to scanning probe micros-copy, or SPM. This well-known method uses a small probe that scans over a surface to measure different properties of the sample mate-rial. The ideal application would combine classical electrochemical measurement methods and SPM to have the ultimate characterization tool on the nanoscale. However, scanning probe microscopes typi-cally depend on the measurement of electron flow, which has prohib-ited their use at the nanoscale for probing electrochemical reactions.

"The problem with most techniques is that they rely on Faradaic currents related to the number of electrons transferred through the system," Kalinin says. "The number of electrons required for measure-ments is actually quite large; they can measure billions of electrons, but probably not millions or thousands. When we study batteries at the nanoscale, we transfer hundreds to thousands of electrons. There-fore, these methods cannot be easily extended to the nanoscale."

To address this problem, Kalinin and Balke, along with ORNL researcher Stephen Jesse, have developed a new SPM technique called electrochemical strain microscopy, or ESM, that relies on the measurement of strain, or volume change, instead of electrons. The technique, based on an R&D 100 award-winning band excitation technology developed by Jesse and Kalinin, is now commercially available through Asylum Research.

"If we want to understand ionic materials like lithium-ion batteries, we need a technique that allows us to measure ionic flows and not electronic flows," Kalinin says. "We want to have a technique that is highly and exclusively sensitive to ions and not electrons."

The ORNL team has used ESM to characterize individual parts of lithium-ion batteries and other electrochemical systems such as fuel cells at unprecedented resolutions—up to a million times greater than was previously possible. But Balke says their application of the ESM technique has only just begun.

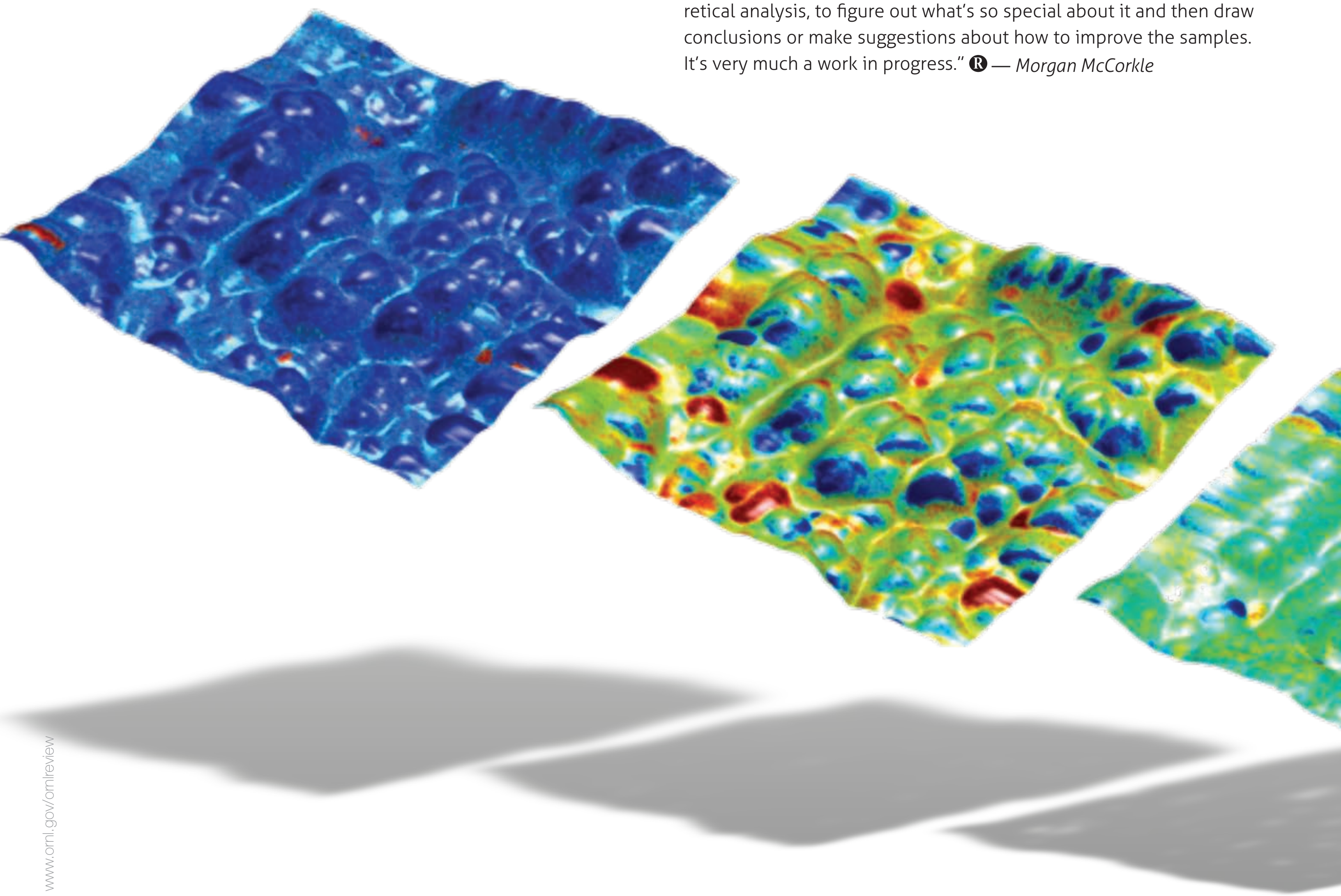
"Right now, we are at the very beginning," Balke says. "We have developed the technique and tried it out on a few model systems. We can take a single battery component and look at it, but we aren't looking at a full battery yet. We have established knowledge that can move us to the next step."

The team's short-term goals include setting up an in-situ SPM to probe a realistic battery surface, which involves a transition to different conditions, given that most electrolytes are liquid. They also plan to start testing new and advanced battery materials instead of analyzing well-known model systems. The microscopy team is already collaborating with ORNL battery researchers, who study the mechanical properties and performance of batteries, with the aim of correlating nanoscale phenomena to overall battery functionality.

Scientists from other institutions are also starting to come to the CNMS user facility to make use of the ESM capabilities. "Battery researchers provide us with samples, and we work with them to improve the samples. They look at the mechanical properties, so if they do something to the sample and see that it results in a better battery, they give it to us to find out if we see an improvement on the nanoscale. We're building up this relationship between the performance and what we see on the nanoscale. We want to understand, from a nanoscale perspective, what makes one battery work and another battery fail," Balke says.

While the microscopy team is dedicated to bringing the ESM technique to its full potential, they note that additional methods are needed to form a complete picture of battery dynamics.

"ESM can only tell you so much," Balke says. "It can tell you that in some areas of the electrode you have much higher ionic transport than in others, but it doesn't tell you why. So you have to combine ESM with other techniques, such as microwave microscopy or theoretical analysis, to figure out what's so special about it and then draw conclusions or make suggestions about how to improve the samples. It's very much a work in progress." Ⓡ — *Morgan McCorkle*



Piezoresponse Force Microscopy workshops build microscopy community

Kalinin addresses a recent PFM workshop in Beijing. Photo: University of Science and Technology Beijing

When Intel invited ORNL's Sergei Kalinin in 2006 to speak to its staff about piezoresponse force microscopy (PFM), he asked how much time he was allowed. "As much time as you'd like," the Intel rep said. After a marathon presentation and discussion that lasted 10 hours, Kalinin recognized there was a glaring need to share knowledge around PFM techniques.

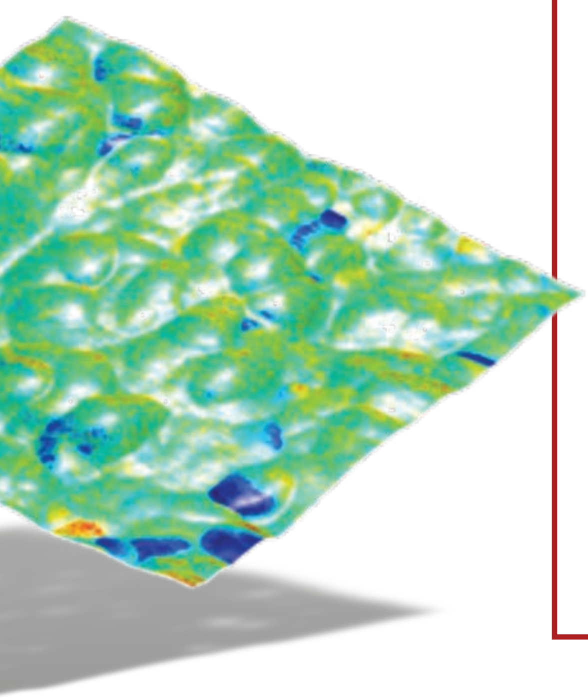
"I started to realize that it's a good idea to have all the community members who are engaged in this technique in one room—at least to talk to each other," Kalinin says. "It wasn't limited to just Intel. PFM was rapidly becoming the mainstream method for exploring ferroelectric memories, hard-drive-like storage and tunneling barrier–based devices in multiple research groups."

The result of this realization was the first meeting of the PFM workshop series, held at ORNL in September 2007, which attracted some 40 attendees from around the globe. PFM, a variant of scanning probe microscopy, was once used primarily to study ferroelectric materials, but its use has now been expanded to include other electrochemical systems, in large part thanks to the PFM workshop series.

"Before we started studying batteries, we spent a lot of time working on ferroelectric materials in terms of technique development and theoretical analysis," Kalinin said. "Many of these techniques can be applied to batteries or fuel cells with insignificant modifications."

Since its humble beginning, the PFM workshop series has grown to include international meetings in Europe and Asia that have attracted more than 100 attendees. The first dedicated PFM conference was held in Aveiro, Portugal, in 2009 and hosted 110 attendees. The 2011 meeting was held jointly with the International Symposium on Applications of Ferroelectrics in Vancouver, Canada, and was attended by 400 participants. Industry participation has led to the commercial availability of PFM techniques that were previously custom-built by individuals. The collaborative spirit of the workshops, however, remains the same.

"It's good to get people together who have a common language—people who understand our problems," ORNL's Nina Balke says. "Since there aren't many people who do these kinds of measurements, it's beneficial to get together to see where we stand and help each other out." Ⓡ — *Morgan McCorkle*



Probing nanopores

Neutrons shine a light on geological nanostructures

Big issues of the day often turn out to be closely linked to small, seemingly mundane facts of life. Consider carbon sequestration, the practice of locking carbon dioxide (CO_2) away in geological formations in hopes of limiting climate change, and hydraulic fracturing, a method of releasing natural gas by cracking layers of rock with high-pressure fluids. Both processes are politically contentious, have global implications, and depend heavily on understanding how liquids and gases behave in the nanopores of rocks located hundreds or thousands of feet underground.

