OAK RIDGE NATIONAL LABORATORY

Review

Probing quantum materials:

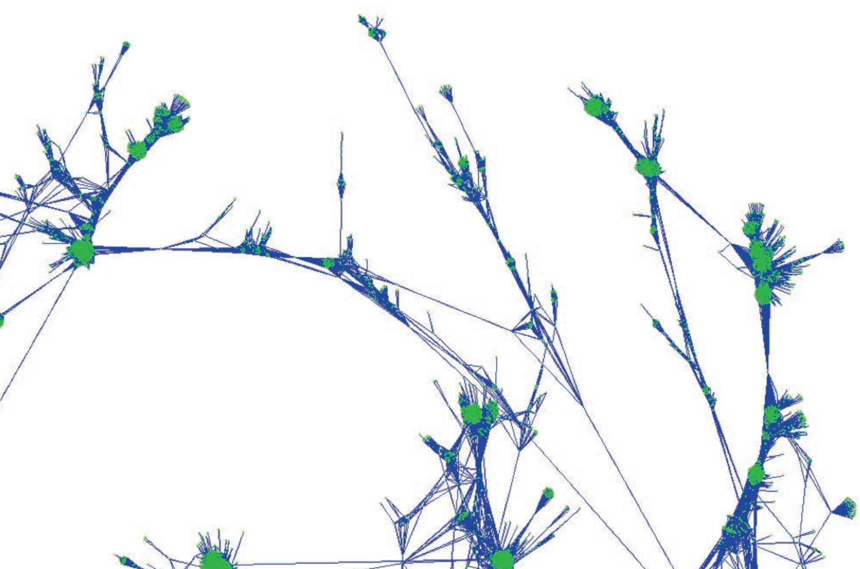
10 • Neutrons help us understand the nanoscale world

Oak Ridge National Laboratory

Vol. 52 | No. 2 | 2019
www.ornl.gov/ornlreview

OAK RIDGE NATIONAL LABORATORY
Review
Vol. 52 | No. 2 | 2019

Contents



On the Cover

Neutron scattering scientist Clarina dela Cruz explores the nanoscale world of quantum materials. Image credit: Carlos Jones, ORNL

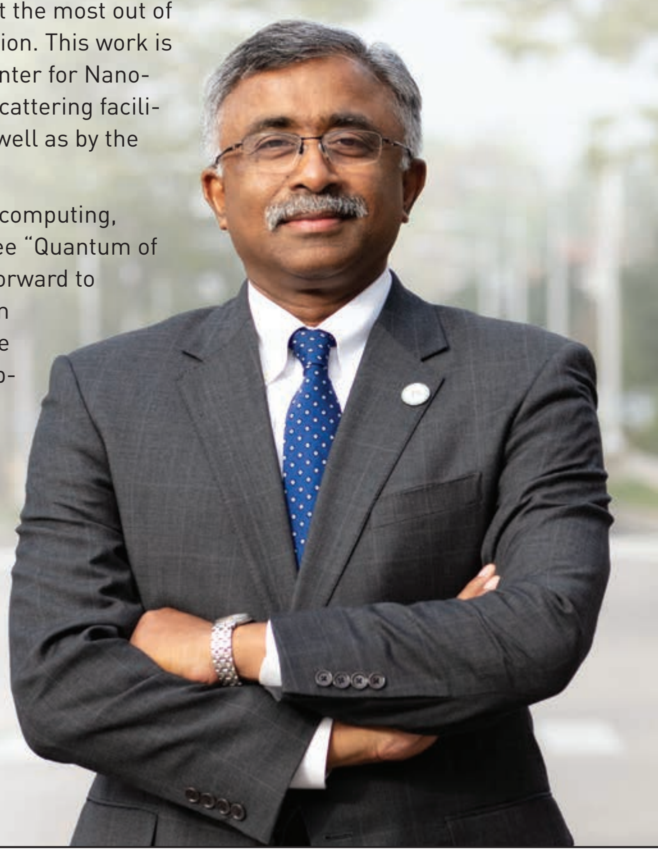
Making the most of quantum science

Matter at the scale of atoms and molecules behaves differently than the world as we experience it. At this scale, particles behave like waves, they can exist in two independent states simultaneously, and they can become entangled with one another at seemingly impossible distances.

The science of this odd behavior—known as quantum mechanics—offers a path to a deeper understanding of matter as well as never-before-seen technologies. Quantum computers promise to someday tackle problems beyond the scope of even the most powerful classical systems, and quantum materials promise powerful encryption, advanced sensors and applications that we cannot yet imagine.

Before we can fully exploit the unique behavior of quantum mechanical systems, however, we will have to overcome serious challenges. While quantum computers may open the way to solving important new problems, we are not there yet. Existing systems may be marvels of physics, but they must be far larger and far more stable to reach their potential. Other quantum technologies, too, are in their early stages, awaiting advances that will help them change the world.

The National Quantum Initiative, signed into law late last year, provides funding for quantum research and development across the federal government, and ORNL researchers are deeply involved in the quantum revolution. Our materials scientists and chemists are working to develop new materials and fully understand their behaviors at the quantum level, while physicists and computer scientists are working to get the most out of both existing and future quantum systems for computing and communication. This work is facilitated at ORNL by Department of Energy user facilities such as the Center for Nanophase Materials Sciences and two of the world's most advanced neutron scattering facilities, the Spallation Neutron Source and the High Flux Isotope Reactor, as well as by the planet's most powerful computer—the Summit system.



In this issue of *ORNL Review*, we take a look at some of the possibilities in computing, information science and materials that are implicit in quantum science (see "Quantum of Science," page 6). We examine the state of quantum computing and look forward to the accomplishments that will develop that technology fully (see "Quantum computing is ideal for quantum problems," page 8). We look at the promise of quantum materials (see "New materials for sensors, computers, encryption and more," page 10). And we reveal how ORNL researchers are creating new quantum materials that may hold the key to future breakthroughs (see "Cooking up quantum materials," page 12).

Elsewhere in the *Review*, we see how ORNL research into callus formation in poplar trees may help us understand human cancer (see "Tree of life: Poplar studies yield human cancer insights," page 36), how the Summit system is giving researchers insights into patients predisposed to substance abuse (see "ORNL team uses supercomputing to fight addiction," page 20) and how ORNL chemists have demonstrated a practical, energy-efficient method of capturing carbon dioxide directly from air.

I hope you enjoy learning about the lab's work in the quantum revolution and other cutting-edge science in this issue.

Thomas Zacharia
Laboratory Director

New ORNL supercomputer will accelerate science and tech

ORNL's next supercomputer, named Frontier, will be capable of more than one and a half billion billion calculations per second, or 1.5 exaflops.

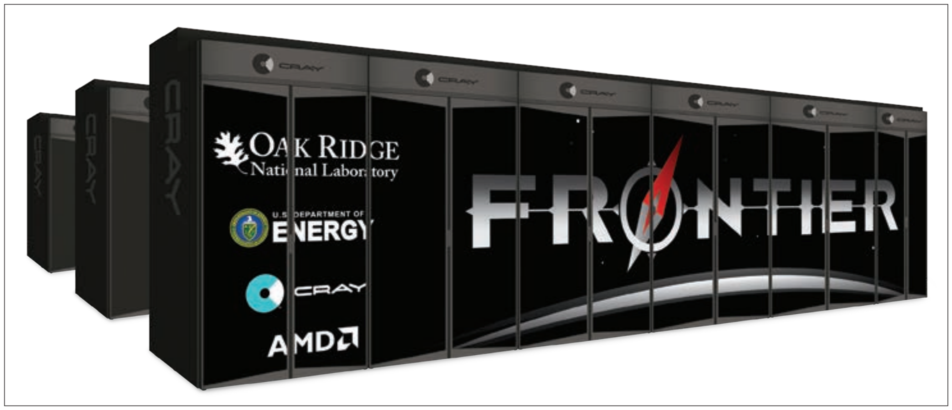
The Department of Energy announced a contract with manufacturer Cray Inc. to build the system, which is anticipated to debut in 2021 as the world's most powerful computer.

Frontier will accelerate innovation in science and technology and maintain U.S. leadership in high-performance computing and artificial intelligence. The total contract award is valued at more than $600 million for the system and technology development. The system will be based on Cray's new Shasta architecture and Slingshot interconnect and will feature high-performance AMD EPYC central processing unit and AMD Radeon Instinct graphics processing unit technology.

By solving calculations up to 50 times faster than today's top supercomputers, Frontier will enable researchers to deliver breakthroughs in scientific discovery, energy assurance, economic competitiveness, and national security. As a second-generation AI system—following the world-leading Summit system deployed at ORNL in 2018—Frontier will provide new capabilities for deep learning, machine learning and data analytics for applications ranging from manufacturing to human health.

"Frontier's record-breaking performance will ensure our country's ability to lead the world in science that improves the lives and economic prosperity of all Americans and the entire world," said U.S. Secretary of Energy Rick Perry, who announced the contract for the new system on May 7. "Frontier will accelerate innovation in AI by giving American researchers world-class data and computing resources to ensure the next great inventions are made in the United States."

Since 2005, ORNL has deployed Jaguar, Titan and Summit, each the world's fastest



Artist's rendition of ORNL's Frontier supercomputer, which is anticipated to be completed in 2021.
Image credit: Jason Smith, ORNL, and Sarah Hager, Cray Inc.

computer in its time. The combination of traditional processors with graphics processing units to accelerate the performance of leadership-class scientific supercomputers is an approach pioneered by ORNL and its partners and successfully demonstrated through ORNL's No. 1-ranked Titan and Summit.

"ORNL's vision is to sustain the nation's preeminence in science and technology by developing and deploying leadership computing for research and innovation at an unprecedented scale," said ORNL Director Thomas Zacharia. "Frontier follows the well-established computing path charted by ORNL and its partners that will provide the research community with an exascale system ready for science on day one."—*Morgan McCorkle*

Logging the miles

ORNL's *Transportation Energy Data Book: Edition 37* reports that the number of vehicles nationwide is growing faster than the population, with sales of more than 17 million since 2015, and that the average household vehicle travels more than 11,000 miles per year.

ORNL researchers compile transportation data from 50 existing sources for DOE, analyzing trends in petroleum, energy, light vehicles (cars, sport utility vehicles, pick-up trucks), heavy trucks, household vehicle characteristics and alternative fuel. This tool provides accurate data on transportation activity that can help inform policy makers and analysts.

"Cars and light trucks account for a significant amount of energy consumption, using 59% of all transportation energy," said Stacy Davis of ORNL's Energy and Transportation Science Division. "Transportation also accounts for almost 16% of all household expenditures."

The annual *Transportation Energy Data Book* is available as a user-friendly online reference.—*Jennifer Burke*

ORNL's More elected fellow of Microscopy Society of America

ORNL researcher Karren More has been elected fellow of the Microscopy Society of America.

Karren More

The MSA fellowships honor those "who have made significant contributions to the advancement of the field of microscopy and microanalysis through a combination of scientific achievement and service to the scientific community and the society itself."

More, who leads the Electron and Atom Probe Microscopy Group in ORNL's Center for Nanophase Materials Sciences, was cited "for her innovative studies of materials for polymer electrolyte membrane fuel cells through the use of advanced analytical microscopy methods."

Her research focuses on using advanced electron microscopy to understand the structure and chemistry of nanomaterials related to their properties of performance, stability and durability. The CNMS is a DOE Office of Science User Facility.—*Bill Cabage*

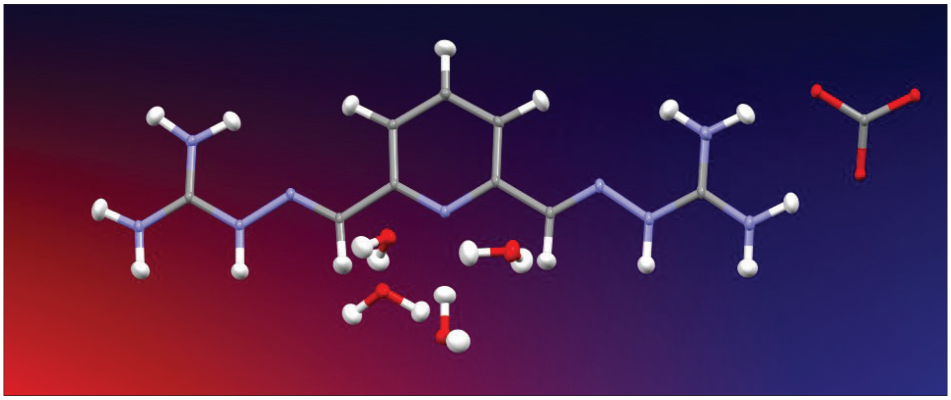
Capturing carbon in midair

Researchers used neutron scattering at ORNL's Spallation Neutron Source to investigate the effectiveness of a novel crystallization method to capture carbon dioxide directly from the air.

Previous studies have demonstrated the feasibility of using an aqueous solution that absorbs carbon dioxide and converts it into insoluble carbonate salt crystals.

"Neutrons from the TOPAZ beamline, which is optimal for locating hydrogen atoms in materials, provided us with precise structural parameters and hydrogen bonding geometries in these crystals, helping us understand the factors determining the low solubility of the carbonate salt and the efficacy of the carbon dioxide capture," said Radu Custelcean of ORNL's Chemical Sciences Division.

Further development could provide a scalable, eco-friendly path to lowering greenhouse gas emissions in the atmosphere, which can help mitigate climate change. The research was published in the *International Union of Crystallography Journal*. The study also included X-ray electron density analysis performed at the University of Toledo.—*Jeremy Rumsey*



Using neutrons from the TOPAZ beamline, which is optimal for locating hydrogen atoms in materials, ORNL researchers observed a single-crystal neutron diffraction structure of the insoluble carbonate salt formed by absorption of carbon dioxide from the air. Image credit: Radu Custelcean and Xiaoping Wang, ORNL

ORNL hosts symposium on quantum networking

Quantum experts from across government and academia descended on ORNL January 16 for the lab's first Quantum Networking Symposium.

The symposium's purpose, said organizer Nick Peters, leader of ORNL's Quantum Communication Team, was to gather quantum and classical networking expertise to better strategize and align capabilities with the nation's needs.

The one-day event featured talks by researchers from ORNL and several universities on various aspects of quantum networking—from components such as integrated optics and ion traps to larger fiber optical networks used for quantum secure communications.

"We have brought together scientists with expertise in the crucial areas which need to progress and interoperate for quantum networks to become a reality," said Peters, who also leads ORNL's Quantum Communications Team.

ORNL was chosen as the setting for the symposium because of its decades of experience in photonic entanglement, quantum communications, quantum networking and quantum key distribution. Because quantum research is inherently interdisciplinary, the laboratory has extensive expertise across its scientific groups, in addition to a concentration within the Quantum Information Science Group, where the Quantum Communications Team resides. The distribution of staff and expertise encourages a culture of deep collaboration.—*Scott Jones*

For more information: https://go.usa.gov/xESN8

ORNL's Hadjerioua elected ASCE fellow

ORNL researcher Boualem Hadjerioua has been elected fellow of the American Society of Civil Engineers.

Boualem Hadjerioua.

Hadjerioua, leader of the Water-Energy Technology Group in ORNL's Environmental Sciences Division, is a water systems engineer focusing on innovations in hydropower and pumped storage research and development. His research advances technologies that address challenges and opportunities in the use of water and energy resources.

ASCE selects fellows from among the top 3% of their membership based on members' contributions to the profession and development of "creative solutions that change lives around the world."—*Bill Cabage*

When air becomes wood

Higher carbon dioxide levels caused 30% more wood growth in young forest stands across the temperate United States over a decade, according to an ORNL-led analysis.

Scientists examined large-scale experimental plots using mixed model analysis to determine if carbon dioxide caused growth in fast turnover tissues such as roots and leaves or if it resulted in

Trees in an ORNL plot and others across the United States were exposed to elevated levels of carbon dioxide. An analysis of four experimental forests shows woody biomass increased 30% over a decade compared with trees in the current atmosphere. Credit: Jeff Warren, ORNL

trees with taller, wider trunks that capture and hold carbon dioxide in the wood.

"We used methods that take site-to-site variation into account and give a population-level result," said Anthony Walker of ORNL's Environmental Sciences Division. "This provided an estimate of the broader response of these ecosystems to the atmospheric carbon dioxide concentrations of the future."

Studying these changes on a decadal scale improves climate modeling. The findings, published in *Nature Communications*, are an outcome of DOE's carbon dioxide enrichment experiments.—*Kim Askey*

AI matches patients with clinical trials

A team of researchers from the ORNL Health Data Sciences Institute has harnessed the power of artificial intelligence to better match cancer patients with clinical trials.

The research team was among 10 teams to develop a digital tool to address complex challenges relevant to medical conditions such as cancer and Lyme disease as part of The Opportunity Project Health Sprint, a 14-week effort sponsored by the Census Bureau, coordinated by the Department of Health and Human Services, and led by two Presidential Innovation Fellows.

The TOP tools rely on emerging technologies and were built using open data from governmental agencies such as the National Cancer Institute and the Department of Veterans Affairs. The sprint was intended to strengthen collaborations among technologists, issue experts and community leaders to address real-world challenges and improve patient lives.

