OAK RIDGE NATIONAL LABORATORY

Review

Discovering element 117

OAK RIDGE National Laboratory

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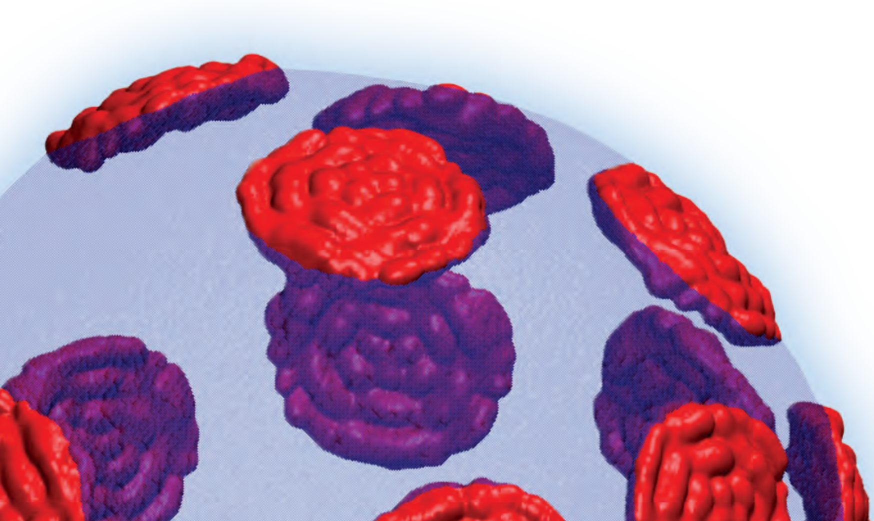
Contents



On the Cover

ORNL's Krzysztof Rykaczewski spent a lot of time in airports while shepherding radioactive targets from Oak Ridge to Russia.

Empowering our next generation

Two-thirds of ORNL's research staff have been with the lab less than a decade. Many of the new staff are young scientists who bring the energy, drive and curiosity of talented professionals in their early careers.

When they come aboard, we become responsible for supporting their career development, including skills that most likely were not a part of their studies, such as locating, obtaining and managing research funding and participating in the leadership of a large organization.

In this issue of *ORNL Review* we focus on the lab's relationship with its early-career researchers—the ways we benefit from their work and the efforts we make, both formal and informal, to ensure they can prosper in a highly demanding and competitive research environment. We also introduce you to four excellent young researchers, recipients of Early Career Research Program awards from DOE's Office of Science, who represent our next generation of science leadership (Pages 6–13).

Also in this edition we look at the logistics of discovering element 117, provisionally named "tennessine" (Pages 26–27). The discovery of a new element requires brilliant science, of course, and world-class facilities such as our High Flux Isotope Reactor. In this case, it also required perseverance and logistical skills to get berkelium targets from Oak Ridge to our Russian collaborators before the targets decayed.

Elsewhere in this issue we discuss research that promises much better access to geothermal energy, an abundant energy source right beneath our feet (Pages 28–29). We highlight neutron research into materials that may be useful in the not-so-futuristic field of quantum computing (Pages 24–25). There's also an interesting look at a project that exploits the odd behavior of some metals—changing temperature when exposed to a magnetic field—to create refrigerators that are more efficient than current models without using environmentally harmful chemicals (Pages 30–31).

Our infographic in this issue explains ORNL's Carbon Fiber Technology Facility, a demonstration plant designed to bring down the cost of a strong, lightweight material with many promising applications (Pages 18–19).

Finally, please check out our other regular features: We talk to young grad students and postdocs who will be part of that next generation of scientific leadership. We hear from a distinguished engineer who spoke at our latest Eugene P. Wigner Distinguished Lecture in Science, Technology, and Policy (Pages 32–33). We conclude, as always, with a look back at a chapter of ORNL history, in this case the quest to quantify the lifespan of an unbound neutron.

I hope you enjoy the *ORNL Review*.

Thomas Mason
Laboratory Director

Vehicle automation will have consequences

Imagine a future in which your car no longer needs someone behind the wheel.

The time you devote to your daily commute—now often a waste—would be available for reading, working, watching videos or even napping. Physical disabilities would no longer keep you homebound. You could send your kids to karate lessons or band practice without having to go along.

Driverless commute.

It's no longer a sci-fi pipe dream. Vehicle automation is making its way onto public roads, and the day of the driverless car seems within our grasp.