ORNL physicist Yuri Melnichenko says there is real significance to studying the physical world at the nanoscale. "We have a good understanding of how materials, like fluids or gases, behave in bulk systems," he says, "but if we reduce the size of the system to a few nanometers, the properties of those liquids or gases become very different. At this scale, there are new effects and properties to understand and make use of."

Melnichenko's recent forays into the realm of the nanoscale involve investigating how fluids, liquids and gases change when confined in nanopores. These changes can be illustrated by imagining a bucket of water, he explains. If you have a big bucket, most of the water molecules aren't affected by the bucket walls. But when you have a nanobucket, there are fewer molecules, and virtually all of them come in contact with the walls. As a result, they don't behave the way as they do in a big bucket. "This is exactly the point of our research," Melnichenko says. "We are trying to understand why various properties of liquids and gases are different, depending on the size of the bucket, the material of the walls, and how molecules interact with the walls."

Carbon sequestration

The properties of nanopores play a major role in carbon sequestration. "Most scientists agree that carbon dioxide emissions constitute some level of threat to the environment by building up in the atmosphere and raising the surface temperature of the earth," Melnichenko says. One approach to limiting the amount of CO_2 in the environment is

ORNL physicist Yuri Melnichenko and postdoctoral associate Lilin He investigate how liquids and gases behave in nanopores using the General Purpose Small-Angle Neutron Scattering (GP-SANS) Diffractometer at ORNL's High Flux Isotope Reactor. Photo: Jason Richards to collect it as it is produced at places like power plants, condense it to a liquid, and pump it into deep, unmineable coal seams where it would permeate the pores of the coal. The hope among proponents of carbon sequestration is that while in these pores, condensed CO_2 would eventually transform into a more stable compound.

"This is all theory of course," Melnichenko says, "so a couple years ago we started a project to study how CO_2 interacts with coal." The research compared the structure of "dry" coal with CO_2-saturated coal to determine CO_2 adsorption rates. The research team also made this comparison for different types of coal and for coals mined from different depths. Although they found variability in adsorption rates, Melnichenko says, they still couldn't determine what makes one type of coal more adsorbent than another or how different nanopore sizes contribute to the adsorption process.

Searching for answers, Melnichenko and his colleagues devised an experiment using neutrons generated by ORNL's High Flux Isotope Reactor and applied the General Purpose Small-Angle Neutron Scattering (GP SANS) Diffractometer to monitor the behavior of CO_2 in small pores. "We built a high-pressure cell to reproduce the high-pressure, high-temperature conditions many hundreds of feet underground," he says. "Then we used the instrument's unique capabilities to analyze samples of various coals under different conditions."

Based on this research, the team developed a method of calculating not only how much CO_2 was adsorbed by the various samples, but also how nanopore size contributed to the adsorption process. This baseline information about the effects of pore size on adsorption is of particular interest to geologists because it provides unprecedented insight into which types of coal are most amenable to carbon sequestration, as well as information about various other processes related to the porosity of coal and other kinds of rock.

Methane recovery

One form of sequestration, called enhanced coalbed methane recovery, involves pumping CO_2 into unmineable methane-saturated coal seams, displacing the methane from the nanopores and forcing it out through a second well. Although this process hasn't been demonstrated on a commercial scale, researchers anticipate that some sequestration costs could be recovered by selling the recovered methane. "Before that happens on a large scale," Melnichenko says, "we will need to know how to make the process effective, what the optimal conditions for CO_2 to replace methane are, and how CO_2 and methane interact with each other and the walls of the nanopores." Research conducted on the GP SANS helps illuminate these questions as well.

In addition to being trapped in coal seams, methane is found in large quantities in geologic formations called "tight gas shales." Methane in this sort of rock is sometimes accessed by a process called hydraulic fracturing or "fracking." It is estimated that the Marcellus Shale formation in the eastern United States, for example, contains a trillion tons of natural gas trapped in small, discrete pores. "It's an enormous amount of clean energy," Melnichenko says. Using their SANS techniques, his team can uncover information about both the structure of the shale itself and the behavior of the methane contained in its pores. This information can then be used by geologists to answer questions about the best way to extract the methane; how the process can be made more efficient; and why there is more methane in one place than another.

Research conducted on the SANS instrument also enables Melnichenko's team to calculate how much methane is contained in non-interconnected pores in any porous material. "So, for instance," Melnichenko suggests, "if 50 percent of the pores of a particular formation are not accessible, perhaps a geologist would rather find another area to work with. There is a lot more research to be done before we can determine how the most efficient release of methane can be achieved."

Judgments based on science

Despite the enthusiasm of commercial geologists for his team's research, Melnichenko makes it clear that the team's focus is on the science, not on solving industry problems. "That's not our job," he says. "But we can provide information to individuals who need to know how fluids behave in nanopores. We are giving these researchers tools that will enable them to understand processes at the fundamental level and let them know what to expect when they drill into coal or shale. Then they can use this information to optimize their processes."

Melnichenko recalls that three or four years ago, when he asked geologists discussing carbon sequestration how they would choose a seam for CO_2 injection, they didn't have much data to guide their judgments. "Our research has given them a better understanding of what will happen when they pump CO_2 into a coal seam," he says. "Now they can make judgments based on science, rather than just educated guessing." Ⓡ — *Jim Pearce*

Designing materials for the future

Analyzing alloys at the atomic level

As energy demands rise, materials scientists are increasingly interested in developing longer-lasting materials for use in the next generation of advanced nuclear and fusion reactors. However, before researchers can think about the big picture, they have to see what's happening with these materials on the atomic level.

One way to do this is to use atom probe tomography (APT), a sophisticated microscopy technology, to zoom in on a material's basic building blocks. In about an hour, APT can characterize millions of atoms, telling researchers what kinds of atoms are present and pinpointing the location of each one. This sort of detailed information improves scientists' understanding of how materials are structured and gives them greater insight into how the properties of these materials can be manipulated and optimized.

In 1986, Michael Miller of ORNL's Materials Science and Technology Division was among several researchers who invented the first instruments capable of doing APT. Today, he's using this technique to study nanoclusters in nanostructured ferritic alloys, a subclass of steels that is being considered for use in next-generation nuclear power applications. The microstructures of these materials will tolerate temperatures of 1000° Celsius and radiation levels well beyond those present in today's nuclear reactors.

Ferritic alloys are expected to provide the first line of defense around nuclear reactor cores, protecting the rest of the reactor from radiation damage. To accomplish this, the alloys need to remain stable in a hostile, extreme-radiation environment. Miller has discovered that the materials best able to provide this stability are those containing chromium for oxidation resistance; titanium, yttrium and oxygen to form nanoclusters; and chromium and tungsten to segregate the grain boundaries.

"Due to their high density of nanoclusters, nanostructured ferritic alloys are one of the most stable iron-based systems materials scientists have discovered so far," Miller says. "However, there's still much to learn about nanoclusters, such as precisely how they tolerate extreme doses of radiation."

APT has revealed that some of the nanoclusters are located in the interiors of the grains and some on the grain boundaries of nanostructured ferritic alloys. This positioning is critical to the durability of the alloys. Under stress, atoms in steel alloys tend to move from grain to grain, causing the grains to grow, which results in deformation of the steel and degradation of its mechanical properties. When nanoclusters are located at the grain boundaries, however, they minimize this movement of atoms and stabilize the structure of the steel. Nanoclusters also provide stability by dispersing potentially damaging helium bubbles, which can form along grain boundaries in a nuclear reactor environment.

Understanding a material's structure helps Miller determine how to change its characteristics. For example, it's common to insert obstacles, such as nanoclusters and precipitates, into a material's crystal lattice to strengthen it. "It's like the story of Goldilocks," Miller said. "You have to find and insert just the right number of obstacles into the material. Too many obstacles and the material becomes brittle, too few and the material may not have enough strength for the application; so it's crucial to introduce the appropriate amount and for them to be stable under extreme conditions. "

A Suite of Techniques

To study nanostructured ferritic alloys, Miller uses a combination of APT and electron microscopy. Miller and his coworkers conduct APT and electron microscopy research at ORNL's Shared Research Equipment (SHaRE) User Facility, which houses the local electrode atom probe (LEAP), the laser-assisted LEAP, a dual-beam focused ion beam (FIB)/scanning electron microscope system, and several electron microscopes.

APT requires a needle-shaped specimen with a tip that is sharp even by nanoscale standards. Miller uses an electropolishing system and the dual-beam FIB system to create his specimens. "This system focuses two beams on one spot," he says. "The electron beam shows me what I'm doing, and the ion bean sputters material away from the specimen in a precise way." Miller can "cut out" a 10-micron-long block this way, then "pencil sharpen" the block into a needle with an end radius of about 50 nanometers. Once Miller has fashioned his specimen, he characterizes the nanoclusters by stripping atoms off the surface one at a time so they fly down a time-of-flight mass spectrometer to a single-atom, position-sensitive detector. The resulting data enables Miller to identify the type of atom and where it was located in the sample. He uses this information to determine the size, number density, distribution, and composition of the nanoclusters in the materials he is studying.