"One of the major obstacles facing cancer trial eligibility is the unstructured nature of the data," said Ioana Danciu, ORNL's TOP Project lead. "Artificial intelligence and natural language processing tools refine and advance the process of matching cancer patients to promising clinical trials."

The team, which includes Georgia Tourassi, Blair Christian and Shamimul Hasan of ORNL's Computational Sciences and Engineering Division, developed a novel knowledge graph that presents information in a way that enables researchers to construct tools to extract meaningful information from vast reams of unstructured text.—*Scott Jones*

For more information: https://go.usa.gov/xES9G

Elements at extremes

In neutron star mergers and supernovae, lighter elements absorb neutrons to create heavier elements with neutron-rich, radioactive nuclei.

To better understand this phenomenon, physicists turned to the tin isotope Sn-132, colliding it with a target at ORNL to assess its properties as it lost a neutron to become Sn-131. The results, published after years of complex data analysis, were combined with a prior experiment in which a nucleus of Sn-132 gained a neutron to become Sn-133.

"Many ambiguities are reduced by systematically studying the addition and subtraction of neutrons," said ORNL's Steven Pain. "This is the first time this technique has been applied to such a heavy neutron-rich nucleus. These results will help benchmark theoretical models and guide future investigations of unstable nuclei with even greater neutron surpluses."

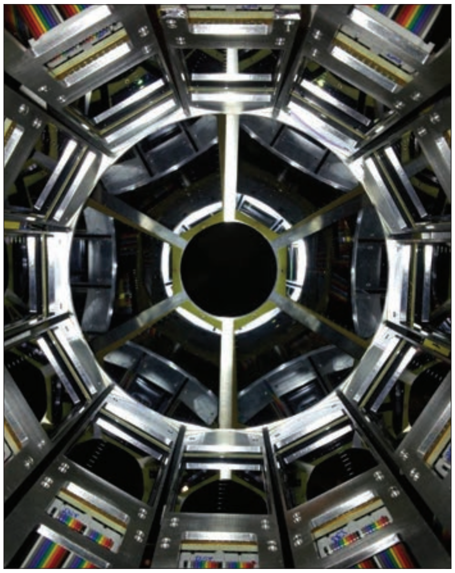
The experiment was the last conducted at ORNL's Holifield Radioactive Ion Beam Facility before it ceased operations in 2012.—*Dawn Levy*

Social media mining

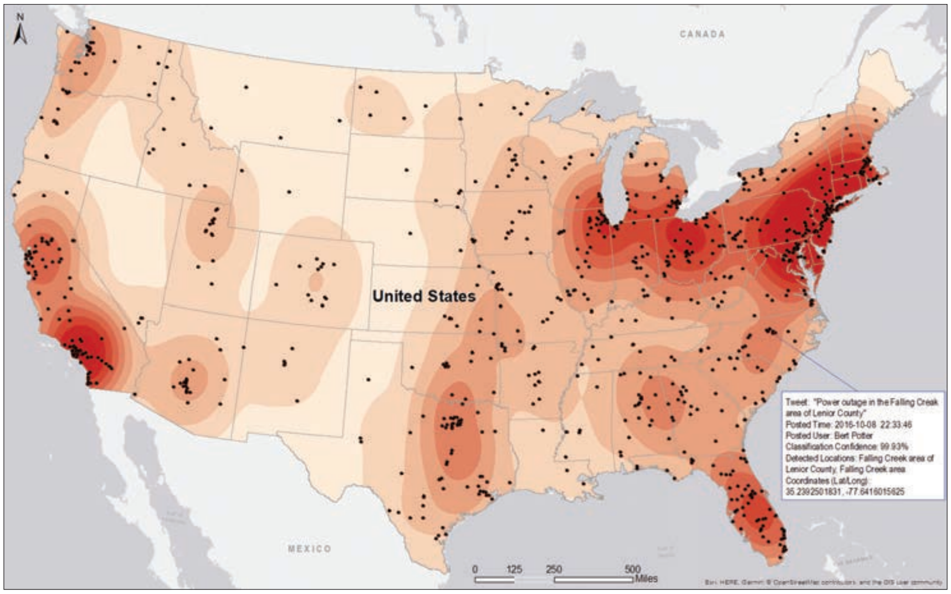
Gleaning valuable data from social platforms such as Twitter—particularly to map out critical location information during emergencies—has become more effective and efficient, thanks to ORNL.

In a preliminary study, geospatial scientists at ORNL built a classification model that can quickly collect, sift through and store large amounts of data—including relevant text, sensor data and images—and automatically detect where a power outage has occurred.

"For this data to be useful in an emergency, it needs to be validated and made available to utility companies or first responders in real time," said Gautam Thakur of ORNL's National Security



Position-sensitive silicon detectors form the "nerves" of the Super Oak Ridge Rutgers University Barrel Array and yield high spatial resolution that enabled the Sn-132 experiment at ORNL—the first neutron-removal reaction on such a heavy, neutron-rich nucleus. Image credit: Steven Pain, ORNL



As part of a preliminary study, ORNL scientists used critical location data collected from Twitter to map locations of certain power outages across the United States. Image credit: ORNL

Emerging Technologies Division. "We developed algorithms through deep-learning methods, ran them on customized hardware and mechanisms designed by ORNL, and successfully extracted outage and location information from informal social media text in near-real time."

This demonstration focused on power outages, but the method could be extended to other disaster analysis.—*Sara Shoemaker*

Company licenses tech that turns CO_2 into ethanol

ReactWell, LLC, has licensed a novel waste-to-fuel technology from ORNL to improve energy conversion methods for cleaner, more efficient oil and gas, chemical, and bioenergy production.

ReactWell will bring ORNL's electrochemical process, which converts carbon dioxide directly into ethanol, into the company's existing conversion solution known as the ReactWell process.

The brainchild of inventor Brandon Iglesias of ORNL's Center for Nanophase Materials Sciences, the ReactWell process is a research and development project involving a reaction that converts organic material to synthetic crude oil. Refineries can use it to upgrade their feedstock or convert biomass to oil.

ORNL's method involves nanofabrication and catalysis science, using tiny spikes of carbon and copper to turn the greenhouse gas into a sustainable liquid.

"Our team's process is complementary to other refining techniques by providing a means to recycle carbon dioxide that would otherwise be released," said ORNL's Adam Rondinone, coinventor of the carbon dioxide-to-ethanol catalyst.—*Sara Shoemaker*

For more information: https://go.usa.gov/xESX3

Speedy motor modeling

ORNL scientists have created open-source software that scales up analysis of motor designs to run on the fastest computers available, including those accessible to outside users at the Oak Ridge Leadership Computing Facility.

The Oak Ridge Software Toolkit for Electromagnetic Devices, or OeRSTED, can be used to design lightweight, low-cost, powerful electric vehicles of the future. This research depends on quickly calculating a challenging mix of electromagnetics and materials for motors with unmatched accuracy.

"What used to take months to design can now take a week or even a day on a supercomputer," said Jason Pries of ORNL's Electrical and Electronics Systems Research Division, who has used the lab's supercomputers to design a motor without rare earth magnets—resolving a critical materials issue for EVs.

The software is available for download at https://code.ornl.gov/p7k/Oersted/wikis/home.—*Stephanie Seay*

Laminations such as these are compiled to form the core of modern electric vehicle motors. ORNL has developed a software toolkit to speed the development of new motor designs and to improve the accuracy of their real-world performance. Image credit: Carlos Jones, ORNL

Quantum of science

Exploring little particles with big promise

by Leo Williams
williamsjl2@ornl.gov

You could say that the quantum science revolution began with a lightbulb, or at least the challenge of making a more efficient one.

The 19th century was closing down, Thomas Edison had patented a longer-lasting incandescent bulb, and each of the world's industrial powers wanted to be at the forefront of this rapidly expanding technology.

Unfortunately for them, they weren't quite sure how a lightbulb worked. They knew, of course, that any object will glow if it gets hot enough—whether it be a lightbulb filament or a fire iron—and will cycle through a well-known sequence of colors as its temperature rises, from red to orange to yellow and, eventually, blue-white. But they could not divine the relationship between temperature and color, especially at higher frequencies. As a result, scientists and inventors were hard-pressed to design a bulb that maximized the light it emitted while minimizing the amount of electricity it required.

Planck starts the quantum ball rolling

The answer came from German physicist Max Planck. In 1900, Planck developed a theoretical foundation for the relationship between temperature and color using what he assumed was nothing more than a mathematical trick. It was commonly understood at the time that light traveled in waves rather than particles, yet to come up with his answer, Planck was forced to assume that light was emitted in little packets.

With this approach, he launched the field of quantum mechanics, though he didn't realize it at the time. Instead, he and his colleagues saw his approach as a stopgap that would soon yield to the real answer.

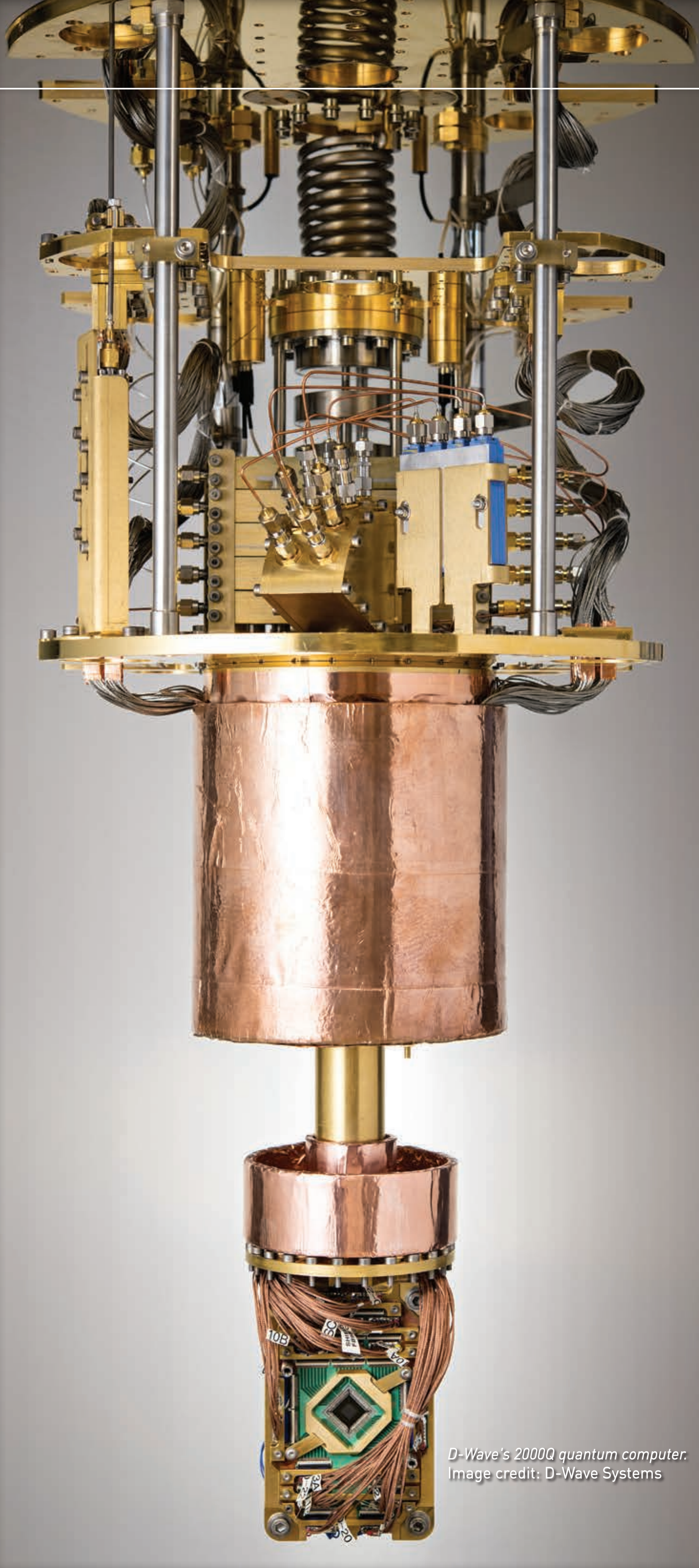
Einstein jumps in

The next step in the evolution of quantum science came from Albert Einstein. In 1905—the same year he introduced both special relativity and science's most famous equation, $E=mc^2$—Einstein published a paper suggesting that Planck's insight was more than mathematical sleight of hand and that light was indeed absorbed and emitted in little packets, or quanta. These quanta would come to be known as photons.

It took several years, but the scientific community eventually accepted Einstein's light quanta and the implications that came with it. As a result, Planck, Einstein and colleagues would uncover a new set of rules for matter at the scale of atoms and smaller.

At this scale—the nanoscale—the world becomes very strange:

- Particles behave like waves.



D-Wave's 2000Q quantum computer.
Image credit: D-Wave Systems

- It's impossible to know both the exact position of a particle and its momentum at any given time.
- A particle can be in two independent states at the same time.
- Particles can become entangled so that a change to one will affect others, even if they're hundreds of miles apart.

As one of the field's pioneers, Niels Bohr, put it, "Anyone who is not shocked by quantum theory has not understood it."

Quantum mechanics in the 21st century

For all its strangeness—or perhaps because of it—quantum mechanics holds enormous technological promise. Computers built on the unique rules of quantum mechanics have the potential to solve problems that are literally unsolvable on even the most powerful traditional computers. Quantum key distribution seems poised to bolster information security, and materials built on the interactions of quantum particles form the basis of extremely sensitive detectors.

Governments are recognizing the value of quantum science as well. On Dec. 21, President Trump signed the National Quantum Initiative Act, which calls for a 10-year plan and $1.25 billion to beef up the country's efforts in quantum information science and technology.

Introducing the qubit

Quantum computers are built on qubits (pronounced CUE-bits), which are both analogous to the bits that control your home computer and fundamentally different. While bits can have only one of two values—typically expressed as 0 or 1—qubits can be 0, 1, or a combination of both. So while a bit can have one of only two values, a qubit is in one of essentially an infinite number of values.

Another odd characteristic of qubits and other quantum particles is that they can be entangled. Entanglement can be useful for a researcher performing a quantum calculation, but it can be a wonder for secure communications.

"Entanglement is monogamous," explained ORNL Quantum Communications Team lead Nicholas Peters. "If entanglement is maximal between two qubits, then any third qubit cannot be correlated to the first two. This property allows us to perform quantum key distribution without a third party being able to guess the key, which enables secure communications."

Finally, qubits and other quantum particles are very, very sensitive to their environment. For a computer scientist, this is a real challenge, because anything from a solar storm to an insufficiently chilled

See QUANTUM OF SCIENCE, page 14

Quantum computing is ideal for quantum problems

by Leo Williams
williamsjl2@ornl.gov

The promise of computers that exploit the strange behavior of subatomic particles has tempted scientists for decades.

In time, quantum computers will likely tackle problems that are difficult or even impossible to solve on a traditional computer—from simulating the behavior of electrons and molecules to advancing artificial intelligence—but daunting challenges must be overcome first.

Building on qubits

The basic unit of computing on a quantum computer is known as a qubit (short for "quantum bit" and pronounced CUE-bit). A qubit is comparable to the bits that govern your day-to-day computer, but there are important differences owing to the quantum mechanical nature of qubits.

For example, a bit (short for "binary digit") must be one of two values, usually stated as 0 and 1. But qubits, because they are quantum mechanical, don't have that restriction. The quantum principle of superposition means a qubit can be a 0, a 1, or some combination of both. As a result, a qubit can represent any one of an essentially limitless range of possible values.

In addition, qubits are subject to quantum entanglement, a special case of superposition in which the two-qubit state is well defined but neither individual state has definite properties. This allows qubits and other quantum particles to establish strong quantum correlations over long distances.

Quantum computers for quantum problems

Researchers have been intrigued by the possibility of quantum computing at least since the early 1980s, going back to the colorful Caltech physicist Richard Feynman's declaration that "nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical."

Nearly 40 years later, experts agree that the quantum world of molecules, atoms and electrons does indeed present an especially fertile ground for this evolving technology.

"A quantum computer is really good at solving quantum mechanics problems," explained ORNL quantum computing scientist Travis Humble.

"So finding what an electron in a molecule is doing—quantum computers are good at that. Looking at the electronic structure of the molecule—the different low-energy levels it has—that information is what we use in chemical reactions."

These problems are especially challenging for classical computers because quantum systems are, by their nature, uncertain. If an electron were a classical particle, for instance, its internal magnet—or spin—would point either up or down, and all you needed to know about that spin could be recorded in a single bit's value of 0 or 1.