But is it entirely a good thing? ORNL public policy researcher Paul Leiby and colleagues at the University of Leeds in Great Britain and the University of Washington in Seattle explored this question for the journal *Transportation Research Part A: Policy and Practice*, looking specifically at energy demand and carbon emissions.

As with many questions, the answer regarding energy use depends on the details. On the one hand, automation can make vehicles far more energy efficient, smoothing traffic flow and reducing fuel-guzzling habits such as stop-and-go driving and heavy acceleration. On the other hand, greater convenience and safety will no doubt lead to more driving. If automation allows us to drive safely at higher speeds, it's also likely we'll want to do that, thereby increasing our energy consumption.

"If you don't get a big increase in travel demand, then the energy-efficiency factors overwhelm," Leiby explained. "But if people become much more interested in driving and much more willing to commute or travel long distances by car, and if we don't get all the anticipated energy efficiency gains, then you could see a big increase in energy consumption.

"We're not sure which way it will go, so we've identified the key factors and estimated some bounding cases to help guide future research and policy."

You can find the article, entitled "Help or hindrance? The travel, energy and carbon impacts of highly automated vehicles," at bit.ly/1RyPCXN.—*Leo Williams*

Laser treatment, bonding potential road to success for carbon fiber

Joining carbon fiber composites and aluminum for lightweight cars and other multimaterial high-end products could become less expensive and the joints more robust because of a new method that harnesses a laser's power and precision.

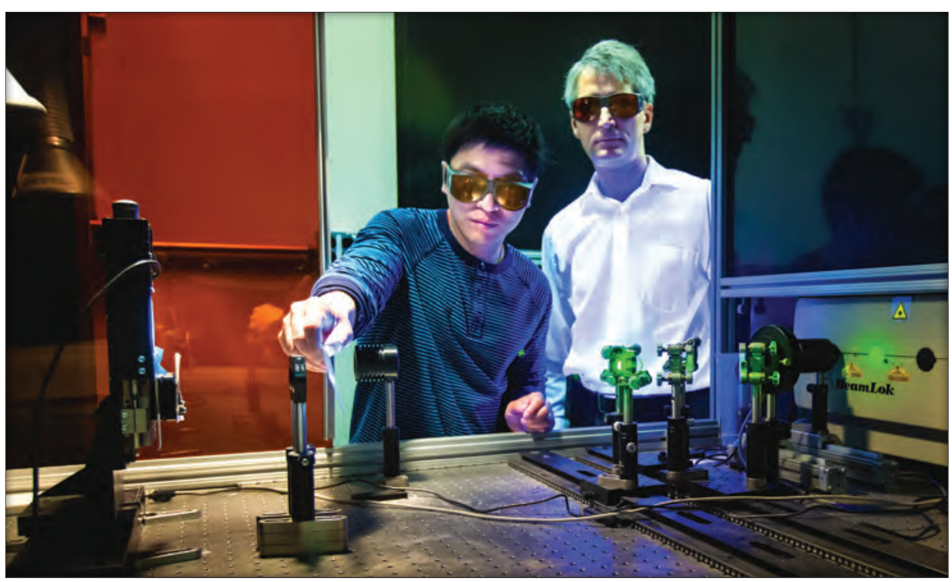
The process, developed by a team led by ORNL's Adrian Sabau, would replace the practice of using abrasive pads, grit blasting and environmentally harmful solvents to prepare the surface of the materials by hand. Using a laser to remove layers of material from surfaces prior to bonding improves the performance of the joints and provides a path toward automation for high-volume use.

"Our technique is vastly superior to the conventional surface preparation methods," Sabau said. "Combined with the potentially dramatic reduction in the cost of carbon fiber polymer composites, this represents an important step toward increasing the use of this lightweight, high-strength material in automobiles, which could reduce the weight of cars and trucks by 750 pounds."

The surface treatment of aluminum and carbon fiber polymer composite is a critical step in the adhesive joining process, which directly affects the quality of bonded joints. Aluminum surfaces typically contain oils and other contaminants from production rolling operations, while carbon fiber surfaces often contain mold releases.

"These surface contaminants affect surface energies and the quality of adhesion, so it is critical that they are removed," said Sabau, adding that the laser also penetrates into the top resin layer, leaving individual carbon fibers exposed for direct bonding to the adhesive and increasing the surface area for better adhesion.—*Ron Walli*

For more information: http://go.usa.gov/chSmJ



Adrian Sabau and Jian Chen work with a laser to prepare the surface of carbon fiber composites and aluminum to create superior bonds that can absorb 200 percent more energy than conventional bonds.
Image credit: Genevieve Martin, ORNL

ORNL hosts Southeast bioenergy meeting, study tour

Researchers and others interested in establishing a sustainable American bioeconomy took part in a five-day study tour in April led by ORNL.