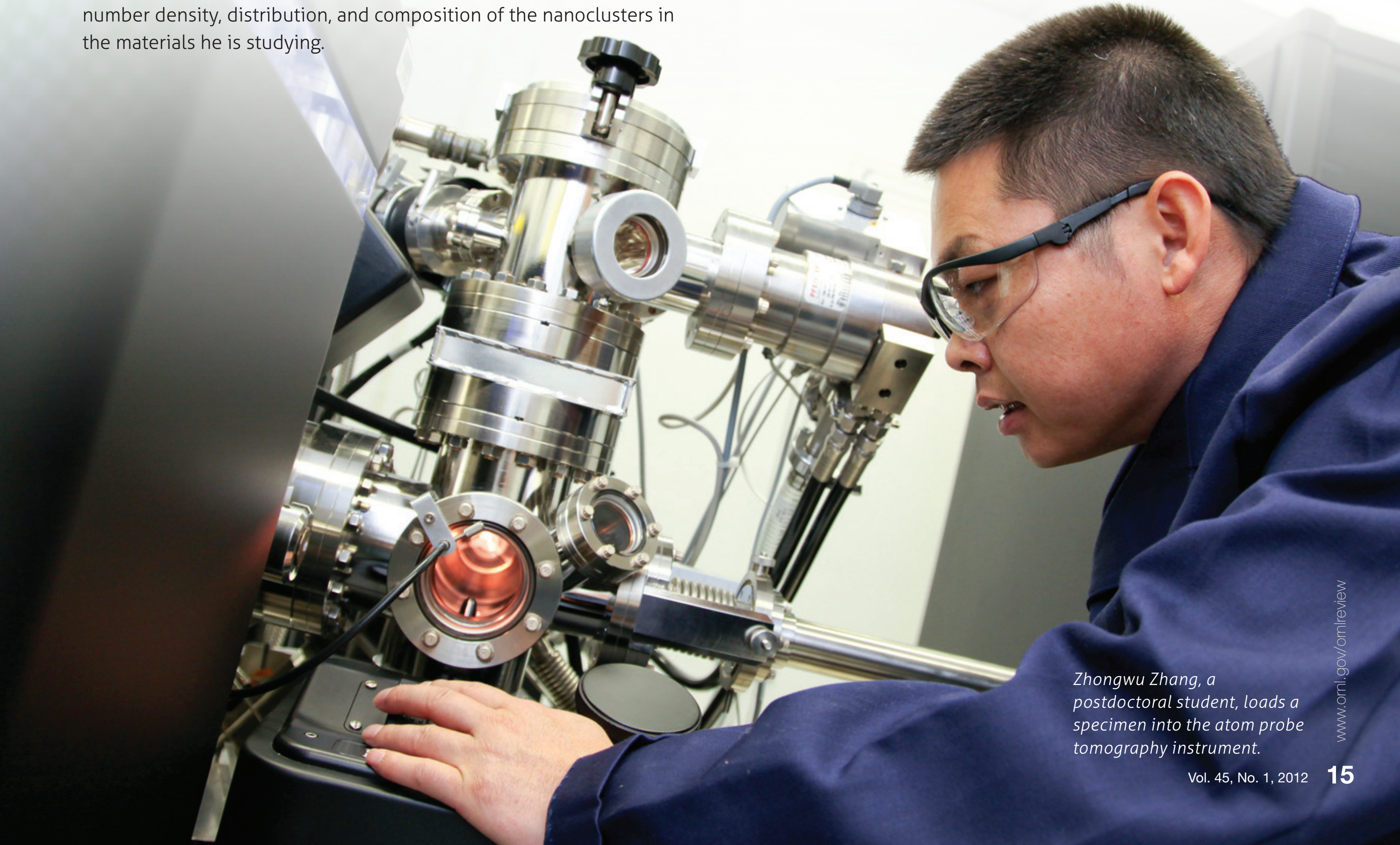
This process allows the APT to produce three-dimensional images of the internal structure of metals and semiconductors by reconstructing millions of two-dimensional slices, each containing a few atoms. Unlike some other analytical techniques, APT also sees all of the elements, without restrictions, allowing Miller and his staff to determine the complete composition and microstructure of materials at the atomic level. Finding tiny nanoclusters can be difficult, but APT detects particles down to a size of five atoms—about one hundred thousand times smaller than the diameter of a human hair.

Room for advancement

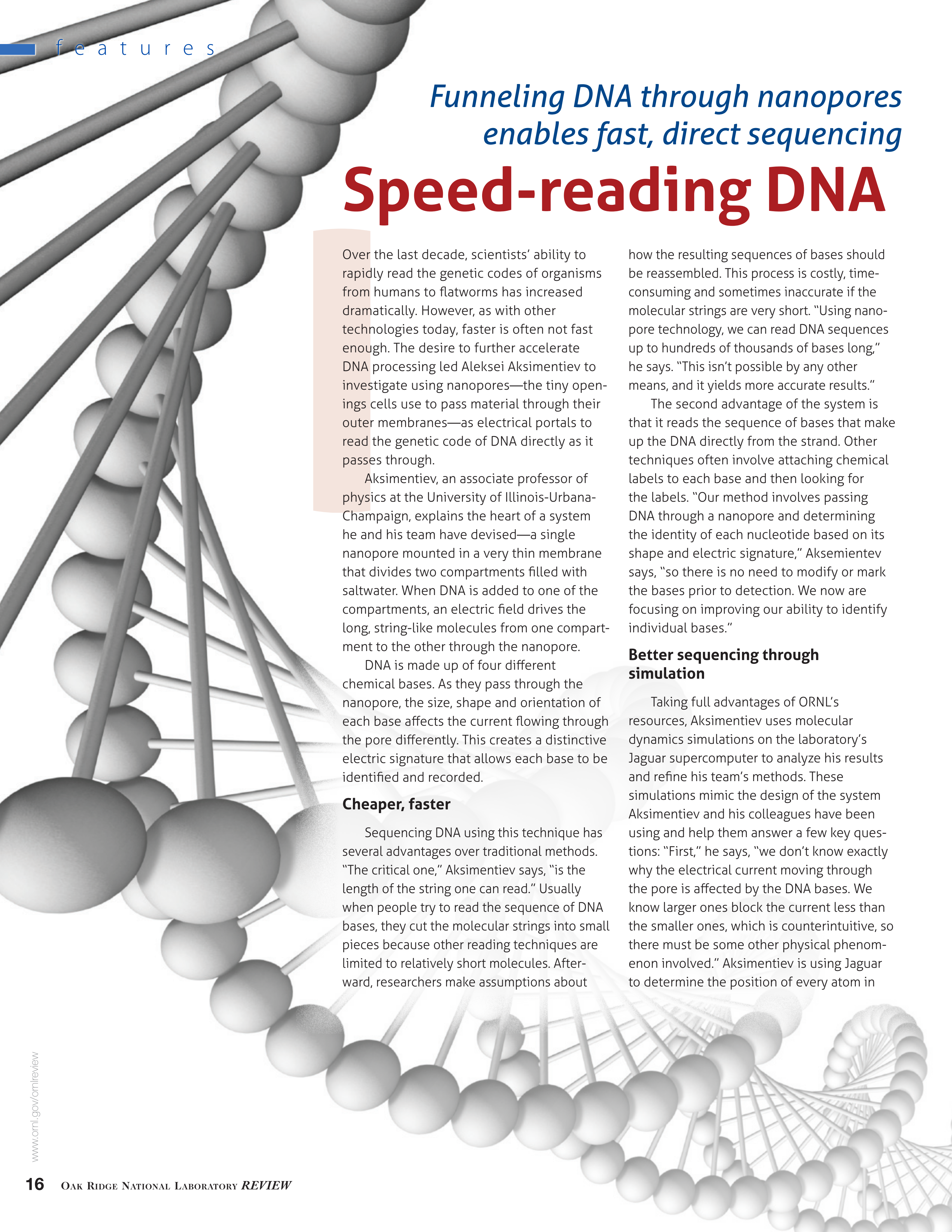
Despite advances made in APT in the past 25 years, Miller says there's still room for improvement. "We're always after higher resolution," he said. "We're also interested in improving our ability to determine the position of atoms."

All of these techniques and atomic-scale characterizations will help materials scientists develop materials that provide the stability and durability needed for the next generation of nuclear fission and fusion reactors.

"We're running short on energy, and consumption's going up, so we need more clean, stable power," Miller said. "These state-of-the-art microstructural characterization tools are critical for understanding and developing new materials for future generations of advanced energy systems." Ⓡ — *Emma MacMillan*



Zhongwu Zhang, a postdoctoral student, loads a specimen into the atom probe tomography instrument.



Funneling DNA through nanopores enables fast, direct sequencing

Speed-reading DNA

Over the last decade, scientists' ability to rapidly read the genetic codes of organisms from humans to flatworms has increased dramatically. However, as with other technologies today, faster is often not fast enough. The desire to further accelerate DNA processing led Aleksei Aksimentiev to investigate using nanopores—the tiny openings cells use to pass material through their outer membranes—as electrical portals to read the genetic code of DNA directly as it passes through.

Aksimentiev, an associate professor of physics at the University of Illinois-Urbana-Champaign, explains the heart of a system he and his team have devised—a single nanopore mounted in a very thin membrane that divides two compartments filled with saltwater. When DNA is added to one of the compartments, an electric field drives the long, string-like molecules from one compartment to the other through the nanopore.

DNA is made up of four different chemical bases. As they pass through the nanopore, the size, shape and orientation of each base affects the current flowing through the pore differently. This creates a distinctive electric signature that allows each base to be identified and recorded.

Cheaper, faster

Sequencing DNA using this technique has several advantages over traditional methods. "The critical one," Aksimentiev says, "is the length of the string one can read." Usually when people try to read the sequence of DNA bases, they cut the molecular strings into small pieces because other reading techniques are limited to relatively short molecules. Afterward, researchers make assumptions about how the resulting sequences of bases should be reassembled. This process is costly, time-consuming and sometimes inaccurate if the molecular strings are very short. "Using nanopore technology, we can read DNA sequences up to hundreds of thousands of bases long," he says. "This isn't possible by any other means, and it yields more accurate results."

The second advantage of the system is that it reads the sequence of bases that make up the DNA directly from the strand. Other techniques often involve attaching chemical labels to each base and then looking for the labels. "Our method involves passing DNA through a nanopore and determining the identity of each nucleotide based on its shape and electric signature," Aksemientev says, "so there is no need to modify or mark the bases prior to detection. We now are focusing on improving our ability to identify individual bases."

Better sequencing through simulation

Taking full advantages of ORNL's resources, Aksimentiev uses molecular dynamics simulations on the laboratory's Jaguar supercomputer to analyze his results and refine his team's methods. These simulations mimic the design of the system Aksimentiev and his colleagues have been using and help them answer a few key questions: "First," he says, "we don't know exactly why the electrical current moving through the pore is affected by the DNA bases. We know larger ones block the current less than the smaller ones, which is counterintuitive, so there must be some other physical phenomenon involved." Aksimentiev is using Jaguar to determine the position of every atom in the system. He expects simulations will reveal explanations for changes in current flow. "Experimentally, it is not possible to tell how the DNA is positioned as it passes through the pore," he explains. "Our preliminary results with the simulation suggest that it's not just the sequence of the DNA, but also its conformation, or structure—and changes in its conformation—within the pore, that contribute to changes in the current."