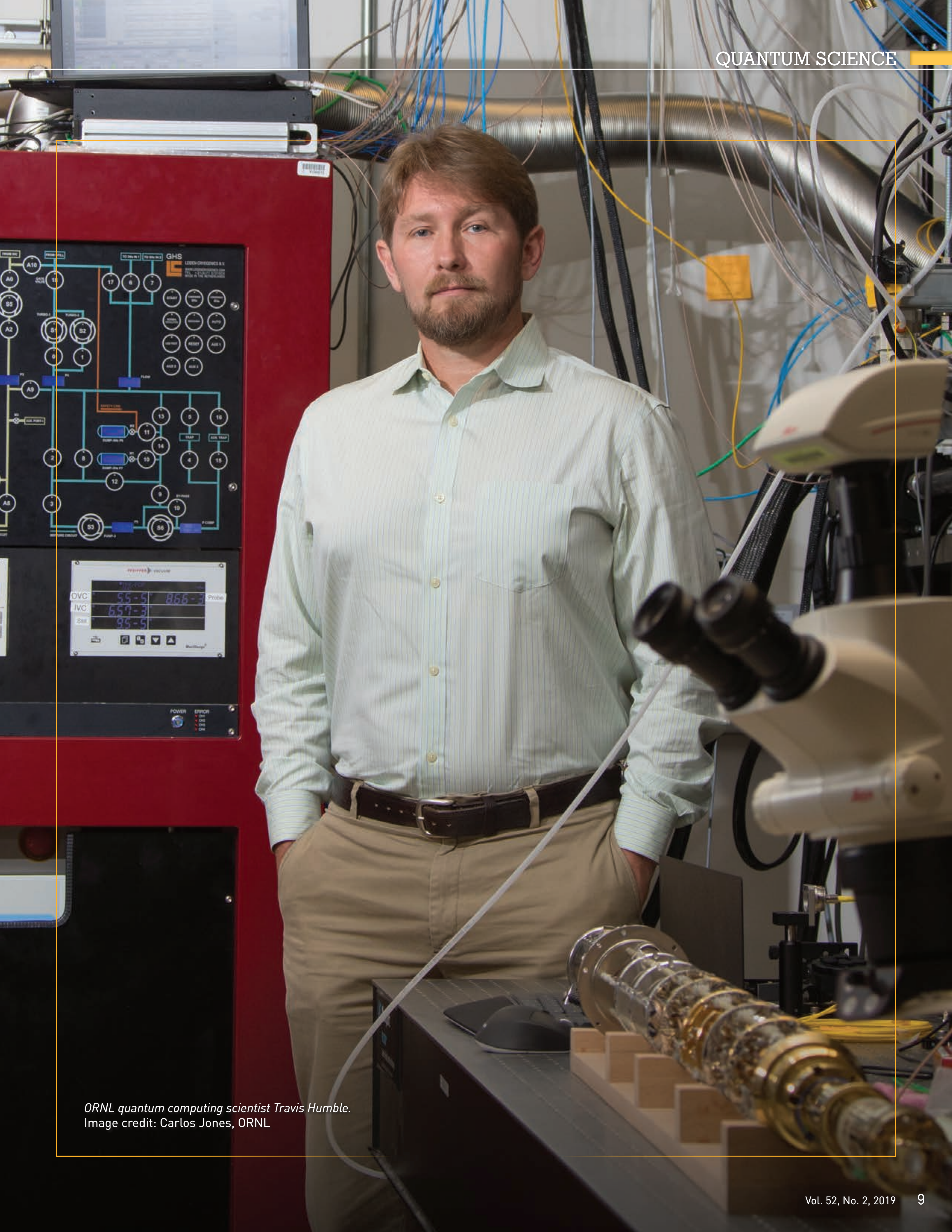
But that electron is not classical, it's quantum, meaning its spin can be up, down, or a combination of both. So, to even begin simulating the complexity of a quantum system, a classical computer must be very powerful and have a vast amount of memory.

Qubits, on the other hand, can more easily reflect the nature of a quantum system because qubits are themselves uncertain.

"Exponential growth is naturally accounted for if you're using quantum systems to simulate quantum systems," explained ORNL quantum information researcher Pavel Lougovski. "You don't have to parse it into classical bits."

Humble noted that quantum computing is also promising in areas like computational chemistry, where the correlated behavior of an atom's nucleus and its electrons determines the

See QUANTUM COMPUTING, page 14



ORNL quantum computing scientist Travis Humble.
Image credit: Carlos Jones, ORNL

New materials

for sensors, computers, encryption and more

by Leo Williams
williamsjl2@ornl.gov

Quantum mechanics may give us powerful computers, but that's not the whole story. Researchers working in the nanoscale world of atoms and molecules are also exploring a variety of materials that show promising, if odd, behaviors because of their quantum mechanical interactions.

With names like spin ice, quantum spin liquid and topological insulator, quantum materials have been around for decades, yet we don't have a universally agreed-upon definition of what the term means. One accepted definition revolves around the behavior of electrons.

> *"A lot of what I've done in the past is make microscopes do things they're not traditionally supposed to do."*
>
> — ORNL materials scientist **Stephen Jesse**

"Quantum materials represent a class of materials that exhibit emergent physical properties due to the quantum mechanical interaction of electrons," explained Ho Nyung Lee, ORNL program manager for the Materials Sciences and Engineering Program of DOE's Basic Energy Sciences.

"The recent rise of interest in quantum materials focuses on uncovering the role of properties that can ultimately provide the avenue to quantum information science and computing. ORNL's materials science research is well positioned to take advantage of synthesis, theory, computation, imaging and neutron scattering."

A spin ice, for example, is not ice as such. In this material, the electrons' magnets, or spins, form a series of connected three-sided pyramids that reminded researchers of actual ice. By the same token, quantum spin liquids are not really liquids. Rather, the structure of their electrons—which are entangled but not ordered—reminds researchers of water.

Topological insulators, on the other hand, are materials that can be distorted without losing their shape. While electrons within the material cannot move, electrons at its edge can.

Exploiting quantum materials

Quantum materials have a variety of potential uses—in novel sensors or powerful quantum computers, for instance—but they no doubt have uses that we haven't even considered yet. According to Steve Nagler, a corporate fellow in ORNL's Neutron Scattering Division, this research is far too early in its development for us to have a clear idea of where it will lead.

"We are at the point of trying to achieve an understanding, and that understanding has moved forward and forward during the intervening years," Nagler said. "Some of these systems could be useful for quantum information systems, and they could be useful for other things. You learn along the way."

He pointed to the evolution of transistors dating back to the 1930s and '40s to illustrate the point.

"That was the same stage as this; it was just basic research. And they worked out the quantum mechanical solu-

See NEW MATERIALS, page 15

ORNL's Clarina dela Cruz uses the lab's neutron scattering facilities to examine quantum materials. Image credit: Carlos Jones, ORNL

Cooking up quantum materials

by Leo Williams
williamsjl2@ornl.gov

Before researchers can experiment with a promising new quantum material, someone has to produce it.

That's where ORNL's Correlated Electron Materials Group comes in. The group uses its lab facilities to manufacture a variety of materials that are attractive to quantum scientists.

> *"The nice thing about Mother Nature is that if you pay attention, sometimes what she gives you may be more interesting than what you were actually trying to grow."*
>
> — ORNL Correlated Electron Materials Group leader **Brian Sales**

"The materials we are interested in are materials that have some functionality," explained group leader Brian Sales. "They're materials that, for instance, become magnetic or become superconducting or have strange topological protected edge states or ground states."

The group pursues a variety of materials, including spin ices, quantum spin liquids and topological insulators (see "New materials for sensors, computers, encryption and more," page 10). Part of the group's job is to decide which materials look the most promising.

"We take input from theory and theoretical calculations," Sales said. "We use crystal chemistry rules. We use experience and intuition to try to select these materials. But there's a certain amount of serendipity involved as to whether the material you select is really going to be interesting and exciting."

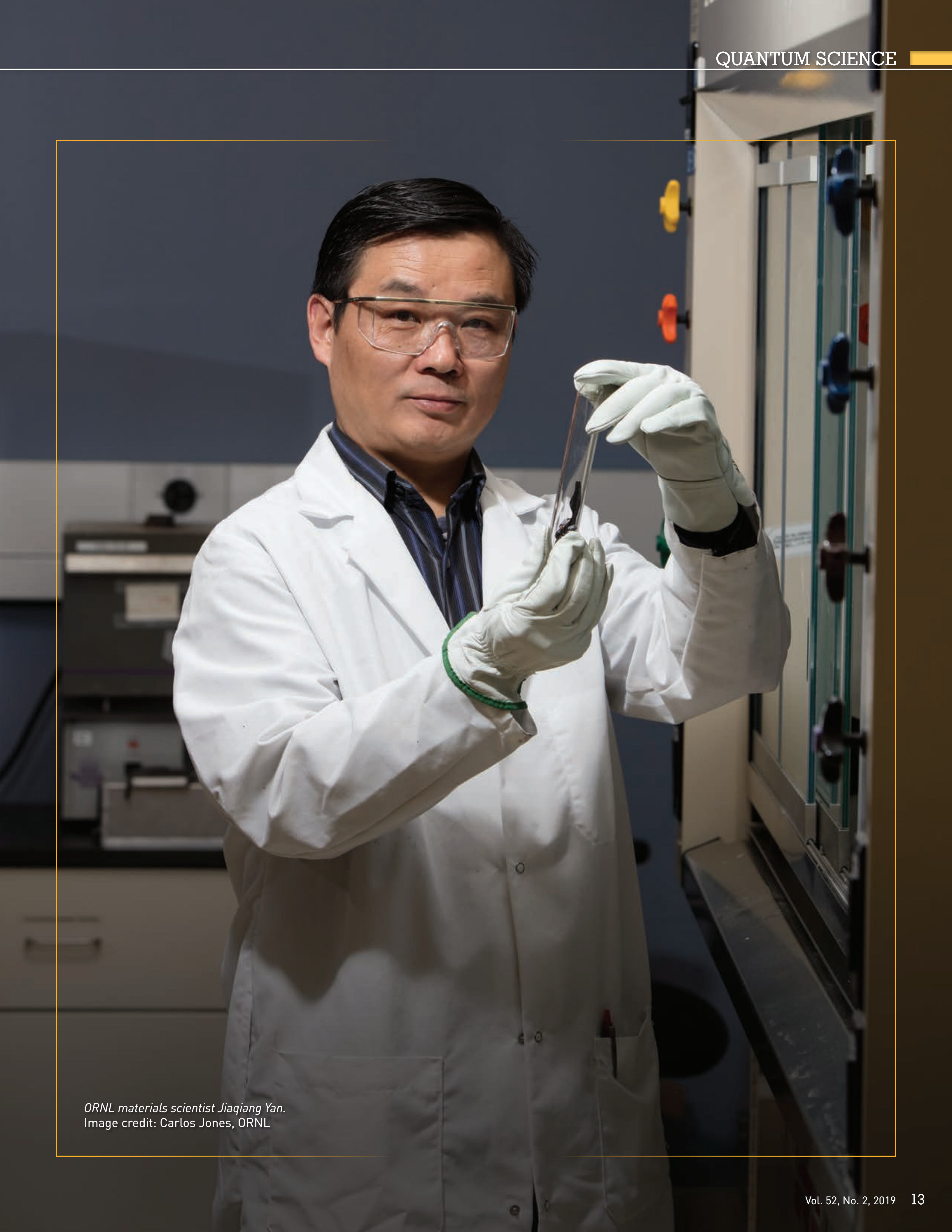
Often, the atoms in an interesting material will be structured in triangular or hexagonal structures that frustrate the magnets—or spins—of individual electrons. Many will also be 2D, with layers only a few atoms thick. As an example, Sales pointed to chromium triiodide, with one chromium atom and three iodine atoms.

"That was grown here as a single crystal, but it grows in layers," he said. "It's similar to the structure of graphene, except you have chromium. So it's kind of a magnetic version of graphene in some sense, and it's very easy to cleave, just like graphene is."

The group has a variety of methods for producing these materials. One—precipitating the crystals out of solution—is similar to the process of dissolving salt in hot water and then letting crystals form as the water cools. But in the crystals produced by Sales and his group, the material is most often dissolved in something like molten tin rather than water, with a temperature a little over 2,000 degrees Fahrenheit rather than 100 or 120 degrees.

In another production method—vapor transport growth—the ingredients are placed in a sealed quartz tube that's hotter at one end than the other, and the crystals are allowed to condense from the vapor phase at the cooler end. And in a third method—production directly from a melt—the material is kept just above its melting temperature, and a cooler tip is slowly pulled out of the liquid material, hopefully pulling a large crystal behind.

See COOKING UP, page 17



ORNL materials scientist Jiaqiang Yan.
Image credit: Carlos Jones, ORNL

QUANTUM OF SCIENCE, page 6

component can destroy your calculation. But for the development of sensors, this can be a boon.

"Any kind of disturbance can knock these guys out of states that they need to be in," ORNL materials scientist Stephen Jesse said. "Because of that, they might be really great sensors. Certainly, for very weak electromagnetic radiation—maybe really weak microwave signals that come from deep space, maybe gravitational waves."

"Anyone who is not shocked by quantum theory has not understood it."

— Quantum mechanics pioneer **Niels Bohr**

The promise of quantum computing ...

The promise of quantum computing is especially exciting to scientists who are bound by the limits of traditional computers, even supercomputers as powerful as ORNL's Summit system, the world's most powerful for the past year.

"Classical computing is defined by Boolean algebra and the ability to add numbers—and do it in zeroes and ones," explained David Dean, ORNL's associate laboratory director for physical sciences. "But there are certain types of problems that can't be solved on a classical computer."

... and the challenge

To get to quantum computers that can solve these problems, however, scientists and engineers will have to overcome enormous challenges—from the fragility of quantum processors that can be rendered useless by something as seemingly inconsequential as an inadequately chilled wire to the fundamental uncertainty of any quantum system.

"The computers we have today are perfect—they rarely mess up," Dean said. "When you add one plus one, you will always get two. The gate fidelity in a classical computer is more than 99.99999 percent correct.

"On the other hand, a single qubit gate—which takes two qubits—is probably at 99.999 percent today. But the minute you have more than a couple of qubits, you get errors. And it's natural, it's inherent, because quantum mechanics is not a definitive—it allows for probabilistic distributions of the particles in some ways."

Computer science will have to adapt

Quantum information science will be fundamentally different not only for the machines, but for the people as well, explained ORNL quantum computer scientist Travis Humble. In fact, computer scientists will have to add a new area of expertise if they expect to work in the field.

"Even if these computers overcome the technical challenge, who's going to use them?" Humble said. "Right now, you have to understand what a qubit is, you have to understand how to program those types of interactions between qubits, and you have to understand the algorithms, which are completely new. If we build these systems and nobody uses them, then it was all for naught.

"We need the physicists to figure out what are the good materials to use for quantum computers. We need the engineers to actually build the devices that can scale up and have low noise levels, and we need the computer scientists to use the devices to solve real problems."

QUANTUM COMPUTING, page 8

stability of a molecule. As an example, he noted that advances in quantum computing may enable scientists to discover more efficient methods to synthesize novel chemicals.

"Finding energy-efficient pathways for molecular synthesis is a hard computational problem," Humble explained. "There are so many different ways for atoms to bond together, and the best configurations often arise from unintuitive quantum mechanical effects. But quantum computing offers a new approach to simulate how molecules react under different conditions, and we expect this to have a significant impact on computational chemistry."

A long way to go

As promising as quantum computing appears, many hurdles must be cleared before it provides important scientific discoveries. There are working quantum computers, created by tech giants such as Google, IBM and Intel as well as smaller companies such as British Columbia-based D-Wave. Yet so far these rudimentary systems serve more to advance research into quantum computing than to provide new scientific knowledge.

"The hardware that is available on the cloud, for example, has numbers of qubits that are on a par with what we can simulate classically," Lougovski said, "so there is, per se, no new science to discover, except for the science of computing—such as how we program those devices, and how we find ways to extract errors and improve the results."

"The rudimentary processors we have right now are basically physics experiments," agreed Humble. "They are almost always located in a laboratory. They do have ways to interface with some—write programs, collect answers and solutions. But it's very finicky.

See QUANTUM COMPUTING, page 16

NEW MATERIALS, page 10

tion for electrons in solids, came up with this concept of energy bands, understood how they could use that to infer what the property of the material would be, and they understood why you had metals and semiconductors and insulators.

"And once this was understood, somebody realized, hey, we can use this knowledge to make a piece of solid material that will do the same thing as a radio tube."

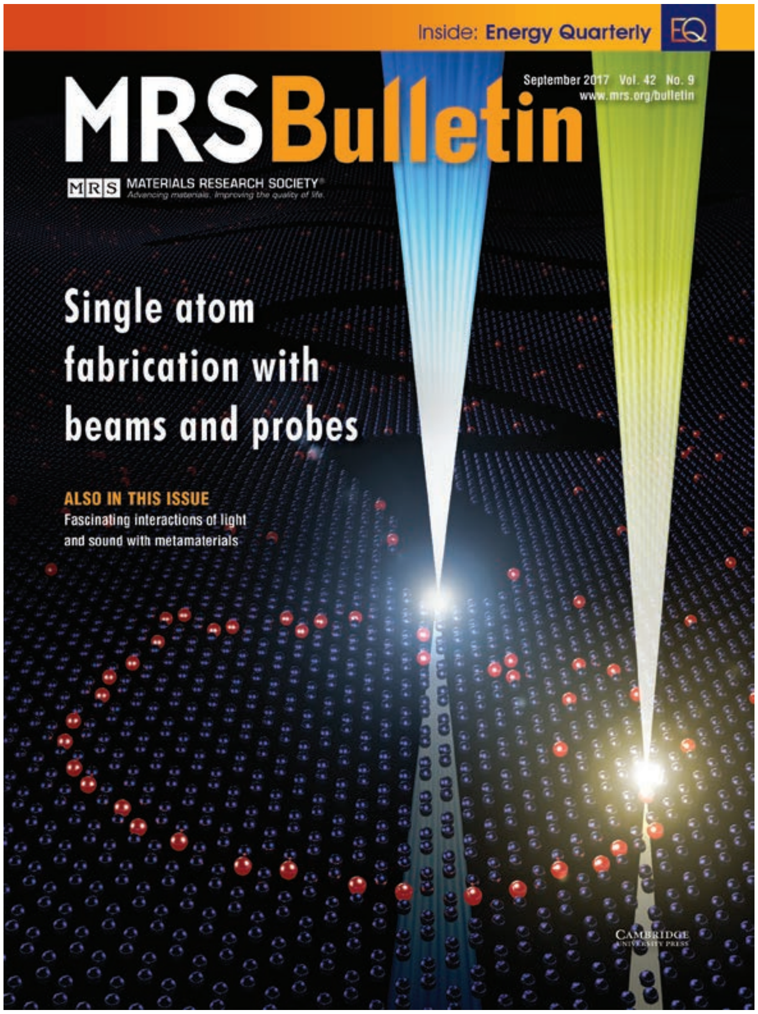
So the job ahead of modern researchers is to understand these materials better. Fortunately, ORNL has powerful tools—specifically neutron scattering facilities and high-powered microscopes—to advance that understanding.