Approximately 70 attendees from DOE and its national laboratories, the International Energy Agency, universities, industry and regional stakeholders such as landowners and nonprofit organizations participated in the Southeast United States Bioenergy Meeting. The meeting and study tour highlighted innovations developed by DOE's Bioenergy Technologies Office in support of deployment of a sustainable bioeconomy.

The BETO-sponsored event highlighted sustainability considerations associated with biomass feedstocks such as perennial grasses and woody residues as well as harvesting operations, logistics and use of the materials.

"The Southeast is the wood basket of the U.S. and serves as a sustainability test case," said Virginia Dale, ORNL corporate fellow and Center for BioEnergy Sustainability director. "The goal of the tour is to have participants develop a better understanding of bioenergy opportunities and constraints in the region."—*Morgan McCorkle*

For more information: http://go.usa.gov/chs9A

Participants visited East Tennessee switchgrass fields and facilities as part of the Bioenergy Study Tour hosted by DOE's Bioenergy Technologies Office and ORNL. Image credit: Jason Richards, ORNL

From tinkering to hackathons

Fernanda Foertter knows from experience that training in high-performance computing often relies on individual effort and is passive in nature. Researchers attend lectures or watch training videos, but little training is done with hands-on learners in mind.

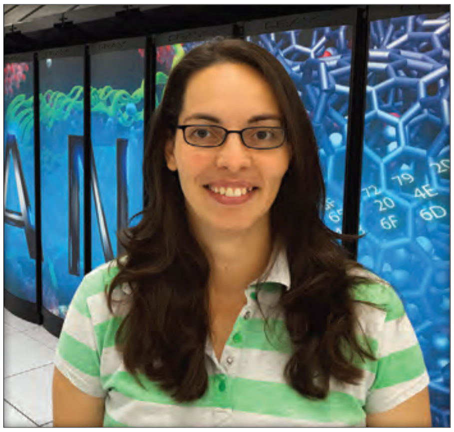
To close that gap, for the past two years she has helped organize hackathons—events that gather researchers to tackle particular coding or programming problems.

"Hackathons represent my love for collaborative work," she said. "The appeal of hackathons might come from my time in the military. The goal is tunnel vision. You work on one aspect of the problem, you trust your team and the process, and you will get a successful outcome."

Foertter is a tinkerer. It started when she was a child, but her innate inquisitiveness still drives her work as a user support specialist at the Oak Ridge Leadership Computing Facility.

Her road to computing expertise began in isolation, after she moved with her mother from Brazil to the United States. She was 12, and the language barrier in those early days left her feeling alone, so she found solace in tinkering—dual-booting her mother's personal computer to run multiple operating systems, for instance, or taking apart old appliances to build circuits.

Her love of learning followed her to the OLCF when she joined the center in 2012, and she soon volunteered to make training one of her main focus areas. "My thinking was, 'This isn't the most high-profile job, but it is really important.'"



Fernanda Foertter

To date, Fernanda has helped organize eight hackathons, some as far away as Switzerland and Germany.—*Eric Gedenk*

For more information: http://go.usa.gov/x3DM3

Large-scale technique produces quantum dots

A method to produce significant amounts of semiconducting nanoparticles for light-emitting displays, sensors, solar panels and biomedical applications has gained momentum with a demonstration by researchers at ORNL.

While zinc sulfide nanoparticles—a type of quantum dot that is a semiconductor—have many potential applications, high cost and limited availability have been obstacles to their widespread use. That could change, however, because of a scalable ORNL technique outlined in a paper published in *Applied Microbiology and Biotechnology*.

Unlike conventional inorganic approaches that use expensive precursors, toxic chemicals, high temperatures and high pressures, a team led by ORNL's Ji-Won Moon used bacteria fed by inexpensive sugar at a temperature of 150 degrees Fahrenheit in 25- and 250-gallon reactors. Ultimately the team produced about three-fourths of a pound of zinc sulfide

Using this 250-gallon reactor, ORNL researchers produced three-fourths of a pound of zinc sulfide quantum dots, shown in the inset. Image credit: ORNL

nanoparticles without process optimization, leaving room for even higher yields.