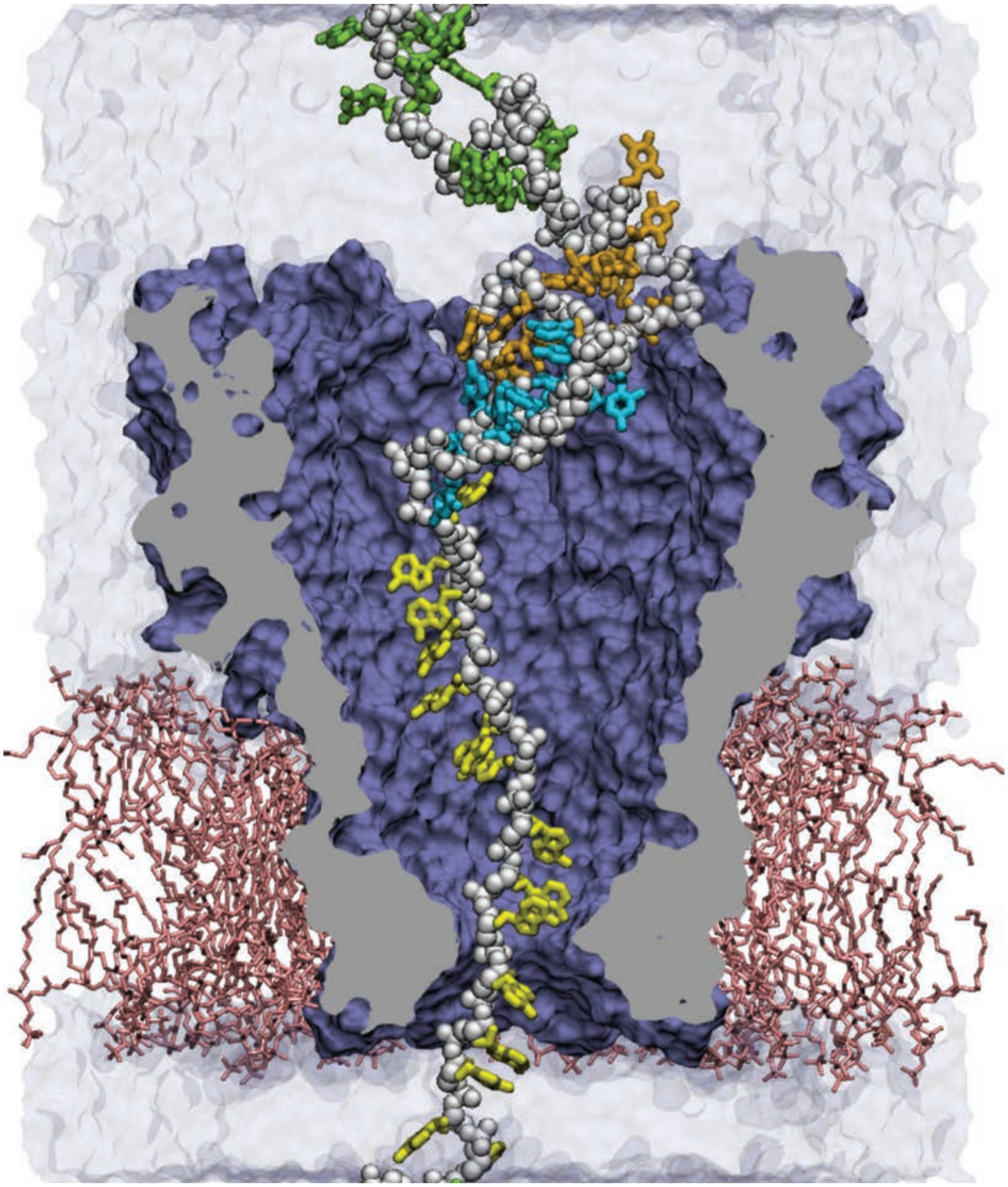
The challenge of speed

"Second," Aksimentiev says, "in our system we're using now, the DNA moves too quickly through the pore, making it hard to read its sequence. We are trying to genetically modify the channel so it interacts more strongly with the DNA, slowing it down as it passes through the pore, so its sequence can be detected more accurately." Simulation was used to design a previous round of genetic modifications aimed at putting the brakes on DNA moving through the pore. Aksimentiev notes that those changes were implemented by his colleagues in the lab and had the desired effect, but more slowing is needed. Even with this reduction in speed, Aksimentiev says the system is still fast enough, in theory, to sequence the entire human genome in an hour.

Finally, Aksimentiev explains that the current passing through the pore is affected by not just a single base, but by a series of three—the base passing through the pore, as well as the one ahead of it and the one behind it. He is using simulation to help determine whether the system can identify these "DNA triplets" by looking at their electric signature or, better yet, whether his colleagues can genetically modify the channel to be sensitive to a single base at a time. "Once we understand which of the three nucleotides passing through the pore provides the dominant contribution to the current," he says, "then we can suggest modifications to the pore that my colleagues can implement. That should improve the accuracy of the detection. We're making progress," he says, "but we will need to do more simulation to pinpoint the origin of each component of the electronic signature."

Next steps

The near-term goals for Aksimentiev and his colleagues include working with an industrial partner to commercialize nanopore sequencing technology. Their goal is to enable any researcher working in a laboratory setting to analyze genetic sequences quickly and easily. He and his colleagues are also trying to develop membranes and pores that last longer than the biologically based materials they're currently using. He says a synthetic membrane and pore combination would integrate more easily with electronics, but there are manufacturing challenges to overcome.

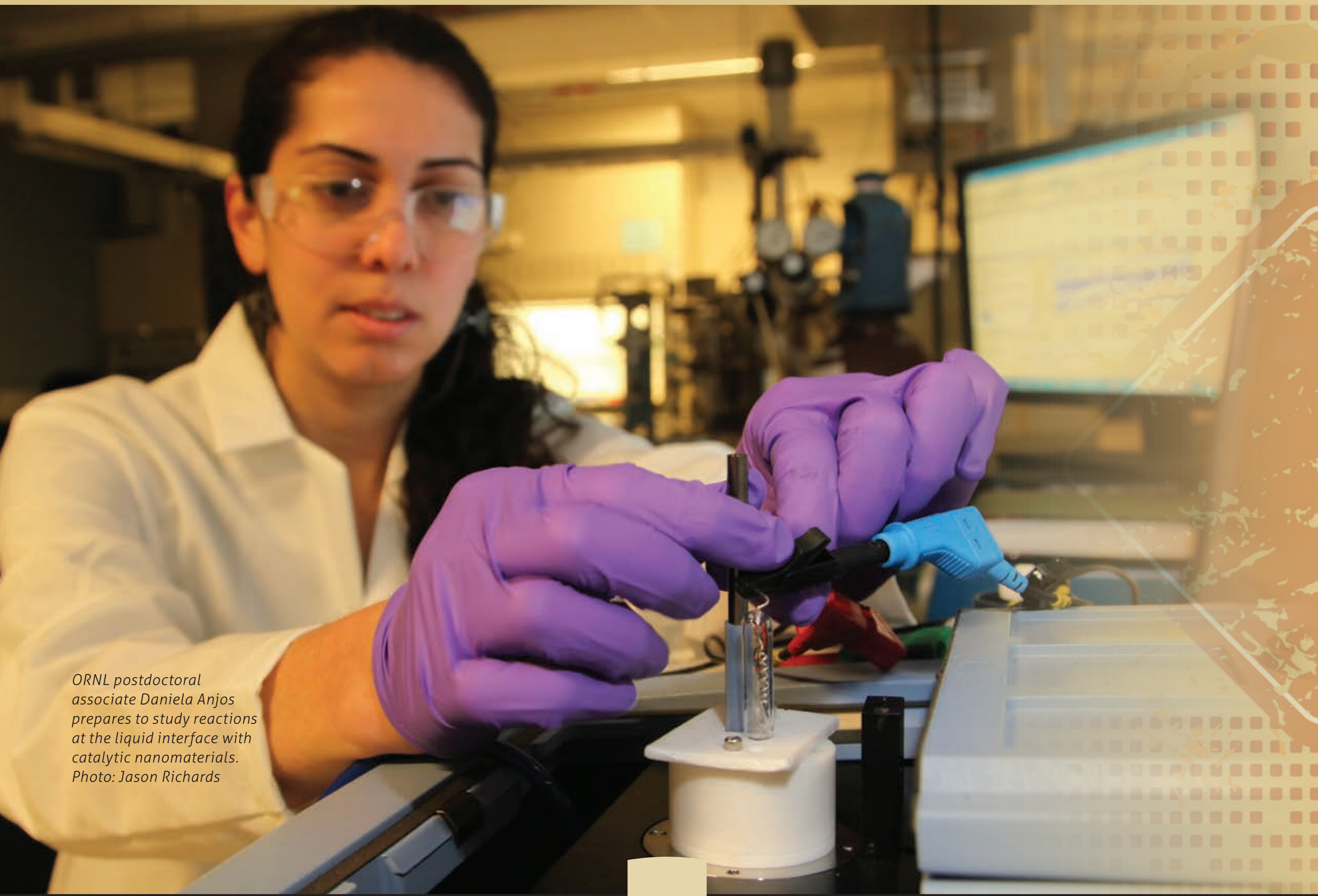


In this molecular dynamics simulation, a single strand of DNA is transported through a nanopore. Simulation: Anthony Ho and Aleksei Aksimentiev, University of Illinois

In the longer term, Aksimentiev anticipates broadening application of the technology to include identifying proteins. "Proteins are also linear polymers," he says, "but instead of just four bases, they have 20 different amino acids to describe their chemical makeup; and they don't carry a uniform electrical charge, so it is more of a technological challenge to move them through a nanopore." More importantly, however, there aren't nearly as many sequencing techniques for proteins as there are for DNA, so the impact of successfully applying this approach to proteins could be even greater."