The value of neutrons

Scattering at ORNL's Spallation Neutron Source and High Flux Isotope Reactor is an especially effective way to study quantum materials, because of neutrons' wavelengths, magnetic properties and energy.

"The key component of these quantum states is the magnetism in the material," explained ORNL neutron scattering scientist Clarina dela Cruz, "and neutrons are the most powerful tool you can have in probing magnetism in any material. This is because neutrons are chargeless; unlike electrons they have some mass, but it's small; and they have an effective magnetic moment."

According to Nagler, the neutrons used in scattering experiments have wavelengths comparable to the spaces between atoms, allowing researchers to use them effectively to study the microscopic structure of materials.



Journal cover showing an artistic rendering of scanning transmission electron microscope-based single-atom-level manipulation and fabrication of 2D materials. Electron beams can be used to cut or remove material and control the position of atoms and dopants on or within a lattice. Image credit: ©2017 Materials Research Society

The same neutrons are also advantageous for studying the motions of atoms and their associated magnetic materials, he said, because the energies of the neutrons and the atomic vibrations are very similar. This can be contrasted to X-ray photons, which are a billion times more energetic than neutrons at the wavelengths needed to study these materials.

Making materials with an electron microscope

Not only are scanning electron transmission microscopes effective at studying quantum materials, noted ORNL materials scientist Stephen Jesse, but they are also good at creating and manipulating these materials.

In particular, he said, these microscopes are especially good at creating and studying materials in which an atom of one element is placed in a lattice made up of another element. While the new atom is typically known as a defect, that is not necessarily bad. In fact, Jesse explained, such materials may be promising for use in quantum information systems.

"Defects are sometimes really, really good," he said. "These optical systems may have, say, a single defect in a material that has special quantum properties, and it emits light in a special way that can be used in a quantum sensor."

The microscope itself has two functions, he said. First, of course, it is used to image the materials, looking at atoms and the atomic structure. But, second, it can also help create the materials.

See NEW MATERIALS, page 17

QUANTUM COMPUTING, page 14

"So the question is, what do they need to get up to before they are ready for the Department of Energy, for example, to say, 'I'm going to build a supercomputing system based on quantum processors.'"

Looking for the right qubit

A qubit can be any particle or system that exhibits superposition and quantum entanglement. To date, the field is dominated by qubits consisting of superconducting circuits, yet researchers are studying a range of possibilities in the hope that one or more will be stable enough to make quantum computing practical.

> *"There are so many different ways for atoms to bond together, and the best configurations often arise from unintuitive quantum mechanical effects. But quantum computing offers a new approach to simulate how molecules react under different conditions."*
>
> — ORNL quantum computer scientist **Travis Humble**

These possibilities include tiny specks of silicon called silicon quantum dots; trapped ions, in which tiny charged particles are held in place by electromagnetic fields; and topological insulators, or materials in which electrons in the center are held in place while electrons at the edge are allowed to form a circuit.

"One major goal is to find materials systems that allow qubits to persist for long periods of time," explained ORNL materials scientist Stephen Jesse. "This may happen at particular defect sites in an otherwise perfect materials system that are inherently immune to external perturbations, or this could be in materials systems where the quantum state is 'protected.'"

Bring in the noise

The search for a more stable qubit is critical because of quantum particles' enormous sensitivity to their environments. While this makes them very promising candidates for advanced sensors, it is a serious challenge for the development of useful quantum computers. Not only must quantum computers harness the delicate states of electrons and other tiny particles, they must also prevent those particles from being disturbed by events such as vibrations, electrical fields and radiant heat.

In fact, Jesse noted, quantum computers must be kept very close to absolute zero, or below minus-450 degrees Fahrenheit. "These qubits are very sensitive to everything that happens around them. They usually have to run these computers at 20 millikelvin, just barely above Kelvin zero, because any kind of disturbance can knock these guys out of states that they need to be in."

Even something as seemingly insignificant as energy emanating from a wire running into a quantum computer can render it essentially useless, explained ORNL Quantum Communications Team lead Nicholas Peters.

"For most qubits, it's expected that we are going to end up having to have them be very, very cold," Peters said. "Just having a wire at room temperature gives you enough noise from the blackbody emission that it will basically ruin your ability to use those as qubits."

In other words, quantum computer developers must figure out how to control and read the processors while at the same time keeping them frigid.

"These are two competing processes," Lougovski said. "You would like to isolate your qubits from the environment so that they are not affected by noise, but on the other hand, you want to be able to send control and readout pulses to those systems to get the information in and out."

According to Peters, this means either generating the signal in this frigid environment or, more commonly, building an interface that carries the signal without carrying the heat.

"At each of these stages, what you end up doing is throwing a whole bunch of attenuators to block the blackbody radiation from higher up," Peters explained. "Then you also have to heatsink it to try to cool that wire down so that it doesn't shine its own blackbody radiation down further into the fridge."

A question of decoherence

These efforts are geared to keeping the qubits from collapsing—or losing their quantum states—long enough to perform useful calculations. So far, this challenge remains daunting.

While current systems can—in theory—perform around a thousand operations before they lose their information, Humble said, the number in practice is dramatically lower—around two operations. As a result, any problem that can be tackled on a quantum computer can also be tackled on a classical computer.

"Going back to the technical challenges, it's that noise. It is really an engineering problem at the moment. Lowering the noise to a level where you could get a hundredfold improvement is where the challenge is."

NEW MATERIALS, page 15

As an example, he said, researchers can use the microscope to punch a hole in graphene, which is made up of a single layer of carbon atoms. If there's carbon present around the sample, it will typically fill in the hole, but if there's a different element present, it, too, can fill in the hole.

"We are figuring out new ways to use this platform to not just image materials, but to actually transform them and add dopants and defects while we're looking at them," Jesse explained. "Our goal is to add defects and then study them and see if we can find new arrangements that give us the optical properties we want, so we're building things atom by atom."

On top of that, he said, researchers are able to use the microscope's electron beam to move specific atoms around the material.

"A lot of what I've done in the past is make microscopes do things they're not traditionally supposed to do," he said.

COOKING UP, page 12

Quality control is a very important element in the group's job, both in verifying the raw materials that they start with—because not all supplies and suppliers are equal—and in characterizing the materials that they cook up.

Sales stressed that it's not necessarily a bad thing if a material the group produces is not what they had in mind, because at this level of research, that unexpected material may actually be more valuable than the one they were trying for.

> *"We take input from theory and theoretical calculations. We use crystal chemistry rules. We use experience and intuition to try to select these materials. But there's a certain amount of serendipity involved as to whether the material you select is really going to be interesting and exciting."*
>
> — ORNL Correlated Electron Materials Group leader **Brian Sales**

"We have two instruments that are extremely important to figuring out what the heck we've made sometimes," Sales noted. "One's an X-ray machine. That gives you how the atoms are arranged, but it doesn't tell you what the chemical composition is. And then we have a little electron microscope, about the size of a tower computer. That lets us look at things pretty small, but it also has something that analyzes the elements that are there."

"The nice thing about Mother Nature is that if you pay attention, sometimes what she gives you may be more interesting than what you were actually trying to grow," he explained. "That's happened several times. So it's important to have an open mind about exactly where the research is going, because sometimes for one reason or another it goes another direction.

"That's why they call it 'research.'"

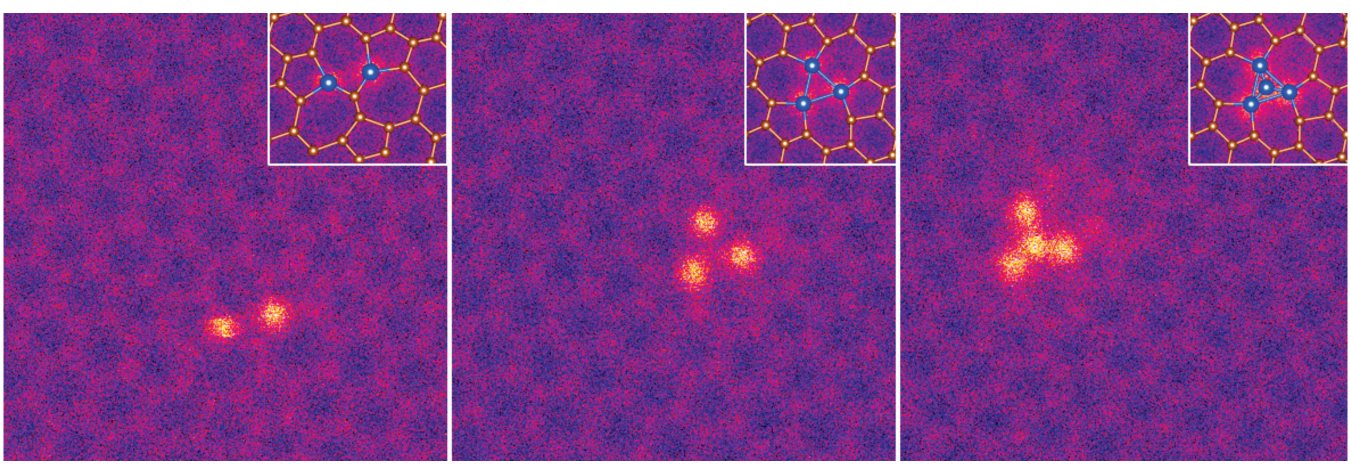


Image showing the assembly of structures at the atomic scale. Silicon atoms within a 2D graphene lattice were moved together to form two-, three- and four-atom structures. Image credit: ORNL

Company pursues unique engine design

with supercomputing

by Katie Jones
joneske1@ornl.gov

With more vehicles in use worldwide than ever before, engine makers are competing to deliver cleaner, more efficient engines at affordable prices. To gain an edge on the competition, California-based small business Pinnacle Engines is laser-focused on a unique design.

"We've been studying more or less the same engine system the entire existence of the company," said Clayton Naber, lead analysis engineer at Pinnacle Engines.

That engine—a four-stroke, opposed-piston, sleeve-valve internal combustion engine—uses an unconventional mechanical design to reduce fuel consumption without increasing emissions. To optimize their engine design, company engineers turned to ORNL's Titan supercomputer.

In a conventional internal combustion engine, a piston reciprocates, or moves back and forth, in relation to a cylinder

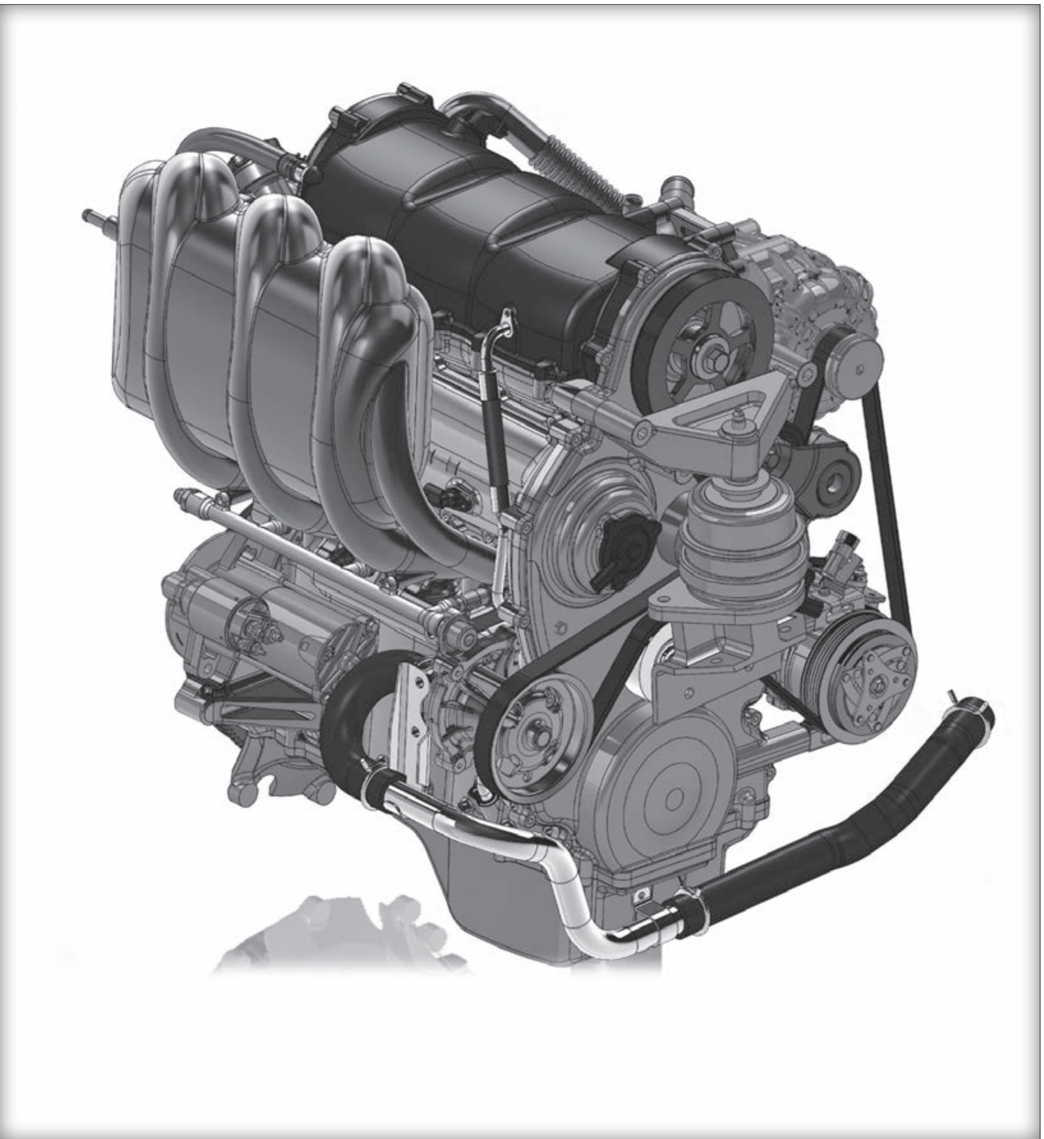
CAD models of the Pinnacle Engines opposed-piston gasoline engine. To optimize the design, Pinnacle Engines researchers used ORNL's Titan supercomputer and Eos cluster to simulate the engine's complex flow of air and fuel during combustion. Image courtesy of Clayton Naber, Pinnacle Engines head that encloses the top of the combustion chamber. In an opposed-piston engine, two pistons move in relation to each other instead of a cylinder head. This design reduces heat loss and allows for a wider range of piston motions that improve efficiency throughout operation.

> *"Part of ORNL's expertise is being able to delve into the more detailed computational physics and provide a better understanding of what is going on at the scale of combustion."*
> — ORNL researcher **Dean Edwards**

For over a decade, Pinnacle Engines has developed opposed-piston engines for small, single-cylinder applications such as motorcycles. Even though it is not the only company developing opposed-piston engines, it is among those striving to overcome the engine's engineering challenges to take advantage of its possibilities.

Now, Pinnacle Engines wants to build an opposed-piston engine for passenger cars and other light-duty vehicles. First, however, the company's engineers analyzed in detail what design choices could improve combustion efficiency and reduce emissions.

The company applied for access to national lab resources through the DOE Small Business Vouchers program, which led to a collaboration with the DOE Vehicle Technologies Office and researchers at ORNL's National Transportation Research Center.



The Pinnacle Engines team worked with NTRC researchers Charles Finney and Dean Edwards to prepare the commercial software package they were using on Pinnacle's in-house cluster for Titan's large-scale architecture.

"Part of ORNL's expertise is being able to delve into the more detailed computational physics and provide a better understanding of what is going on at the scale of combustion," Edwards said.

The team conducted thousands of computational fluid dynamics simulations on Titan and ORNL's Eos cluster to reduce the amount of time needed to survey the design space. The ORNL computations took about six months, but Naber estimates they would have taken eight times longer in-house.

Researchers simulated key design options for a multi-cylinder, 1.2-liter gasoline engine. To achieve high efficiency and low emissions, their opposed-piston design uses variable valve timing and compression ratios, as well as a gas intake method that creates a "swumble mode"—a combination of swirling and tumbling gas in the combustion chamber.

With variable valve timing and compression ratios, the pistons responsively move to adjust gas compression, optimizing combustion for different engine speeds and work outputs. The swumble mode, which was enhanced based on Titan simulations, improves fuel and air mixing and reduces fuel usage and emissions under certain operating conditions.