Aksimentiev notes that computer simulations run on Jaguar are by far the best tools for exploring complex interactions like those involved in protein sequencing. To date, only a few protein sequencing experiments that involved nanopores have provided useful data, but the cause of the problem isn't clear. "We need help in understanding how to move proteins through the pore in a controlled way," he says. "That's something that Jaguar can clearly help to explain." — *Jim Pearce*

A closer look at catalysts



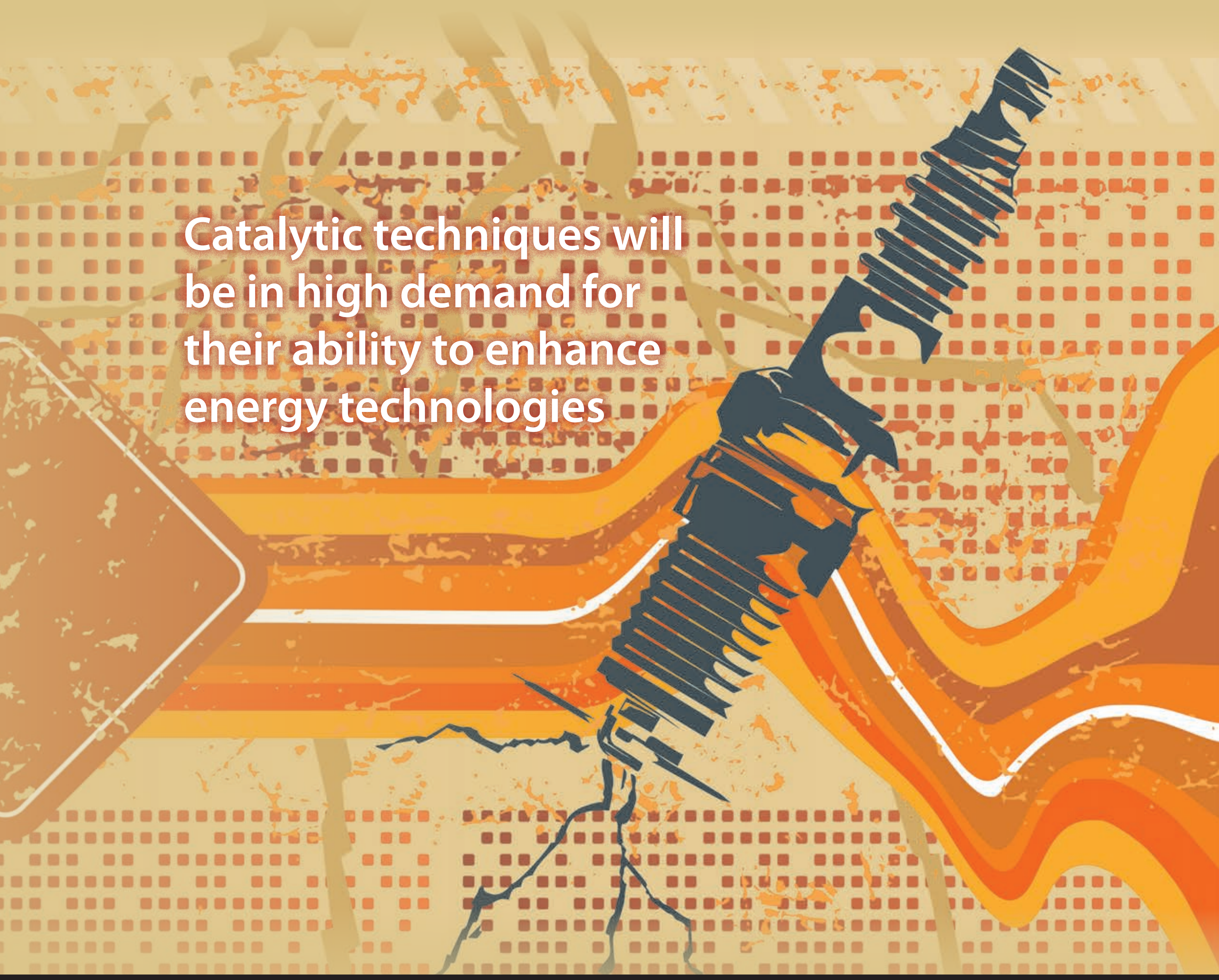
ORNL postdoctoral associate Daniela Anjos prepares to study reactions at the liquid interface with catalytic nanomaterials. Photo: Jason Richards

Understanding and improving chemical reactions

It's almost redundant to talk about chemistry at the nanoscale, because that region of the physical world is where all chemical reactions occur. You could say that chemists have been working with nanotechnology for centuries without ever actually seeing what they were doing. However, new techniques allow researchers to watch reactions on the atomic level as they occur and provide new insights into chemical reactions in general, as well as into the particular role of catalysts as accelerators of these interactions.

Catalysts work by providing an environment that encourages specific chemical reactions. Usually this means that catalytic materials are broken down into nano-sized pieces to maximize their surface area and then placed in the mix with the other chemical reactants. The greater the surface area of the catalyst, the faster the reaction will proceed. ORNL chemist Steve Overbury explains that his research team is trying to understand, on a very basic level,

Catalytic techniques will be in high demand for their ability to enhance energy technologies



how molecules interact with catalytic surfaces. "For example," he explains, "a catalyst could be used to remove oxygen from liquids in the biofuel production process or to promote a reaction between carbon monoxide and oxygen." In order for a catalytic reaction to happen, reactant molecules have to attach themselves to the surface of the catalyst; then a bond has to form between them; finally, the new molecule has to release itself from the catalyst's surface. "There are a number of steps in most catalytic reactions," Overbury says. "Knowing exactly how they occur allows researchers to apply, modify and improve them."

A better understanding

This kind of insight is illustrated by Overbury's ongoing work with cerium oxide particles. His team uses these particles to accelerate the process of removing hydrogen from ethanol—another biofuel-related application of catalysts. To help understand the effect of the catalyst's structure on the interactions occurring on its surface, Overbury's group produces two kinds of cerium oxide nanoparticles: some cube-shaped and others in the form of octahedrons. Overbury wants to determine how differences in shapes and the structure of surfaces affects the catalytic activity of nanoparticles. "We have already seen some differences in the way the catalytic reaction occurs on the differently shaped particles," Overbury says. "Surface structure definitely plays a role in this process."

To gain a better appreciation of the nuances of catalytic surfaces, Overbury also collaborates with researchers at ORNL's Center for Nanophase Material Sciences. These experiments often involve using electron microscopy, as well as neutron and x-ray-based analytical tools, to study catalytic nanoparticles attached to supports or substrates. "Surprisingly," Overbury says, "one of the most inter-

Anjos prepares nanoparticles for electrochemical studies. Photo: Jason Richards

esting catalysts we have been working with is gold." Scientists have found that gold's ability to catalyze reactions is heavily dependent on the size and shape of the gold particle and the composition of the material supporting the particle. "If the particle is very small," he says, "it can be very catalytically active. Larger particles are much less active—even if you take into account differences in surface area." There has been a huge amount of interest in understanding why this happens and whether the effect is related to the structure of the particle's surface or its electrical charge or something else entirely. This question is interesting not only in terms of basic research, but also because it could help determine whether gold could be used to catalyze certain types of chemical reactions.

"We ask the same basic questions in each experiment," Overbury says. "Does the reaction occur? Does it occur on the surface of the nanoparticle? Does it occur on the support? Does it occur at the interface between the two? Are there differences in reaction based on the type of support or on the size of the particles?" Ultimately, Overbury and his colleagues will use the answers to these questions to advance their understanding of how molecules react on the surfaces of these catalysts. However, this research has considerable practical value as well. "If someone wants to create a new catalyst to decrease exhaust emissions, or a photocatalyst to produce hydrogen from water," he says, "they will need to know, at a fundamental level, what is going on in these reactions. The chemical industry is based on creating catalysts that can make a particular reaction occur. Understanding these properties and applying them to technological challenges is what the nanoscale revolution is about."

Accelerating energy technologies

Overbury expects that catalytic techniques will be in increasingly high demand for their ability to enhance energy technologies.

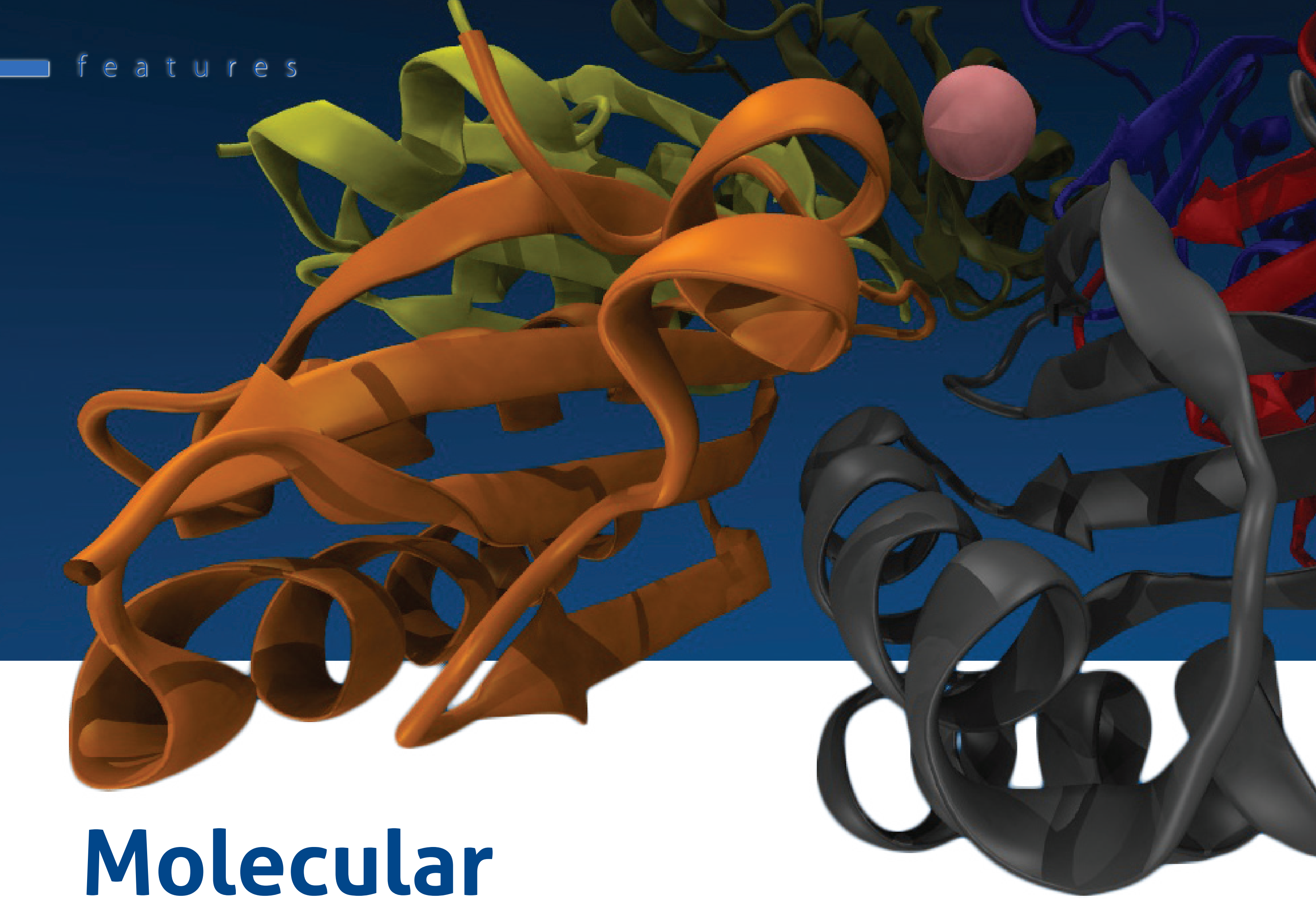
One of these technologies is producing hydrogen for fuel cells and other applications. "ORNL is home to the Fluid Interfaces Reactions Structure to Transport (FIRST) center," Overbury says. "So our group is particularly interested in reactions that occur at the fluid–solid interface in processes like water splitting—extracting hydrogen from water." He notes that the main stumbling block in the way of creating a hydrogen-based economy is the lack of an efficient means of producing hydrogen. "People want to be able to use photons from the sun to split water and create hydrogen," he says, "but we can't do this economically. Before hydrogen power can be made practical, we have to understand how water interacts with other molecules at semi-

Chemists have worked with nanotechnology for centuries without ever seeing what they were doing

conductor surfaces that harvest photons." Overbury anticipates that understanding the fundamentals of the water splitting process will increase the practicality of both applying solar energy to hydrogen production and using hydrogen fuel to meet our energy needs.