With a firm design concept, the team modeled the entire combustion system over typical operating conditions to evaluate whether the design could meet emissions and fuel-economy standards as well as other efficient engines on the market.

"Ultimately, we were able to find a design to achieve very low emissions while also maintaining high efficiency," Naber said. "This was a design that we did not have prior to embarking on this project."

The team is building a prototype engine for experimental testing.

"For us, it's really about commercialization next," Naber said.

ORNL team uses supercomputing to fight addiction

by Jonathan Hines
ornlreview@ornl.gov

In 2017, drug overdose deaths in the United States hit a record high, surpassing 70,000 and contributing to a drop in overall life expectancy for Americans. Most of these overdoses can be attributed to opioids, a drug class that includes prescription painkillers, heroin and synthetic drugs such as fentanyl.

Despite the grim figures, it's estimated only about 10 percent of people exposed to opioids develop an addiction. Scientists believe a major indicator of who is at risk of addiction lies in our genes.

Genes, DNA segments that encode for proteins and determine everything from eye color to height, also play a role in more complex traits such as addiction and disease. Deciphering which genes contribute to which traits, however, can be perilously complicated. An ORNL team led by computational systems biologist Dan Jacobson is poised to lead a revolution in our understanding of the role genes play in disease.

Using ORNL's Summit supercomputer, which debuted as the most powerful system in the world, the team is leveraging population-scale genomic data sets to uncover hidden networks of genes at record-breaking speeds. Its work could inform treatment for patients predisposed to substance abuse. For example, a quick genetic test at the doctor's office could one day indicate who should be prescribed alternative forms of pain management.

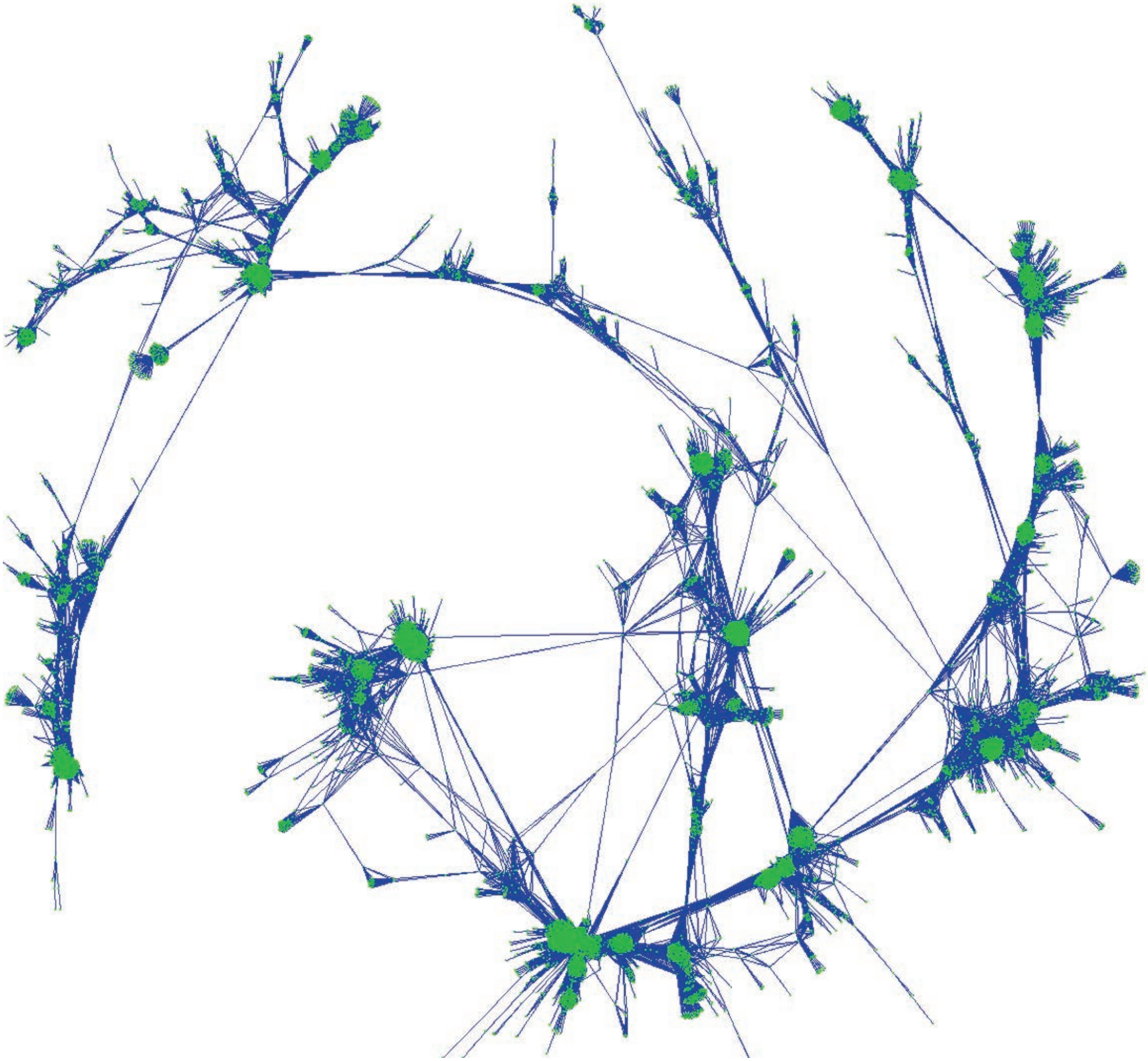
The same research could also guide treatment for other conditions, including diabetes, heart disease, Alzheimer's and dementia, and could improve practices to prevent disease from occurring in the first place.

Critical to realizing this future is growth in genomic data and advances in computing hardware. On Summit, the ORNL team's genomics application—Combinatorial Metrics, or CoMet—analyzed a large-scale data set faster than any application ever, achieving a peak throughput of 2.36 exaops—or 2.36 billion billion mixed-precision calculations a second.

"For the first time, we have the capability to discover new relationships between genes at a scale that has never been approachable before," Jacobson said.

As scientists have learned more about how genetic interaction, or epistasis, gives rise to observable traits, the human genome has come to seem less like a list of instructions and more like a hopelessly knotted ball of string.

Untangling these epistatic networks, which are composed of two or more genes, has required scientists to look beyond individual genes and to study multiple genes tested across a population. To complicate matters further, the same gene can take



A visualization of a network depicting correlations between genes in a population. These correlations can be used to identify genetic markers linked to complex observable traits. Image credit: Dan Jacobson, ORNL

on multiple forms within a population. These variations, called single nucleotide polymorphisms, or SNPs, are characterized by changes to a single nucleic acid at a specific location in the genome. The human genome contains millions of nucleic acids, the basic building blocks of DNA.

"Only when you look at mutations and the whole set of genes responsible for a complex phenotype are you going to find the sophisticated patterns we are looking for," Jacobson said.

Fortunately, Summit can untangle huge combinatorial problems like no previous system, making feasible the million billion correlations that must be calculated to test one SNP pair.

Through a partnership between ORNL and the U.S. Department of Veterans Affairs, Jacobson's team will use CoMet to analyze approximately 600,000 genomes—one of the largest human genome data sets in the world. It was compiled under the VA's Million Veteran Program, a voluntary research program focused on studying how genes affect health.

As epistatic networks are identified within population data sets, they can then be tested against known phenotypes, including opioid addiction.

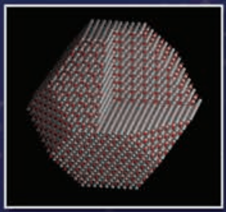
"We're really on the cusp of a whole new level of understanding," Jacobson said.

Using a Quantum Computer

Scientific use cases

Quantum computers are especially important for modeling quantum systems of atoms and subatomic particles.

Catalysts

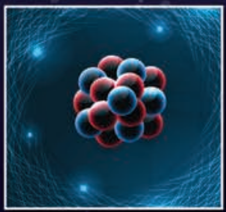


Catalysts, which promote chemical reactions without being changed by them, are used in products throughout the economy, from petroleum to margarine. The process often relies on complex quantum states as one molecule is transitioned to another.

Superconductivity

Superconductors have especially strong magnetic fields and conduct electricity without loss—as long as they are kept very cold. Superconductivity relies on the quantum relationship between electrons.

Computational chemistry



The correlated behavior of an atom's nucleus and its electrons determines the stability of a molecule, opening the door for discovering more efficient methods to synthesize novel chemicals.

Smashed atoms

The collisions created by particle accelerators cause particles to break up and scatter according to the quantum mechanical forces within them. Scientists want to discover the laws governing these fundamental states of matter.

Programming controls

Inputs must be able to control the qubits without introducing heat or other interference.

Examples of input controls include:

- Lasers
- Electric fields
- Magnetic fields

Qubits

Whereas a classical bit can be either of two values (e.g., 0 or 1), a qubit (short for "quantum bit") can be 0, 1 or a combination of both. Qubits rely on the rules of quantum mechanics (e.g., superposition, entanglement, uncertainty).

Superconduting circuit (a)

The superconducting current can behave as a qubit by flowing clockwise, counterclockwise, or a superposition of the two.

Trapped ion (b)

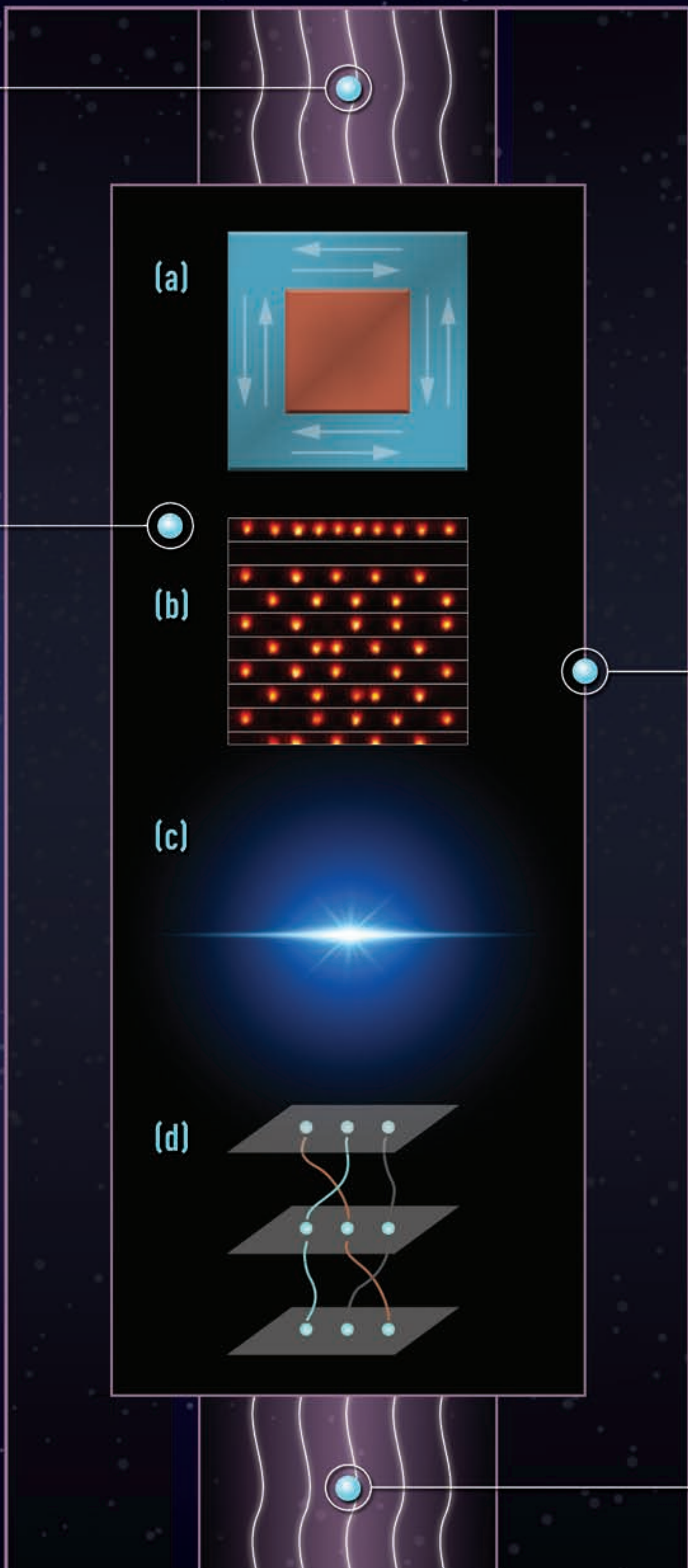
A charged particle can be suspended by electromagnetic fields, with qubits stored in its electronic states.

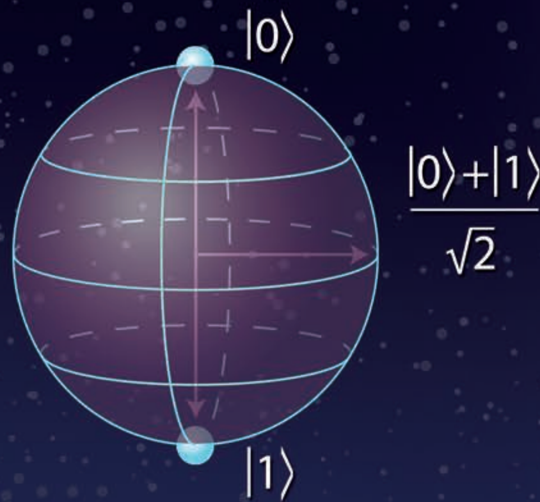
Photons (c)

Particles of light encode quantum information in their spectral and temporal properties.

Topological materials (d)

Two-dimensional materials may exhibit virtual particles—or quasiparticles—to store the quantum information.





A Bloch sphere gives a geometrical representation of a qubit.

Image credit: Brett Hopwood, ORNL

Containment

Quantum information is sensitive to noise and must be protected to minimize interactions with the environment that contribute to decoherence.

Electromagnetic interference

Containment must shield electronic and magnetic noise.

Vibration

Containment must minimize vibrational motion.

Heat

Quantum computers are cooled to sub-Kelvin temperatures (i.e., close to absolute zero, or –459.67°F) to reduce vibrations even further.

Result

The computation ends with a measurement of the quantum state to produce the classical result of the program.

UT–ORNL team measures accelerator beam

in six dimensions

by Jeremy Rumsey
rumseyjp@ornl.gov

The first full characterization measurement of an accelerator beam in six dimensions will advance the understanding and performance of current and planned accelerators around the world.

A team led by researchers at the University of Tennessee conducted the measurement in an ORNL beam test facility using a replica of the Spallation Neutron Source's linear accelerator, or linac. The details are published in the journal *Physical Review Letters*.

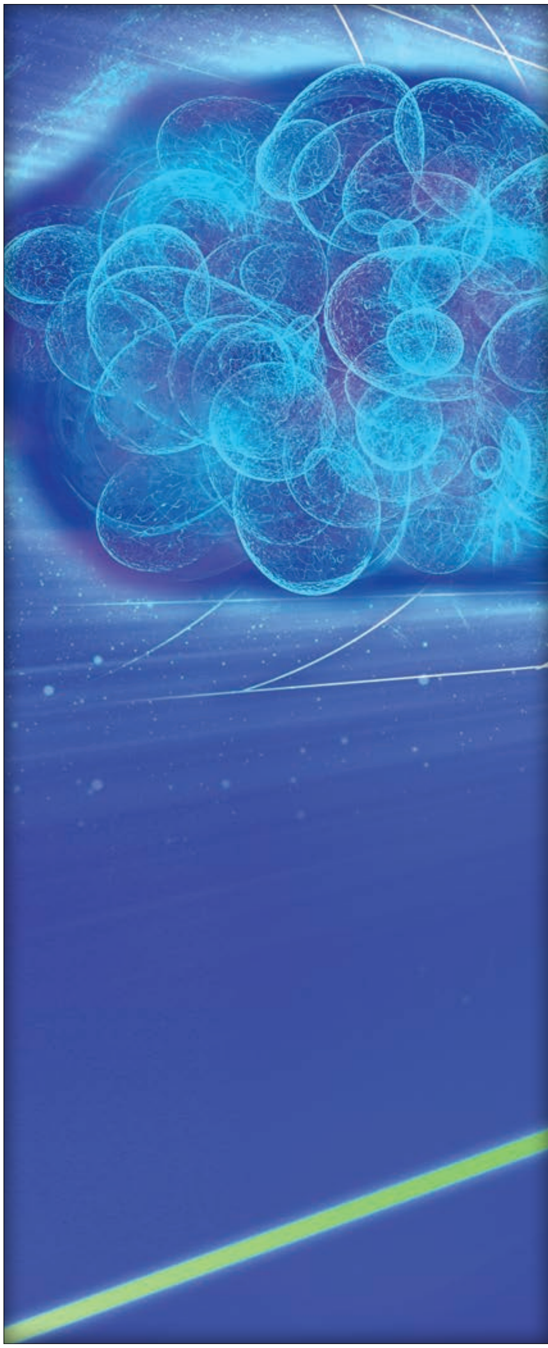
"Our goal is to better understand the physics of the beam so that we can improve how accelerators operate," said Sarah Cousineau, group leader in ORNL's Research Accelerator Division and UT joint faculty member. "Part of that is related to being able to fully characterize or measure a beam in 6D space—and that's something that, until now, has never been done."