Another promising prospect for the application of catalytic technologies is the process of converting biomass to biofuel. The biomass fermentation process creates a number of different types of molecules that are heavily loaded with oxygen. "These aren't very good for fuel," Overbury says. "However, if we convert them catalytically, stripping out the oxygen and putting the small molecules together to make long-chain molecules, we can make something that's a lot like gasoline." There are already technologies available to do this, but they are relatively inefficient. By developing a deeper scientific understanding of these catalytic transformations, Overbury hopes to develop a more elegant and efficient means of converting biomass to fuel.

All of the catalysis research in Overbury's group has the same basic aim: applying an improved understanding of the underpinnings of chemical reactions to the job of streamlining catalytic processes. "We're always looking for ways to reduce the energy needed to run a catalytic system," he says. "This can involve increasing the speed or efficiency of the catalyst or increasing the selectivity of the reaction. Process improvements like these are what catalysis is all about." R — *Jim Pearce*



Molecular machinery

Synthetic biology, nanostructures could boost biofuel production

Over the centuries humans have used microorganisms for activities from making wine and beer to baking bread. Common microorganisms like yeast and bacteria can carry out surprisingly complex chemical transformations in the space of a few nanometers. Today, scientists working in the field of synthetic biology are developing methods of modifying and controlling the molecular machinery within these organisms. Their goal is creating nanoscale chemical factories that are more efficient than traditional production methods and can be easily modified and reproduced.

One of these efforts, aimed at boosting the efficiency of biofuel production, is a collaboration between ORNL physicist Miguel Fuentes-Cabrera and Qing Lin, associate professor of chemistry at the University at Buffalo, The State University of New York.

Investigating microcompartments

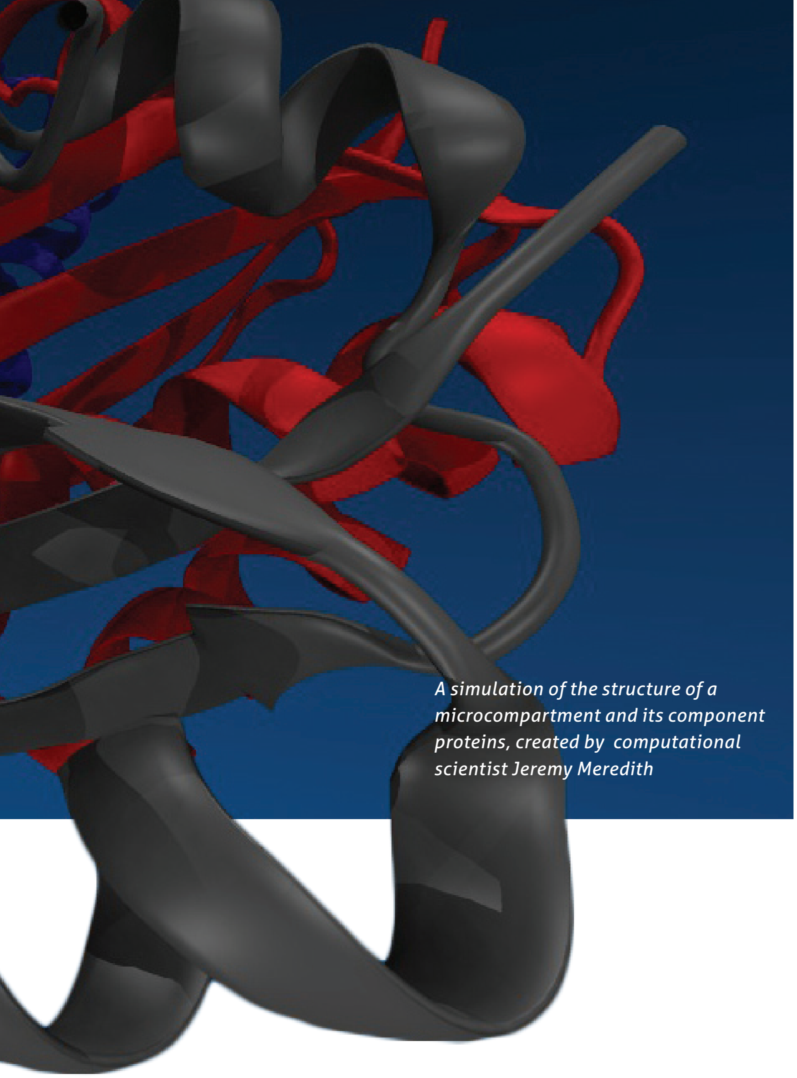
The pair's research, begun under a grant from the Keck Foundation, is focused on transplanting the chemical processing capability of nanoscale bacterial structures called microcompartments into a strain of yeast used in commercial biofuel production. "These microcompartments usually have a specialized function associated with cellular metabolism," Lin says. "The structures act like completely isolated entities—small machines within a big factory," Fuentes-Cabrera adds. "They take material from the host bacteria, perform various enzyme-catalyzed metabolic reactions, and then release the resulting products into the host organism."

"For example," Lin says, "we know that under certain conditions bacteria use microcompartments to convert ethanolamine to acetaldehyde and ammonia for nourishment. By performing this essential metabolic function in a segregated compartment, the bacteria are able to tolerate levels of acetaldehyde which would otherwise be toxic. Because the ethanol production pathway in yeast also involves acetaldehyde, we thought a good way to demonstrate the potential of these microcompartments would be to import them into yeast to boost ethanol production and improve ethanol tolerance. That's the goal we're working toward."

Both researchers note that the ability to engineer these organisms to produce ethanol, propanol or other biofuels hinges on gaining access to the chemical processing capabilities of the nano-sized microcompartments—and that requires understanding how molecules move in and out of these structures.

Understand then modify

Computer simulations may hold the key to understanding the ins and outs of microcompartments. That's where Fuentes-Cabrera's



A simulation of the structure of a microcompartment and its component proteins, created by computational scientist Jeremy Meredith

primary contribution to the collaboration comes into play. The simulated microcompartments he creates not only improve the general understanding of these structures, but also help Lin's team determine how to proceed in unlocking their function.

Microcompartments are made of collections of proteins, which include a number of pores. Some researchers suggest that these pores act like "gates" that allow molecules to move in and out; however, they're not sure what causes the pores to open and close. The gates could be regulated by metabolites—materials produced by the bacterium during digestion and other chemical processes—in reaction to concentrations of these materials within the cell. "That's what our simulation is helping to determine," Fuentes-Cabrera says. "There is a lot of speculation as to how metabolites are transported through the microcompartments." His post-doctoral assistant, Yungok Ihm, is investigating this process by creating a simulation of ions and metabolites passing through the pores in the microcompartments. "This will allow us to determine how the size and electrical charge of these objects affect their passage through a pore." To gain greater insight into the question, Fuentes-Cabrera plans to build a simulation of a microcompartment comprising millions of atoms. "This kind of large-scale simulation is precisely what ORNL's computational capabilities are designed to do," he says. "We are optimistic that we will be able to simulate an entire microcompartment."

Once they understand how molecules are transported in and out of the compartments, Fuentes-Cabrera and Lin plan to turn their attention to understanding other aspects of the structures. Using simulations, Fuentes-Cabrera will investigate the proteins that spontaneously self-assemble into the microcompartments. For his part, Lin will attempt to introduce new enzymes into the interior of the microcompartments to enable the production of ethanol or propanol. "The critical first step is to determine whether the native metabolic pathway present in these structures can be re-engineered to facilitate the bioethanol production," Lin says. "First we understand, then we modify," Fuentes-Cabrera says.

Bacteria to yeast

If the biofuels production capability of microcompartments can be achieved in bacteria, Lin's goal is to reproduce the same process genetically in yeast used to produce biofuels. Providing yeast with the added metabolic capability of microcompartments could reduce the number of steps involved in the biofuels production process and, therefore, its cost.

However, genetically engineering new qualities into an organism can be problematic. "Often when researchers try to genetically modify an organism to do something that it doesn't normally do, it dies," Fuentes-Cabrera says. Despite that note of caution, he and Lin feel they have a good chance of having bacterial microcompartments work in yeast because of their self-contained nature. He explains this optimism by pointing to the fact that all of the engineered metabolic reactions occur within the confines of the microcompartments. "We are more confident of success because we are not interfering with the yeast's normal metabolic processes," he says.

So far, the two researchers have been able to express the five compartment-related proteins in yeast. Their assumption is that, once expressed, these proteins should spontaneously assemble themselves into microcompartments—which is what occurs in bacteria. The researchers are now in the process of isolating the potential microcompartments from the yeast in order to study them using transmission electron microscopy. To gain additional molecular-level insight into the protein self-assembly, they are also using simulations to model the interactions among the proteins. "When we have a better understanding of how the proteins interact," says Fuentes-Cabrera, "we will be able to suggest genetic modifications to facilitate the self-assembly process."

Biological advantage

Both Fuentes-Cabrera and Lin maintain that biofuel production is just one of many potential applications of this relatively new facet of synthetic biology. They emphasize that one of the goals of the field is to learn from nature and then apply what you have learned to your advantage. "In this case," Fuentes-Cabrera says, "we are showing that we can harness natural biological processes to provide us with technologies we need. Much of the system we are working with occurs naturally. We didn't have to invent it. It was already there."

Lin notes that the biggest advantage of a purely biological approach to biofuel production over those using artificial or manufactured components is the ease with which changes to the system can be implemented. "Because microcompartments are naturally produced by certain microorganisms," Lin says, "they are part of a genetically encoded system. If we want microcompartments to do other tasks, we can simply modify the genes that control the biological parts in the system and scale up the production by growing more microorganisms. Ramping up production for a new generation of nanomaterials, on the other hand, could be far more difficult." Ⓡ — *Jim Pearce*

Sean Smith,

the Director of ORNL's Center for Nanophase Materials Sciences, came to ORNL from the University of Queensland in Australia where he was the Director of the Centre for Computational Molecular Science. His decision to take a new job half a world away was based on the enormous possibilities offered by the laboratory's critical mass of research capabilities in several different areas of nanoscience. "Working at ORNL," he says, "offers the opportunity to collaborate across a large scope of nanoscience and in activities that can potentially have a significant impact on society at large."

We asked Smith about what's behind the surge of interest in all things "nano" and how research at the nanoscience center impacts other research at the laboratory, as well as our everyday lives.

Nanotech has been hugely popular in the last few years. What about nanoscale phenomena makes them so interesting across a range of disciplines?

The essence of why nanotech is interesting to so many different disciplines is that many physical and even biological processes play out on a scale that falls between molecules and bulk materials. The nanoscale is that in-between space. It's where we can see aggregations of molecules interacting in ways that can't be explained from a bulk macroscopic point of view or from an atomic or molecular perspective. At the CNMS, we integrate these domains of knowledge by studying the structure and dynamics of what is happening on this intermediate scale.

Where can the average person see the benefits of nanotechnology?

I think the earliest applications of the technology that everyone could see were fabrics that had nanoparticles incorporated in them to strengthen them and to improve their flexibility. Nanoparticles have also found their way into cosmetics and sunscreens. Nanostructures, such as carbon nanofibers and nanotubes, have been incorporated into composite materials such as those in sporting and military equipment, automobiles and planes, to reinforce and strengthen while retaining lightness. Today, nanotechnology is being used to develop longer-lasting batteries for mobile phones, tablet computers and other portable appliances. Less obvious, but important from a quality-of-life perspective, are the nanoscience-enhanced catalytic materials used to filter air in the passenger cabins of airplanes. There are many nano-engineered products all around us, and we never even know they're there.

Many ORNL research groups are doing research at the nanoscale. How do they interact with CNMS?

The most common scenario for this kind of cooperation arises when a group needs access to an instrument at CNMS to gain new insights into the process or materials they're working with. CNMS is a user facility, so like any other research group from any other institution, prospective ORNL users write a user proposal. The proposal goes through peer review and, as long as the science behind the proposal impresses the reviewers, it's accepted and the research group is allocated time to come to the nanoscience center and work with our staff and equipment. Sometimes, if there are genuinely common research interests between users and the staff scientists at CNMS, we establish a formal collaboration. These collaborations often grow into research projects that involve our science program, users' science programs, grant proposals, new funding and so on.

What kinds of research are your visiting scientists primarily interested in?

The big research drivers are energy and materials sciences. There is also an increasing amount of interest in the biological sciences because the medical applications of nanotechnology are potentially very important. The full spectrum of research interests we support is incredibly broad because our center supports many users from academia, and individual professors and universities are pursuing nanotechnology research in any number of areas.

Where do your users come from?

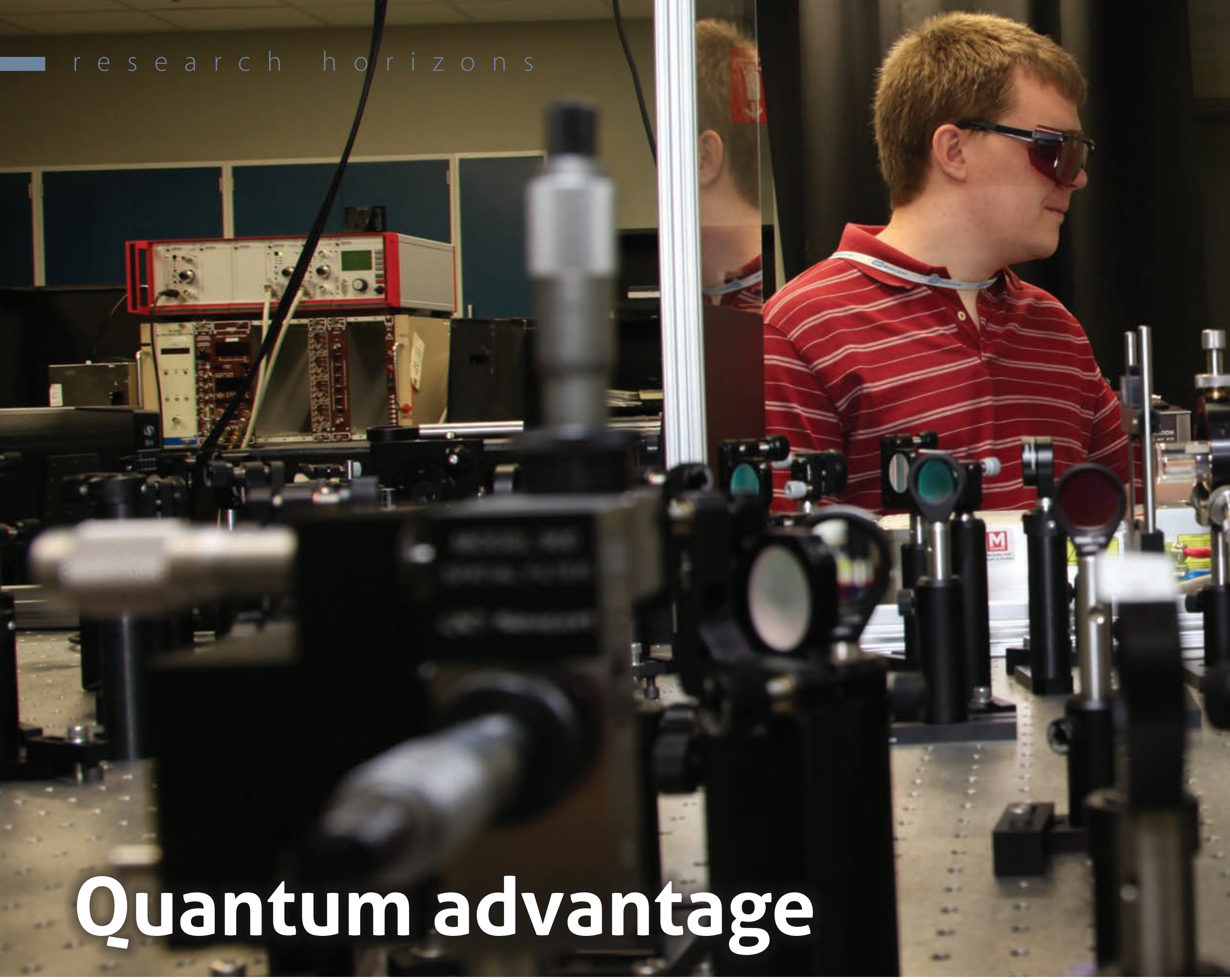
Although we have users from around the world, our users are primarily domestic. Because CNMS supports nanoscience research at ORNL, we have a lot of users from the laboratory. We also have many users from universities who want to get access to a specialized piece of equipment or take advantage of our specialized skills. One of the things that distinguishes the Department of Energy's five nanoscience centers from other nanoscience centers is that they have not only very specialized equipment but also staff scientists with an enormous amount of skill and experience. As a result, some users come to CNMS not for the facilities but for the opportunity to work with our research staff.

What's the biggest difference between leading CNMS and your previous job at the University of Queensland?

At the University of Queensland, I headed up a laboratory that focused on computational nanotechnology and nano-bio research. CNMS has a broader mandate, encompassing six groups with different domains of experimental activity in nanoscience. This gives me both the challenge and the opportunity to interface, in a much more direct way, with a range of different experimental areas of nanoscience. It expands my horizons. It's a challenge, and it's a great reward to see interactions developing among these areas.

Where do you see nanotechnology having the most impact over the next few years?

I think nanotech will have the largest impact in energy and medicine. The next generation of batteries, supercapacitors and fuel cells will be critical to the ongoing development of our economy and to the sustainability of our energy demands. Nanoscience will drive advances in this area by enhancing the properties of the materials that go into these devices. Medical research at the nanoscale is going to be an area of keen interest, both because of its potential benefits for society and because it involves collaborative research among physical and material scientists, biologists and clinicians. Our experience suggests that, through this kind of cross-disciplinary interaction, questions are asked that wouldn't be asked otherwise, and solutions are found that couldn't be found in any single research domain. Ⓡ



Quantum advantage

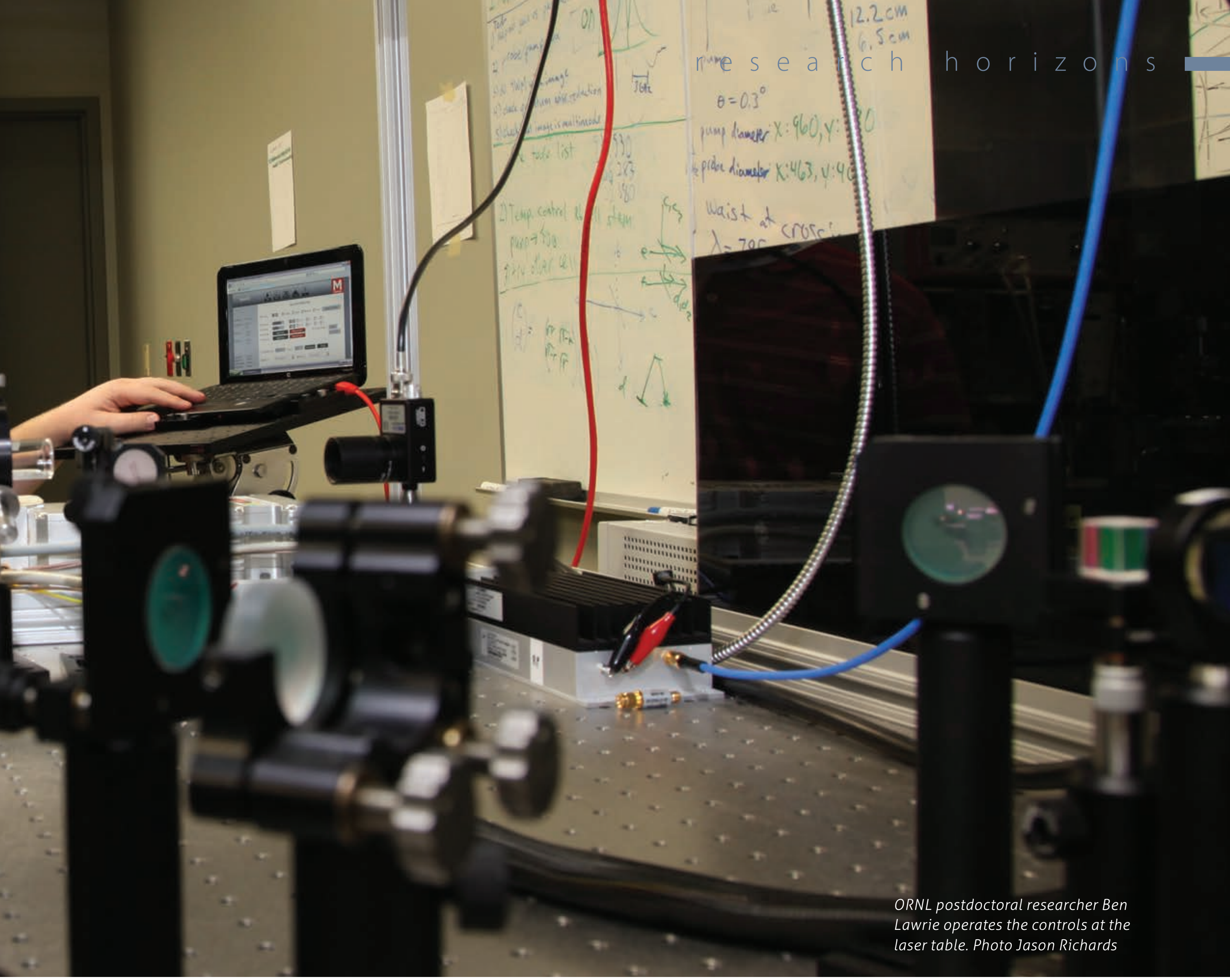
Small-scale phenomena drive next-generation computing technology