Six-dimensional space is like 3D space but includes three additional coordinates on the x, y, and z axes to track motion or velocity.

"Right away we saw the beam has this complex structure in 6D space that you can't see below 5D—layers and layers of complexities that can't be detangled," Cousineau said. "The measurement also revealed the beam structure is directly related to the beam's intensity, which gets more complex as the intensity increases."

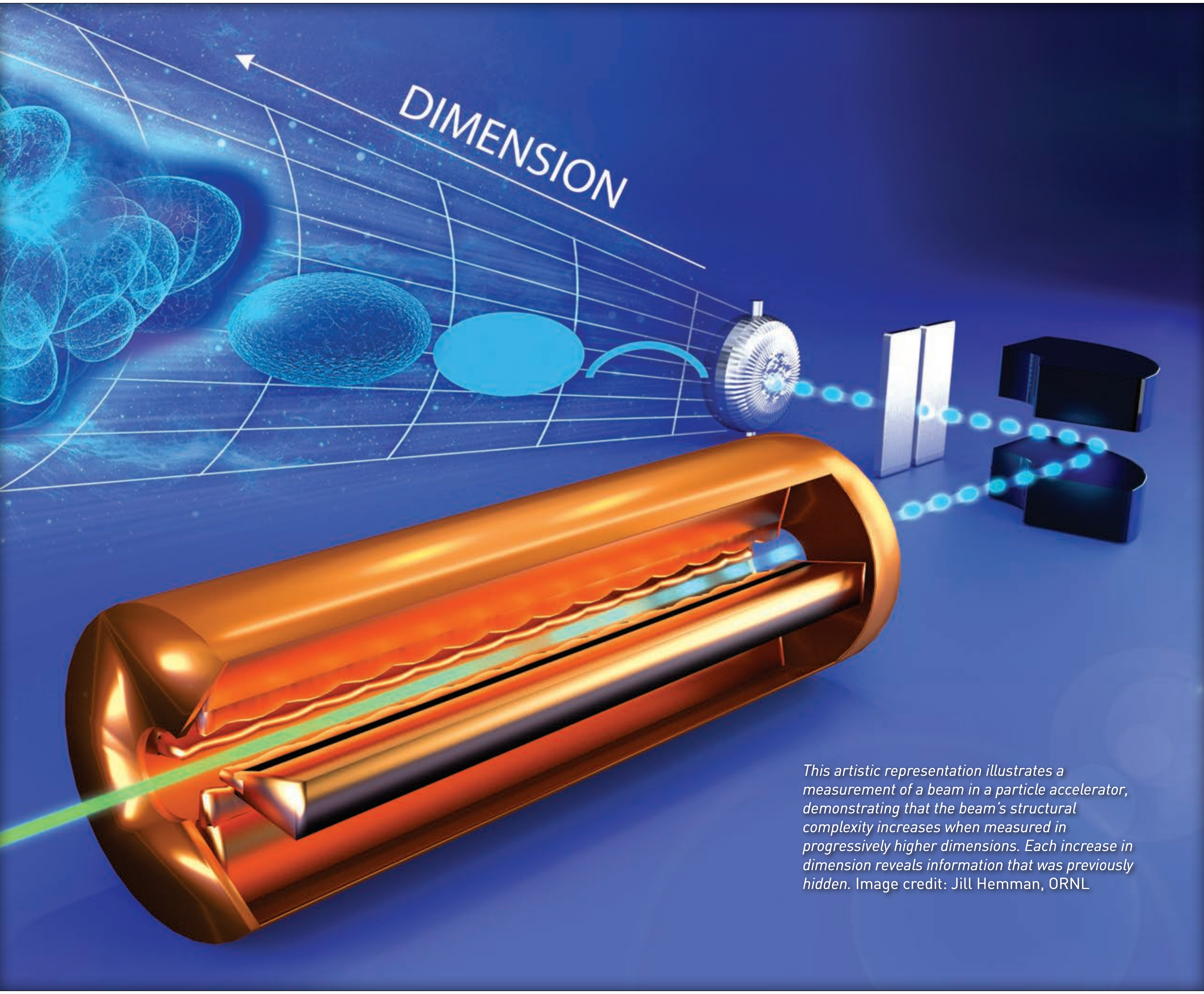
Previous attempts to fully characterize an accelerator beam fell victim to "the curse of dimensionality," in which measurements in low dimensions become exponentially more difficult in higher dimensions. Scientists have tried to circumvent the issue by adding three 2D measurements together to create a quasi-6D representation. The UT–ORNL team notes that approach is incomplete as a measurement of the beam's initial conditions entering the accelerator, which determine beam behavior farther down the linac.

As part of efforts to boost the power output of SNS, ORNL physicists used the beam test facility to commission the new radio frequency quadrupole, the first accelerating element located at the linac's front-end assembly. With the infrastructure already in place, a research grant from the National Science Foundation to UT enabled researchers to outfit the beam



test facility with the state-of-the-art 6D measurement capability. Conducting 6D measurements in an accelerator has been limited by the need for multiple days of beam time, which can be a challenge for production accelerators.

"Because we have a replica of the linac's front-end assembly at the beam test facility, we don't have to worry about interrupting users' experiment cycles at



This artistic representation illustrates a measurement of a beam in a particle accelerator, demonstrating that the beam's structural complexity increases when measured in progressively higher dimensions. Each increase in dimension reveals information that was previously hidden. Image credit: Jill Hemman, ORNL

SNS. That provides us with unfettered access to perform these time-consuming measurements, which is something we wouldn't have at other facilities," said lead author Brandon Cathey, a UT graduate student.

The researchers' ultimate goal is to model the entire beam, including mitigation of the so-called beam halo, or beam loss, which occurs when particles travel to the outer extremes of the beam and are lost. The more immediate challenge, they say, will be finding software tools capable of analyzing the roughly 5 million data points the 6D measurement generated during the 35-hour period.

"When we proposed making a 6D measurement 15 years ago, the problems associated with the curse of dimensionality seemed insurmountable," said ORNL physicist and co-author Alexander Aleksandrov. "Now that we've succeeded, we're sure we can improve the system to make faster, higher-resolution measurements."

"This research is vital to our understanding if we're going to build accelerators capable of reaching hundreds of megawatts," Cousineau said. "We'll be studying this for the next decade, and SNS is better positioned to do this than any other facility in the world."

'Chemical sponge' removes toxic gases from our air

by Paul Boisvert
boisvertpl@ornl.gov

Removing greenhouse and toxic gases from the atmosphere is a challenge both because they have relatively low concentrations and because moisture in the air can hamper the separation of targeted gas molecules from other atmospheric gases.

Another obstacle has been finding a practical way to release captured gases for use as industrial feedstocks or for long-term sequestration in underground locations such as depleted oil reservoirs and saline-filled rock formations.

A relatively new class of materials known as metal-organic frameworks, or MOFs, has shown promise in such applications. A team led by the University of Manchester is working with scientists at ORNL's Spallation Neutron Source to test an MOF material, developed by the group, that behaves like a "chemical sponge."

The MOF can adsorb a gas—in this case, nitrogen dioxide—directly from the atmosphere in ambient conditions, then release the gas as the MOF is heated. Experiments show the MOF can be loaded and unloaded repeatedly without any reduction in performance.

"This material is the first example of a metal-organic framework that exhibits a highly selective and fully reversible capability for repeated separation of nitrogen dioxide from the air, even in the presence of water," said Sihai Yang, a lecturer in inorganic chemistry at Manchester's School of Chemistry.

The MOF—known as MFM-300(Al)—captures nitrogen dioxide selectively at ambient pressures and temperatures, even at concentrations lower than one part per million, and in the presence of moisture, sulfur dioxide and carbon dioxide. Despite the highly reactive nature of nitrogen dioxide, the MOF proved extremely robust and capable of being fully regenerated, or degassed, multiple times without loss of crystallinity or porosity.

"Other studies of similar porous materials typically found performance was degraded in subsequent cycles by nitrogen dioxide, or that regeneration was too difficult and costly," said Professor Martin Schröder of Manchester's School of Chemistry

The scientists used neutron scattering techniques at ORNL's VISION vibrational spectroscopy instrument to confirm and precisely characterize how MFM-300(Al) captures nitrogen dioxide molecules.

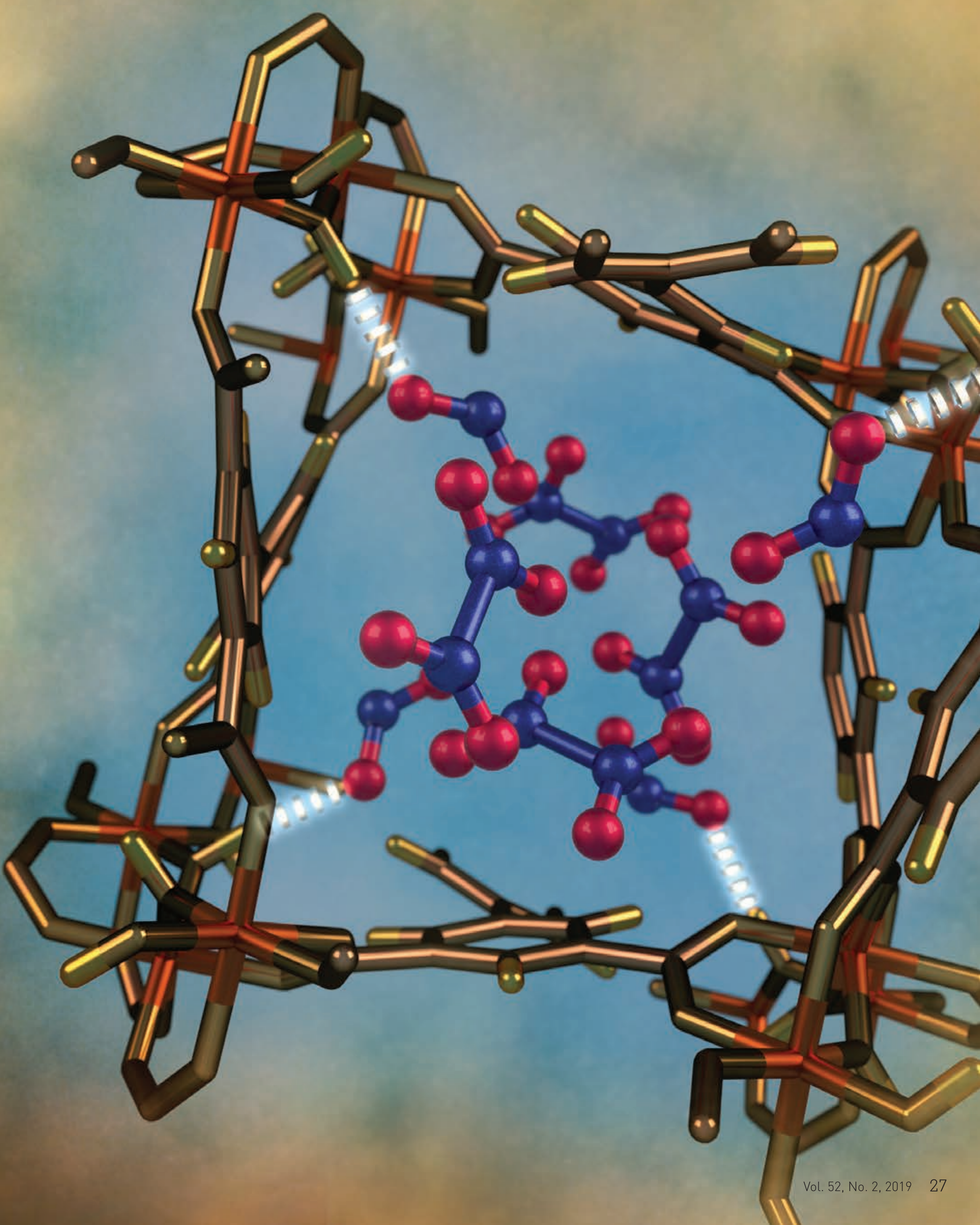
"Neutrons can easily penetrate dense materials such as metal containers where we put the MOFs to study them, and neutrons are extremely sensitive to lighter elements, such as the hydrogen atoms inside the MFM, which enabled us to observe how the nitrogen dioxide molecules are confined within the nanosize pores by tracking the motions of the hydrogen atoms next to them," said Timmy Ramirez-Cuesta, a coordinator for the chemistry and catalysis initiative at ORNL's Neutron Sciences Directorate.

The ability to directly observe how and where MFM-300(Al) traps nitrogen dioxide is helping the researchers validate a computer model of the MOF gas separation process, which could help identify how to produce other materials to capture a variety of different gases.

"Computer modeling and simulation played critical roles in interpreting the neutron scattering data by helping us connect subtle changes in the vibrational spectra to interactions between the MFM-300 and the trapped molecules," said Yongqiang Cheng, an ORNL neutron scattering scientist. "Our goal is to integrate the model with experimental data to deliver results that are otherwise difficult to achieve."

"This research could lead to practical air filtration technologies that capture large quantities of targeted gases, including carbon dioxide and other greenhouse gases," Ramirez-Cuesta said. "It has the potential to facilitate capturing atmospheric gases for use by industry and for long-term sequestration, which could help mitigate air pollution and global warming."

Illustration of a nitrogen dioxide molecule (depicted in red and gold) confined within a nanosize pore of an MFM-300(Al) metal-organic framework material, as characterized using neutron scattering.
Image credit: Jill Hemman, ORNL



Antibacterial nanoparticles

on a mission to save your teeth

by Paul Boisvert
boisvertpl@ornl.gov

Few people realize that upon leaving the dentist's office, their new filling, implant, or other dental restoration is already under attack by millions of oral bacteria.

To help address the problem, Oak Ridge National Laboratory researchers are using neutron scattering to study how nanoparticles with antibacterial properties can be added to adhesive resins, which are used by dentists to strengthen the bond between a tooth and its polymer composite filling.

> *"Thanks to the user program at ORNL, even someone like me, a dentist with limited training in advanced scientific technologies, can test a hypothesis with the help of some of the top scientists in the field while using world-class neutron scattering facilities."*
>
> — **Fernando Luis Esteban Florez,** University of Oklahoma

Soon, the bacteria form biofilms, where they metabolize sugars and other carbohydrates into acids that can dissolve tooth structures and cause cracks—half of all restorations fail within 10 years—or lead to new decay and cavities called "secondary caries."

Replacing restorations that fail due to cracking and secondary caries accounts for about 60 percent of all dental restorations performed in the U.S., at a cost of over $5 billion each year.

"The adhesive layer applied by a dentist prior to filling a cavity is fundamental to the success of the restoration, because the polymer materials used in fillings can promote the growth of biofilms," said Fernando Luis Esteban Florez of the University of Oklahoma Health Sciences Center. "Also, tiny imperfections in the adhesive surface can lead to early-stage cracking that also contributes to the failure of restorations."

Ideally, said Esteban Florez, an adhesive resin would have antibacterial properties and support the growth of dentin—the soft layer beneath a tooth's hard enamel surface—to help eliminate small gaps in the adhesive layer.

Working with Adam Rondinone, a scientist at ORNL's Center for Nanophase Materials Sciences, the researchers developed an experimental dental adhesive resin containing modified nanoscale titanium dioxide (N_TiO_2) particles. They studied samples of the adhesive resin using small-angle neutron scattering at ORNL's High Flux Isotope Reactor to determine the optimal shape, modifications, and dispersion for the particles.

"In creating the adhesive resin, we modified the surface of the N_TiO_2 nanoparticles with silanes and proteins, to improve both the function of the nanoparticles within the polymer matrix and the ability of these materials to establish covalent bonds to a tooth's naturally occurring proteins," Rondinone said.

"The benefit of using the Bio-SANS beamline instrument at HFIR is that the neutrons can tell us how the proteins bond to the N_TiO_2 and how the particles disperse."

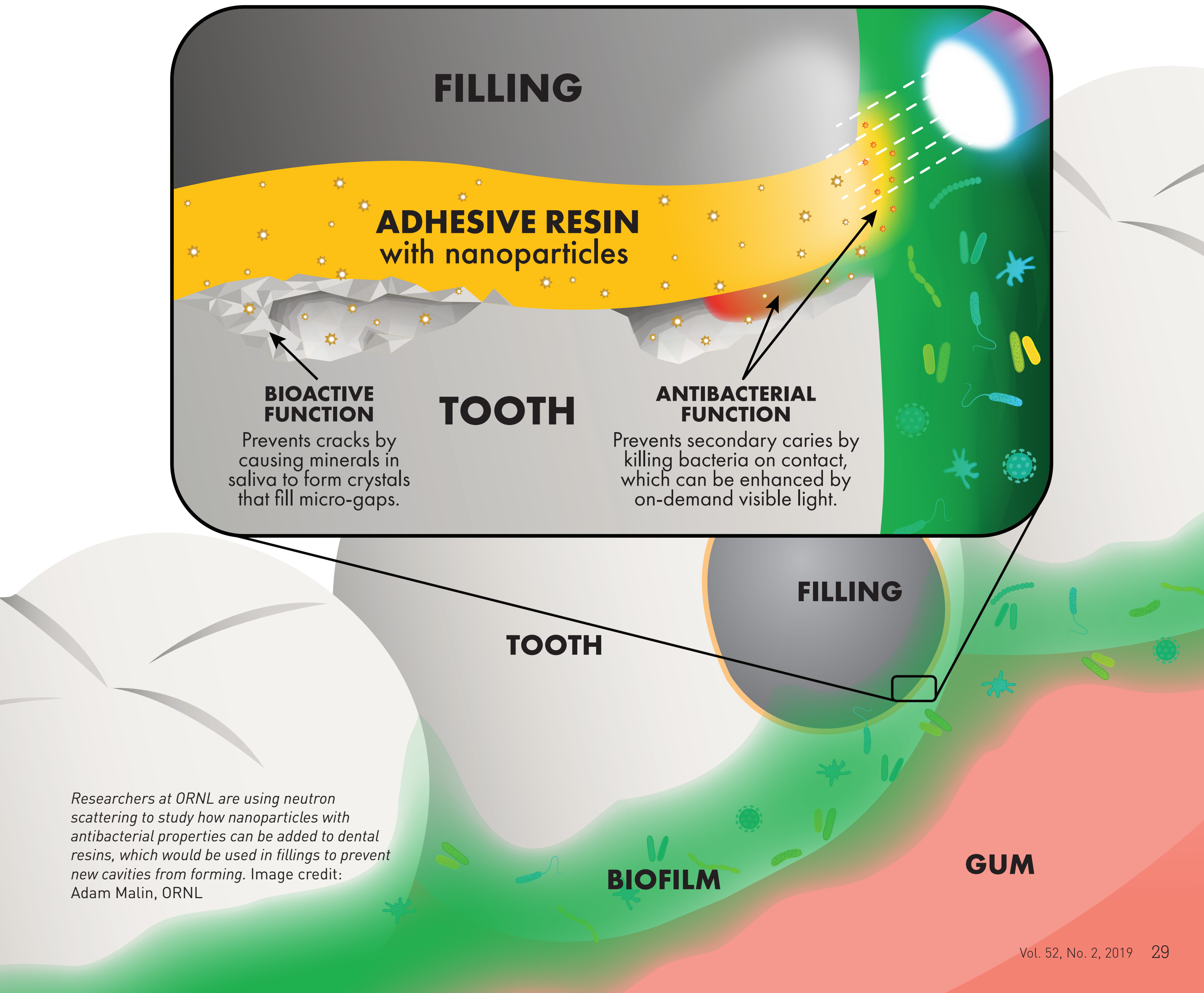
Early results show the nanoparticles disperse well and are compatible with the adhesive resin, a commercially available brand commonly used by dentists.

Other experiments have shown that the new adhesive resin exhibits active, on-demand antibacterial activity when irradiated by visible light, and passive, on-contact antibacterial effects even in darkness. Such a dual capability could enable a dentist to use light to jump-start the adhesive's antimicrobial activity before filling the cavity, and afterward the adhesive would serve as a long-term, contact-based antibacterial barrier.

One of the next steps for the researchers is to use neutron scattering to evaluate the nanoparticles for potential bioactivity, including the ability to promote self-assembly of natural tooth material adjacent to the restoration.

"Studies have shown that nanoparticles can initiate the growth of crystalline structures and guide them to become chemically bound to teeth," said Esteban Florez. "We plan to functionalize our N_TiO_2 particles to produce crystals of hydroxyapatite, the primary component of dentin, which could promote the growth of the dentin layer to minimize gaps at the adhesive interface."

He added, "Thanks to the user program at ORNL, even someone like me, a dentist with limited training in advanced scientific technologies, can test a hypothesis with the help of some of the top scientists in the field, while using world-class neutron scattering facilities. Together, hopefully, we can soon offer dentists a new and better tool that will give their patients longer-lasting-smiles."



Researchers at ORNL are using neutron scattering to study how nanoparticles with antibacterial properties can be added to dental resins, which would be used in fillings to prevent new cavities from forming. Image credit: Adam Malin, ORNL

Chemists improve carbon dioxide capture

by Dawn Levy
levyd@ornl.gov

ORNL chemists have demonstrated a practical, energy-efficient method of capturing carbon dioxide directly from air. If deployed at large scale and coupled to geologic storage, the technique may bolster the portfolio of responses to global climate change.

"Negative emissions technologies—for net removal of greenhouse gases from the atmosphere—are now considered essential for stabilizing the climate," said Radu Custelcean of ORNL, who conceived and led the study. This opinion echoes conclusions of a recent report from the National Academy of Sciences.

"Our direct-air-capture approach provides the basis for an energy-sustainable negative emissions technology," Custelcean added.

The accomplishment builds on a proof-of-principle study the chemists conducted last year, which was improved through a two-cycle process that dramatically enhances the speed and capacity of CO_2 absorption and completely recycles both the amino acid sorbent and the guanidine compound.

It's cheaper and easier to cut CO_2 emissions at their source than to recapture them from the atmosphere. Regardless, large-scale deployment of technologies such as direct air capture of CO_2 is now considered necessary to limit the rise in average global temperature to 2 degrees C (or about 4 degrees F).

Solar collector. Image credit: Carlos Jones, ORNL

Limiting warming to 2 degrees C would require grabbing billions of tons of CO_2 from the atmosphere. In principle, trees could do it. However, to capture CO_2 at this scale, "you'd need to plant trees on a surface the size of India," Custelcean said.

Capturing a billion tons of CO_2 per year with industrial scrubbers would require a relatively modest 2,700 square miles or so—an area less than the big island of Hawaii, said co-author Neil Williams.

For the recent ORNL study, Williams and Flavien Brethomé mixed amino acids with water to make an aqueous sorbent to grab CO_2 from air. Amino acids are safer than caustic sodium or potassium hydroxides, or smelly amines, the sorbents used in industrial CO_2 scrubbers.

The scientists put their aqueous sorbent in a household humidifier to maximize contact between air and sorbent and thus speed CO_2 uptake. Once absorbed into the liquid, the CO_2 formed a bicarbonate salt.

Colleague Charles Seipp had designed and synthesized an organic compound containing guanidines, chemical groups common in proteins that can bind negatively charged ions. Williams and Brethomé added Seipp's guanidine compound to the loaded amino acid sorbent solution containing the bicarbonate. The reaction created an insoluble carbonate salt, which precipitated out of solution, and regenerated the amino acid sorbent, which could be recycled.

ORNL's Radu Custelcean, left, and Neil Williams used a solar-powered oven to generate mild temperatures that liberate carbon dioxide trapped in guanidine carbonate crystals in an energy-sustainable way. Image credit: Carlos Jones, ORNL

A critical part of the study was a thorough thermodynamic analysis of the process by Custelcean and Michelle Kidder, who determined how much energy was needed to drive each chemical reaction. The last step—releasing CO_2 from the carbonate crystals so it can be stored long-term—is especially important for developing an energy-sustainable process.

Because the CO_2 is bound in a guanidine carbonate solid, it can be liberated at much lower temperatures (80–160 degrees C, or 176–320 degrees F) than the 800 degrees (1,472 degrees F) required to release CO_2 from the inorganic salts used in current capture technologies. Nevertheless, the analysis showed the heat needed to release the CO_2 from the guanidine carbonate crystals is still significant.

> *"Negative emissions technologies—for net removal of greenhouse gases from the atmosphere—are now considered essential for stabilizing the climate."*
>
> — ORNL Researcher **Radu Custelcean**

To make the overall process energy-sustainable, Custelcean decided to employ concentrated solar power. He acquired a solar-powered oven, normally used to cook foods using a parabolic mirror to concentrate the sun's rays. The guanidine carbonate crystals were placed on a tray inside the solar oven, and the CO_2 was liberated in as little as 2 minutes, in a process regenerating the guanidine compound for recycling.

ORNL's bench-scale process currently can capture as much as 100 grams of CO_2 in 24 hours. The researchers have applied for patents describing the process.

For more information: https://go.usa.gov/xEQc7

Self-sensing materials

can monitor their own well-being

by Dawn Levy
levyd@ornl.gov

Carbon fiber composites—lightweight and strong—are great structural materials for automobiles, aircraft and other transportation vehicles.

They consist of a polymer matrix, such as epoxy, into which reinforcing carbon fibers have been embedded. Because of differences in the mechanical properties of these two materials, the fibers can detach from the matrix under excessive stresses or fatigue. That means damage in carbon fiber composite structures can remain hidden below the surface, undetectable by visual inspection, potentially leading to catastrophic failure.

"Carbon fiber composites fail catastrophically, so you won't see damage until the entire structure has failed," said Chris Bowland, a Wigner Fellow at ORNL. "By knowing what's going on within the composite, you can better judge its health and know if there is damage that needs to be repaired."

Recently, Bowland and Amit Naskar, leader of ORNL's Carbon and Composites Group, invented a roll-to-roll process to coat electrically conductive carbon fibers with semiconducting silicon carbide nanoparticles. Composites made with this nanomaterial-embedded fiber are stronger than other fiber-reinforced composites and imbued with a new capability—the ability to monitor their own structural health.

Next-generation fiber-reinforced composites may be self-sensing and able to issue warnings about structural threats. Image credit: Christopher Bowland and Sherry Razo, ORNL

When enough coated fiber is embedded in a polymer, the fibers create an electrical network, and the bulk composite becomes electrically conductive. The semiconducting nanoparticles can disrupt the electrical conductivity in response to applied forces, adding an electromechanical functionality to the composite.

If the composite is strained, the connectivity of the coated fibers is disrupted and the electrical resistance in the material changes. Should storm turbulence cause a composite airplane wing to flex, for example, an electrical signal may warn the plane's computer that the wing has endured excessive stress and prompt a recommendation for an inspection.

ORNL's roll-to-roll demonstration proved in principle that the method could be scaled up for high-volume production of coated fibers for next-generation composites. Self-sensing composites, perhaps made with a renewable polymer matrix and low-cost carbon fibers, could find themselves in many products, even including 3D-printed vehicles and buildings.

To fabricate nanoparticle-embedded fibers, the researchers loaded spools of high-performance carbon fiber onto

From left, Amit Naskar, Ngoc Nguyen and Christopher Bowland in ORNL's Carbon and Composites Group bring a new capability—structural health monitoring—to strong, lightweight materials promising for transportation applications. The spools contain fibers from various stages within the carbon fiber production process. Bottles contain neat epoxy resin (white) and nanoparticle-loaded epoxy (gray) in which fiber tows will be dipped and dried to create a thin coating on the fibers. Image credit: Carlos Jones, ORNL

rollers that dipped the fiber in epoxy loaded with commercially available nanoparticles about the width of a virus (45–65 nanometers). The fiber was then dried in an oven to set its coating.

To test the strength with which nanoparticle-embedded fibers adhered to the polymer matrix, the researchers made fiber-reinforced composite beams with the fibers aligned in one direction. Bowland conducted stress tests in which both ends of this cantilever were fixed while a machine assessing mechanical performance pushed on the beam's middle until it failed.

To investigate the sensing capabilities of the composite, he affixed electrodes on both sides of the cantilever. In a machine called a "dynamic mechanical analyzer," he clamped one end to hold the cantilever stationary. The machine applied force at the other end to flex the beam while Bowland monitored the change in electrical resistance.

ORNL postdoctoral fellow Ngoc Nguyen conducted additional tests in a Fourier-transform infrared spectrometer to study chemical bonds within the composites and improve understanding of the enhanced mechanical strength that was observed.

The researchers also tested composites made with different amounts of nanoparticles for the ability to dissipate energy—as measured by vibration-damping behavior—a capability that would benefit structural materials subjected to impacts, shakes, and other sources of stress and strain. The nanoparticles enhanced energy dissipation by 65 to 257 percent.

Bowland and Naskar have applied for a patent for the process to make self-sensing carbon fiber composites.

For more information: https://go.usa.gov/xEQ4B

Seeing double:

Digital twin for a secure, resilient grid

by Stephanie Seay
seaysg@ornl.gov

For critical infrastructure such as the nation's power grid, the delay between identifying a cyberattack and mounting a defense could be catastrophic. ORNL scientists are working to solve this dilemma with a platform known as a "digital twin" that provides a real-time simulation of the grid so that system aberrations can be identified almost immediately.

The grid is often called the world's largest machine. It is a complex, interdependent network made up of power generation, transmission lines that carry electricity across vast distances, substations where voltages are stepped down for utility systems, distribution lines that connect communities, and devices that convert electricity for customer usage.

But the grid has become increasingly vulnerable to cyber disruption as more of its controls have moved into the digital realm and are connected to the internet.

The digital twin—an active model fed by real-time sensor data and running side-by-side with the actual grid in a control room—could give utility operators the ability to detect a zero-day attack, or one that has just been discovered, for which there is no patch.

"No one knows what the next attack will look like, because it will be brand new," said Ryan Kerekes, project lead for ORNL's digital twin framework and leader of ORNL's RF, Communications and Intelligent Systems Group. "But we do know that a cyberattack will cause the system to behave in a way that we didn't expect. Having this live comparison of how the system should be performing can give you a crucial edge in detecting attacks."

A digital twin would initially recommend courses of action for operators to take, added Mark Buckner, leader of the Power and Energy Systems Group. "But eventually as the system is trusted and validated, we could use artificial intelligence to create a self-aware, self-healing network that would automatically quarantine abnormalities so they can be examined, while preventing issues such as cascading outages."

In a demonstration of the digital twin, the researchers launched a cyberattack on the model, spoofing values that a grid operator would see. The values were valid, but they didn't make sense in the context of the larger system. The digital twin was able to identify those values as aberrations that didn't make sense, based on its model of how the system's components should be interacting, Kerekes said.

"It's like in the movies, when someone has installed a loop of footage showing an empty hallway on the camera—when in reality there are people walking through," Buckner said. "But let's say you also had a simple infrared sensor monitoring temperature in the area. The system knows if there are no warm bodies in the hallway, then the temperature should be consistent. So the system is looking at a combination of things that the camera might not see."

The digital twin framework uses the same dynamics as the larger grid at a lower, safe voltage for researchers. It is now being leveraged to design and test cyber resilience solutions for critical infrastructure.

"The digital twin framework is already proving useful for our work with the power grid," said Mason Rice, leader of the lab's Cyber Physical Systems Group. "We are also leveraging it more generically for industrial controls systems to have a larger impact on the nation's diverse critical infrastructure."

The system could be used to build a grid more resilient to disruption, including physical damage from storms, the scientists noted. Using the projected path of a storm, for instance, operators could use the digital twin to turn off power to portions of the system so that cascading faults do not occur.

The digital twin is an active model fed by real-time sensor data and running side by side with the actual grid. Image credit: Jason Richards, ORNL

Tree of life:

Poplar studies yield human cancer insights

by Kim Askey
askeyka@ornl.gov

ORNL researchers studying the genes that control callus formation in poplar trees have made an extraordinary discovery: genetic networks that are also at the root of tumor formation in several human cancers.

Surprisingly, plants and humans share genes that trigger or suppress the uncontrolled growth of cell clusters—forming callus in poplar and tumors in humans. The genes originated billions of years ago, when plants and animals shared a common ancestor.

"We'd never thought about such genes being conserved," said ORNL plant biologist Wellington Muchero. "But what we are seeing is this really surprising conservation of function between plants and humans."

As a result, the research may aid both in engineering better plants for bioenergy production and identifying new targets for cancer treatment.

A boon for bioenergy

Populus—or poplar trees—show great promise as a bioenergy crop. Scientists at the Center for Bioenergy Innovation at ORNL are studying genetic variations in these perennials that can increase drought and disease resistance and yield more biomass for biofuels and other products. To enhance these characteristics, researchers modify the genes in callus cells, which then grow into a whole new plant.

"Callus formation is an important step in creating new genetically engineered plants," Muchero said. "Without the ability to form callus, you are at a dead end. You can introduce your gene, but you cannot grow the plant."

Some plants grow callus easily. Others grow none at all. The research team used leaves cut from poplars of different genotypes to determine which genetic variations result in callus formation. Their analysis identified genes that trigger rapid cell division and genes that restrict it.

Targeting new cancer treatments

What is healthy for poplar—active callus inducers paired with inactive callus suppressors—can be a recipe for cancer in humans.

All eight of the key genes for poplar callus formation have equivalents in humans—genes associated with diseases like chronic myeloid leukemia, breast cancer and stomach cancer. Although these cancer-causing hub genes are well

Poplar callus. Image credit: ORNL

ORNL plant biologist Wellington Muchero and colleagues have discovered that genes that control callus formation in poplar trees are also at the root of tumor formation in several human cancers. Image credit: Carlos Jones, ORNL

known, it was only by examining them in poplar that scientists could see the connections between them and the array of associated genes that play a role in their regulation.

"We were able to build these networks showing how these genes were related to each other and the intermediate signals that were co-occurring," said corporate fellow and CBI director Jerry Tuskan. "With this library of co-expressed genes, pharmaceutical companies could begin identifying new targets for therapy."

A new drug could inhibit an associated enzyme from functioning, for instance, and switch off or block the genetic pathway that triggers a tumor to form. Studying poplar trees can help root out the best targets for drug development.

New platform for testing

Since poplars have never been domesticated, individual poplar trees vary widely in their genetic makeup. Scientists can often identify the genetic variant that results in a specific phenotype, or characteristic, by examining a few hundred trees. In comparison, it would take hundreds of thousands of individuals to make a similar finding in humans, who are 99.9 percent identical in their DNA.