From smartphones to supercomputers, users of digital devices are united in their need for speed. For decades, that has meant creating silicon-based computer chips that pack more circuitry into increasingly smaller spaces. Recently, however, the recognition that the density of circuitry on silicon chips is nearing its theoretical limit has accelerated research in the field of quantum computing.

Although still in its infancy, quantum computing has demonstrated the potential to handle certain types of computational problems many times faster than traditional methods. The key to this advantage is its reliance on esoteric physical interactions that occur among particles like photons and electrons on a vanishingly small scale.

Creating quantum entanglement

To generate these quantum interactions in the laboratory, ORNL quantum scientist Raphael Pooser fires a laser into a cloud of



ORNL postdoctoral researcher Ben Lawrie operates the controls at the laser table. Photo Jason Richards

vaporized rubidium atoms. The laser beam, like all light, is composed of individual photons. Under tightly controlled conditions, the atomic vapor acts like a nonlinear crystal, splitting the laser into twin beams of light, each with a frequency slightly different from that of the original. Pairs of photons—one in each beam—are created by this process. Each member of the pair is linked to the other by a phenomenon known as quantum entanglement. "These entangled pairs are the fundamental building blocks of quantum optics," Pooser says. "They enable us to do quantum computing with photons."

The notion of quantum entanglement is difficult for most people to take in. Even Albert Einstein wasn't a big fan of the concept. In a paper published in 1935, Einstein and his colleagues disputed the completeness of the new theory of quantum mechanics because they claimed it failed to define all elements of reality accurately. Among their misgivings were reservations about the implications of equations indicating that measuring the position or momentum of one quantum object (such as a photon) allows one to calculate the position or momentum of another—regardless of the distance between the two. Einstein skeptically called this phenomenon "spooky action at a distance." "We call it 'entanglement,'" Pooser says.

Encoding quantum information

Pooser explains that the "spooky" relationship between the entangled photons in terms of position and momentum extends to their polarization as well. In classical computing, the distinction between horizontally and vertically polarized light could be used to express a unit of digital information known as a binary digit, or "bit," represented by a zero or a one. In quantum computing, however, a quantum bit, or qubit, is much more versatile. With vertical polarization, the value of the qubit is zero; horizontal polarization yields a one. "What is interesting," Pooser explains, "is that the bit can have not only horizontal or vertical values, but both, and any intervening values, at the same time. That is the probabilistic nature of quantum mechanics." This ability to express simultaneous or superimposed values illustrates the advantage quantum computing has over classical computational methods. "Superimposition means we can do calculations for all possible values of the qubit at once," Pooser says. "That's what we call massive parallelization."

The challenge for Pooser is determining how to extract all of the answers. "If we can't access all of the results at the same time, what good is this massive parallelization?" he asks. That's where entanglement comes in.

The difficulty in extracting multiple results arises as a result of the inherent uncertainty of quantum measurements. An oft-cited example of this ambiguity is offered by one of Einstein's contemporaries, the physicist Werner Heisenberg. Heisenberg's uncertainty principle states that it is impossible to measure both the position and the velocity of a quantum object at the same time. Similarly, researchers cannot read all possible values of a qubit at the same time. However, as noted above, entanglement makes it possible to make a measurement on one entangled object and then to infer the value of the same measurement for its entangled partner. As a result, a pair of entangled photons enables simple calculations to be made. As Pooser and his colleagues succeed in entangling greater numbers of photons, they will use them to address progressively more complex computational problems.

This ability to express simultaneous values illustrates quantum computing's advantage

Quantum calculations

Quantum calculations are made by the optical equivalent of algorithms—specialized mathematical equations. Pooser uses an apparatus called a laser table to direct beams of entangled photons through a network of optical components, like beam splitters, lenses and filters, to create these optical algorithms. These components enable the photons to interact with one another so that, when they complete the circuit of the table, the results of the equation are encoded in their final optical characteristics.

"Most quantum algorithms use entanglement to get results," Pooser says. One of the most highly touted applications for this technology is finding large prime numbers—numbers that can be evenly divided only by themselves and 1. Large prime numbers are of interest in computing circles because they are used to create, and decode, encrypted data. "It turns out that quantum computing is particularly good at that," he says.

As computational requirements become more complex, the number of optical components required to reach a solution increases as well. This and other practical considerations are fueling a drive toward miniaturization of these optical circuits. Most of Pooser's computational research has been conducted at the macro scale—on a laser table. However, he and his colleague, quantum information scientist Phil Evans, have made considerable progress in scaling down these optical algorithms to the point that a tabletop experiment can be recreated on an optical chip the size of a fingernail. These chips have microscopic waveguides etched into their surfaces to channel laser light as it undergoes optical permutations that mirror those used on the full-sized laser table.

Quantum simulations

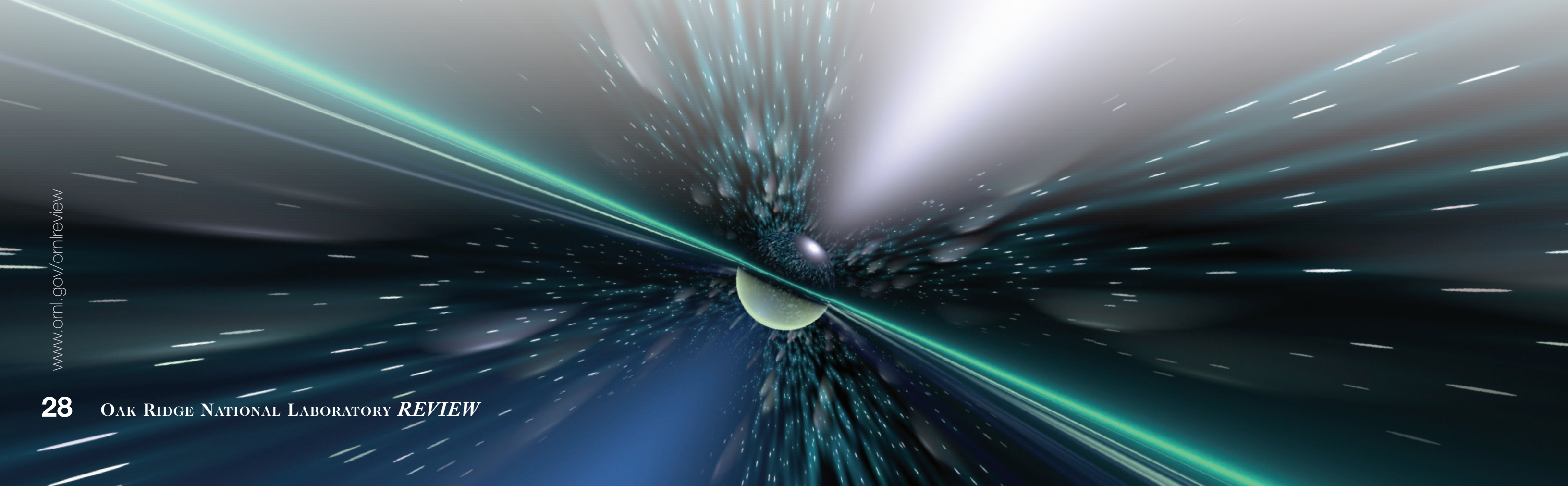
One of the primary applications of complex quantum calculations is expected to be creating quantum simulations. Pooser explains that programmers can write routines for classical computers that simulate quantum systems, but they will never be exactly right because classical computers are designed to operate under the physical laws of classical physics, not quantum physics. "If we really want to simulate a quantum system accurately," he says, "we need to build a computer that obeys the laws of quantum mechanics. For example, if I build a quantum mechanical simulation that demonstrates high-temperature superconductivity, the fact that I could build the simulation proves that the system could exist in nature. This is one of the ways a quantum simulator would provide insight into the quantum world in ways classical computers can't."

The potential for eventually producing quantum simulations has been a big motivation for developing quantum computing. Pooser expects that the area will continue to be of interest to the Department of Energy because scientists are finding that quantum mechanical processes are intertwined with critical energy technologies. "For example," he says, "photosynthesis involves quantum entanglement, and generating solar energy depends on the photoelectric effect, which is also a quantum mechanical process. If we want to conduct the most accurate possible analyses of systems like these, we'll need a quantum computer."

Technology of tomorrow

Pooser says he and his colleagues in ORNL's Cyberspace Science and Information Intelligence Research group are on the cutting edge of quantum optic science. "Only one or two other groups in the world have the capability to do this kind of research," he says. "This is the technology of tomorrow."

Looking ahead, Pooser estimates that, in five years, complex calculations will be carried out on optical chips—or a series of chips. In 10 years, he hopes to be able to consolidate complex algorithm processing on a single chip. He suggests that the timeline for quantum computing's becoming a viable analytical platform could be anywhere from 15 to 20 years down the road if there is a big breakthrough, longer if there's not. "The world is waiting for this," he says. "There's no question that it will happen. It's just a question of when." ® — *Jim Pearce*



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