Stresses that cannot be applied to humans or laboratory rats can be used in controlled plant experiments to verify that a gene results in a phenotype under various conditions. This richer understanding of how these genetic networks function could complement results from traditional mice studies to increase the efficacy of new drugs going to clinical trials.

"While we at CBI are focused on new knowledge and technologies for biofuels and bioproducts, it is very rewarding to know our work has broader applications to improve human health," Tuskan said.

3D printing shapes building industry

by Jennifer Burke
burkejj@ornl.gov

A residential and commercial tower under development in Brooklyn is changing the New York City skyline, and its origins exist in ORNL research.

The tower's white precast concrete façade—rising from the site of the former Domino Sugar Factory along the waterfront—evokes the form of a sugar crystal, a pattern created from 3D printed molds at DOE's Manufacturing Demonstration Facility at ORNL.

Working under collaborative research and development agreements with industry partners Gate Precast and Precast/Prestressed Concrete Institute, ORNL researchers used carbon-fiber–reinforced acrylonitrile butadiene styrene, or ABS—a common thermoplastic compounded with chopped carbon fibers—to make the molds for the project.

ABS molds for the Domino Sugar Factory site were produced on ORNL's Big Area Additive Manufactured machine. Image credit: Gate Precast

The Big Area Additive Manufactured—or BAAM—molds were used to cast close to a thousand precast concrete parts for the façade of the 42-story tower. ORNL researchers from the Building Technologies Research and Integration Center and MDF collaborated to produce the molds.

"We didn't know if 3D printed molds could be made to work for the precast industry," said Diana Hun, lead buildings researcher on the project. "But we thought it was worthwhile to examine the potential."

To do so, ORNL needed a project to demonstrate that BAAM technology could rapidly manufacture molds suitable for precast concrete manufacturing. Gate Precast, one of PCI's members, was awarded the contract to construct the Domino building façade, and the tower provided ORNL with the perfect platform to demonstrate the viability of 3D printed molds.

For Gate Precast, ORNL developed the process science to reliably manufacture 3D printed molds and transferred that knowledge to a commercial enterprise, Additive Engineering Solutions, to print additional molds.

Precast concrete parts, poured from molds developed at ORNL, are installed in a residential and commercial tower on the site of the Domino Sugar Factory along the waterfront in Brooklyn. Windows in the tower resemble sugar crystals. Image credit: Gate Precast

"With the Domino project, the challenge was to find the right solution for a job that required durable molds that could be used numerous times," Hun said. "We proved that 3D-printed molds could cast at least 200 concrete parts, which was key to meeting the project's schedule."

Within a year, the project progressed from designing prototypes to printing actual molds used to cast concrete parts for the Domino tower.

Conventional wood molds are manually produced by skilled carpenters, a profession in short supply in the labor force. In general, wood molds produce fewer castings, as they are significantly less durable than the molds printed with carbon-fiber–reinforced ABS.

"The carbon fibers help improve the strength by two times and stiffness by four times of the molds, relative to the ABS plastic, allowing the inserts to support the weight of the poured concrete and the force of the demolding operations over repeated cycles," said Brian Post, advanced manufacturing engineer for the project.

3D-printed molds begin from computer-aided design models that are sliced, layer by layer, to develop tool paths that drive the printhead. The printer executes these tool paths layer by layer by extruding molten polymer to form the final part.

"Each mold insert takes between eight and 11 hours to print and eight hours to machine to the desired surface finish," Post said.

As the Domino development takes shape in New York, it's attracting attention not only for its unique look and design but also for its potential.

"With 3D printing at hand, architects can now unleash their creativity and design complex façades that they have not previously explored," said Hun.

The Domino tower is expected to be completed in 2020. ORNL continues to work with PCI as part of a five-year research program to determine how new technologies can improve insulated precast panels.

Sir Richard Roberts was awarded the Nobel Prize in Physiology or Medicine in 1993 for his contribution to the discovery of introns in eukaryotic DNA and the mechanism of gene-splicing.

A native of England, Roberts received a Bachelor of Science in chemistry in 1965 and a Ph.D. in 1969, both from the University of Sheffield. He has served as consultant and chairman of the Scientific Advisory Board at New England Biolabs since 1974 and has been the board's chief scientific officer since 1992.

Roberts's current research interests focus on enzyme discovery using bioinformatics, combined with the experimental testing of function. He also gives lectures and presentations worldwide and investigates potential opportunities for both scientific and commercial collaborations.

Roberts delivered the Eugene P. Wigner Distinguished Lecture February 6, 2019, on the topic "Precision Agriculture and Genetically Modified Organisms." This is an edited transcript of our conversation following his lecture.

Distinguished

Richard Roberts

1. What are GMOs, and how are they created?

GMO stands for genetically modified organism. They are created by taking genes from one organism—usually a single gene—and putting it into a recipient, usually a plant. In this way, you can introduce new traits encoded by the gene into the plant. So, for instance, if you wanted it to grow much taller, then you would try to put in a gene that would make it grow much taller.

2. What are the benefits?

The benefits are that it's much more precise than traditional breeding methods. You can be absolutely certain that the gene you want to go in, goes in. You can test easily that it's gone into the right place, and that it's working. And that becomes a very big advantage; it's a big advantage not to have the relatively nonprecise breeding methods that are the traditional way of doing things.

One of the greatest advantages is that you can make a new plant very quickly. Typically, using precision agriculture with the methods offered by GMOs, in a matter of one, two, three years, you can generate a new hybrid plant that is useful for production. Whereas, if you do it by traditional methods, it can take anywhere from 10 to 20 to 30, maybe even 40 years to develop a new variety that has just the properties that you want. So it's much, much faster.

3. How do GMOs differ from plants created through traditional crossbreeding?

In the traditional way, you basically take two plants, cross them in much the way that you cross a man and a woman when you're making a baby, the genes get mixed up, and you end up with a progeny plant that has half the genes from one parent and half from the other. In addition to getting maybe the gene you wanted, you get a lot of genes that you don't want. And so, you have to keep backcrossing to get rid of the genes that you don't want, and usually you never get rid of all of them. But that's what they've been doing for a long time.

That is good if you've got two varieties that you can cross—that is, they are compatible with one another. But if the gene you want to put in isn't present in one of the parents, then you have to use an alternative method, and the GMO method is the way to do it.

4. You said during your lecture that this is a critically important technology for developing countries. Why is that?

The big agricultural companies have gone out of their way to make sure that farmers could grow the very best crops possible; and all of this was

Lecturer

done in markets controlled by Europe, the USA, Canada, Japan—the developed countries. The agricultural companies realized that they could make better crops, and in this way they could make more money for themselves because people would buy them.

In the developing world, that's not the case. In the developing world, first, they don't eat the crops that we eat in the West most of the time; and second, they don't have the money to pay the cost of having crops bred specifically for them. This is why GMOs are so nice: local scientists can do it, they can make the new hybrids, they can make better crops. It doesn't cost a lot of money, because the method is not that expensive. And you can do it relatively quickly. So they can do it all themselves, and they are not reliant upon big agribusiness from the West in order to provide food for their people.

5• Why have GMOs become a political issue?

I think the reason they became a big political issue was because Greenpeace and the other anti-GMO parties realized that this was a way of mixing two issues: one, big agribusiness, which nobody particularly liked, especially in Europe, and two, GMOs, which were being pushed by big agribusiness.

And so, they took this as a wedge issue, because they thought, already everybody's against big agribusiness, and so it's easy to conflate the two and make the two as though they were one. In fact, that's not true. You don't need big agribusiness in order to make GMOs. It was just that when Monsanto first rolled them out, they didn't do it in a very clever way.

6• Why was it important to visit ORNL, meet with researchers here, and participate in the Wigner lecture series?

I came because I was invited by your CEO, if you like, [ORNL Director] Thomas Zacharia. And I had been to Oak Ridge previously. But in general, I enjoy going around and meeting new scientists, especially people in fields remote from my own. And I was curious to see what Oak Ridge had turned into—I was last here in 1969, and so, as you can imagine, there have been a few changes in the meantime.

The Eugene P. Wigner Distinguished Lecture Series in Science, Technology, and Policy gives scientists, business leaders and policymakers an opportunity to address the ORNL community and exchange ideas with lab researchers. The series is named after Eugene Wigner, ORNL's first research director and recipient of the 1963 Nobel Prize in Physics.

ORNL is proud of its role in fostering the next generation of scientists and engineers. We bring in talented young researchers, team them with accomplished staff members, and put them to work at the lab's one-of-a-kind facilities. The result is research that makes us proud and prepares them for distinguished careers.

We asked some of these young researchers why they chose a career in science, what they are working on at ORNL, and where they would like to go with their careers.

Elizabeth Skoropata

Postdoc, Materials Science and Technology Division
Ph.D., Physics, University of Manitoba
Hometown: Winnipeg, Canada

What are you working on at ORNL?

My work focuses on examining the magnetism created at interfaces between nanoscale materials with dissimilar physical properties. Currently, I am working to understand how ingredients like heavy elements and structural symmetry at an interface work to change a conventional magnet into something more complex.

What would you like to do in your career?

I would like to continue to do research in either an academic or industry setting and investigate how atomic properties can be used to create new magnetic behaviors that are not found in nature.

Why did you choose a career in science?

I have always been passionate about learning new things and solving problems. I enjoy working on magnetic materials because they are essential to our everyday lives, but we also have a lot left to understand about them; and that makes me excited for what we can discover in the future.

Paritosh Santosh Mhatre

Graduate student, Energy and Transportation Science Division
Master's student, Industrial & Systems Engineering, Rochester Institute of Technology
Hometown: Mumbai, India

What are you working on at ORNL?

My work at ORNL focuses on the development of fieldable and scalable large-scale additive manufacturing systems capable of extruding concrete. I'm working on the design of the control system and a trajectory planner for the system aimed at smoothing the required motion and thus minimizing the induced vibrations.

What would you like to do in your career?

I would like to pursue a career in research and development of additive manufacturing systems and contribute toward increasing their adoption in mainstream manufacturing.

Why did you choose a career in science?

Since a very young age, I've had a desire to understand the working principle of things around me, which got me interested in science. Further, I was fascinated by high school physics, which confirmed my decision to choose science as a career.

Debanjana Nayak

Graduate student, National Security Emerging Technologies Division
Ph.D. student, Computer Science, North Carolina State University
Hometown: Kolkata, India

What are you working on at ORNL?

I am working on improving the accuracy of various navigational solutions (e.g., GPS, SLAM, odometry) through data analysis. My research experience involves analysis of time-series or spatiotemporal data, such as detecting change points or anomalies or creating forecasting models. I am applying the same techniques to the problem of navigation.

What would you like to do in your career?

I would like to build a research-oriented career in the field of data science and analytics, with a focus on solving the major problems that modern society is dealing with, such as climate change, clean energy, socio-economic development and so on.

Why did you choose a career in science?

Since my childhood, I had a passion for numbers. This later developed into a deep interest in the areas of mathematics and computer science. Besides, I sincerely believe science can solve most of today's real-world problems. And I want to contribute to that process as much as I can.

Patrick Caveney

Graduate student, Center for Nanophase Materials Sciences
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Johnson City, Tennessee

What are you working on at ORNL?

My research is about understanding how molecular resources are used among genes to make proteins. Using fluorescent, confocal microscopy, I observe protein production in a simplified, synthetic, cell-free system encapsulated in lipid membranes the size of mammalian cells. This work helps inform the designs of gene circuits that could be used to make bioproducts.

What would you like to do in your career?

In parallel with research, I cofounded a company to explore entrepreneurship. We licensed technology created at ORNL, improved it with a DOE grant, but failed to commercialize it. I would like to apply this experience to continue to work to bring scientific discoveries to market through small companies.

Why did you choose a career in science?

My parents encouraged academics and scientific curiosity. My high school AP biology teacher sparked my interest in cell biology with an experiment transforming E. coli with a fluorescent protein. It is fun to be, for a moment, the only person in the world to learn something new about nature.

Rachel L. Seibert

Postdoc, Reactor and Nuclear Systems Division
Ph.D., Condensed Matter Physics, Illinois Institute of Technology
Hometown: Gig Harbor, Washington

What are you working on at ORNL?

My research at ORNL focuses on development of nuclear fuel concepts and understanding the behavior of nuclear fuels under irradiation. I primarily work on post-irradiation examination— for example, using microscopy to study fission product behavior and microstructural evolution in silicon carbide for fuel containment in both fuel and surrogate systems.

What would you like to do in your career?

I want to work jointly in academia and at a research institute like ORNL in nuclear and alternative energy. I'd like to continue my work in nuclear fuels, and I want to see my work making a contribution to the energy sector.

Why did you choose a career in science?

It was natural. I always excelled when I was doing hands-on work, and my mind was geared more for math and problem-solving and puzzles. I was one of those kids who dreamed of saving nature, so I knew I wanted to be involved in alternative energy.

Oluwaseun Ogunro

Postdoc, Computational Science and Engineering Division
Ph.D., Chemistry, New Mexico Tech
Hometown: Oka-Akoko, Nigeria

What are you working on at ORNL?

I'm developing the International Ocean Model Benchmarking tool and evaluating marine biogeochemical processes in Earth system models (ESMs). This tool helps to identify areas of uncertainty in ESMs and enables the modeling community to make informed decisions on uncertainty reduction that could improve future model development.

What would you like to do in your career?

My desire is to work on the cutting edge of science to inform decision makers. We live in an extraordinary time, with a lot of interesting science questions such as the global impact of geoengineering. My objective is to lend my expertise to advance the current understanding in ocean model development.

Why did you choose a career in science?

Most times I wonder how the choices we make every day could influence our environment. Science has always helped me to answer intriguing questions on climate feedback.

When Oak Ridge was gated, but muddy

by Tim Gawne
gawnetj@ornl.gov

Oak Ridge in its earliest days was a quintessential planned community, and a gated one at that.

Born of the wartime necessity to house the thousands of workers who would construct and operate the region's three Manhattan Project facilities, the city itself was a secret. It had gates, too—guarded ones.

At its peak, Oak Ridge was home to 75,000 men, women and children, a number that far exceeded the government's initial projections. As a result, the town hosted a patchwork of housing types, from prefabricated houses to dormitories, trailers and the euphemistically named "victory cottages," which each bunked five workers around a coal stove. If you were lucky enough to land a spot in a victory cottage, you also found yourself sharing bathroom and shower facilities with the rest of the neighborhood.

Despite its rushed construction, Oak Ridge had many of the same facilities as other communities in the 1940s: schools, a pool, recreation centers, churches, cafeterias and a full-service hospital. It also had a few features other communities lacked: security fencing, a curfew, armed guards at each town entrance, and its own military intelligence force.

It was a love-it-or-hate-it kind of place; you either saw the frontier town it appeared to be, or you saw the thriving community it had the potential to become. While many early residents were happy to bid it goodbye when they had the chance, the ones who stayed carried a sense of pride for having roughed it in "Dogpatch."

Magnesium ribbon electrified at Elza Gate. Image credit: ORNL

Nobel Prize-winning physicist Arthur Compton belonged to the former group. In his book *The Atomic Quest*, Compton recalled a rainy ride from the nearby city of Knoxville carrying a cake to his child's birthday party. A fellow passenger looked down at his muddy boots and said, "Oh, you are from that place." Compton was happy to put distance between himself and Oak Ridge once the war no longer required his services.

Another early staffer—the lab's chemistry director at the time—was even more blunt. His view of the residential area was so dim that he suggested the Army build a better development next to the lab called "Clinton Village."

Beyond housing, the bigger obstacle to long-term sustainability was that Oak Ridge's three plants—X-10 (which eventually became ORNL), Y-12 and K-25—faced an uncertain future until 1949, when their continued operation was guaranteed by the newly formed Atomic Energy Commission.

The town would have growing pains. For one, it had to choose whether to remain behind the security perimeter established during the war or to open up and let the public in.

Some opposed opening the town, but they were in the minority. On March 19, 1949, at what was Elza Gate, a magnesium ribbon was ceremoniously electrified by ORNL's Graphite Reactor, the world's first continually operating nuclear reactor.

The ribbon split in a blaze, formally opening the city to the public. The celebration included parades and public tours. *Good Housekeeping* magazine even came out and gave the town a good review and a rating of "must see."

www.ornl.gov/ornlreview

OAK RIDGE NATIONAL LABORATORY REVIEW
PO Box 2008, Oak Ridge, Tennessee 37831-6266

Editor—Leo Williams
Writers—Kim Askey, Paul Boisvert, Jennifer Burke, Tim Gawne, Jonathan Hines,
Katie Jones, Dawn Levy, Jeremy Rumsey, Stephanie Seay, Leo Williams
Designer—Brett Hopwood
Illustrators—Jill Hemman, Brett Hopwood, Adam Malin
Copy editors—Deborah Counce, Wendy Hames, Laurie Varma
Photographers—Carlos Jones, Jason Richards
Stock images—iStockphoto™

Phone: (+1) 865.574.8891
Fax: (+1) 865.574.0595
E-mail: ornlreview@ornl.gov
Internet: www.ornl.gov/ornlreview

Oak Ridge National Laboratory is managed by
UT-Battelle LLC for the US Department of Energy under contract
DE-AC05-00OR22725

ISSN 0048-1262