The ORNL biomanufacturing technique is based on a platform technology that can also produce nanometer-size semiconducting materials as well as magnetic, photovoltaic, catalytic and phosphor materials. Unlike most biological synthesis technologies that occur inside the cell, ORNL's biomanufactured quantum dot synthesis occurs outside the cells. As a result the nanomaterials are produced as loose particles that are easy to separate through simple washing and centrifuging.—*Ron Walli*

For more information: http://go.usa.gov/xTYuw

Opening neurotransmission's gatekeepers

In an era of instant communication, perhaps no message-passing system is more underappreciated than the human body, which relies on a network of neurons to efficiently relay signals to the brain.

Neurons communicate by emitting signals composed of chemicals called neurotransmitters. To save energy these chemicals are released and recaptured by so-called neurotransmitter transporters, membrane proteins that act as chemical "gatekeepers."

Understanding how these proteins function—both as energy-driven systems and as key machinery in biological processes—is one of the primary aims of Harel Weinstein's laboratory at the Weill Cornell Medical College of Cornell University. Using the Titan supercomputer at ORNL, Weinstein's team produced the first comprehensive 3-D simulation of a specific type of neurotransmitter transporter called the dopamine transporter, or DAT.

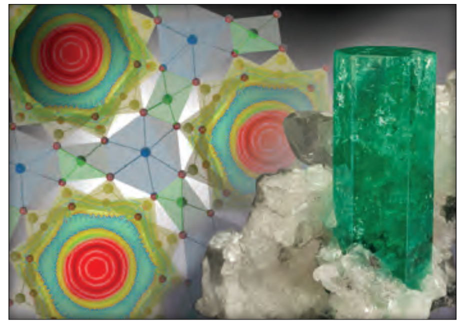
By simulating DAT, Weinstein and his collaborators are not only learning how cells harness energy to move molecules against a concentration gradient but also uncovering potential strategies for treating DAT-related disorders such as addiction and depression.

"In our simulation on Titan, we were able to incorporate new experimental data into our DAT model and follow its movements over long periods of time, which made all the difference," Weinstein said.—*Jonathan Hines*

For more information: http://go.usa.gov/chHjQ

Researchers discover new state of water molecule

Neutron scattering and computational modeling have revealed unique and unex-



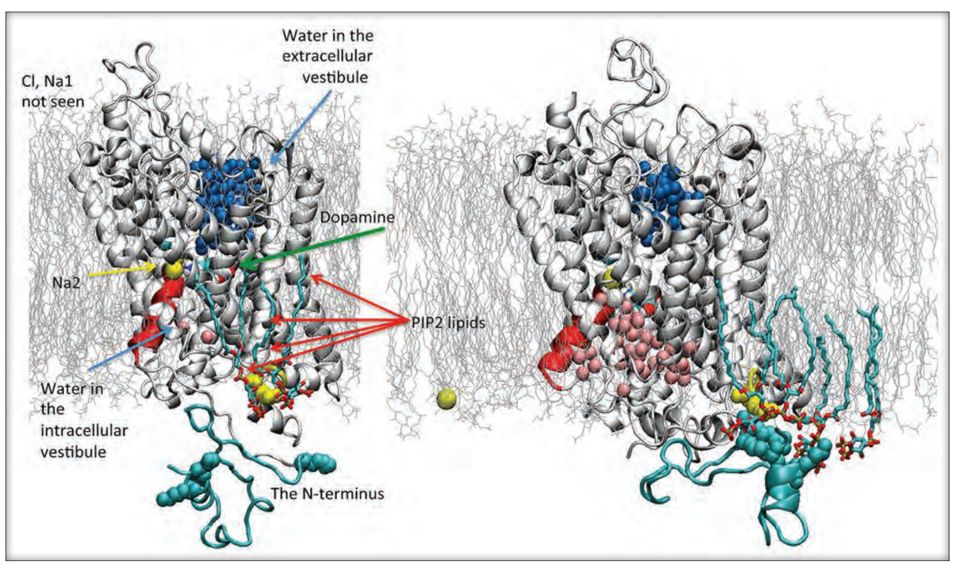
Water in beryl displays some unique and unexpected characteristics. Image credit: Jeff Scovil

pected behavior of water molecules under extreme confinement that is unmatched by any known gas, liquid or solid states.

In a paper published in *Physical Review Letters*, ORNL researchers describe a new tunneling state of water molecules confined in hexagonal ultra-small channels—5 angstroms across—of the mineral beryl. An angstrom is 1/10-billionth of a meter, and individual atoms are typically about 1 angstrom in diameter.

The discovery, made possible with experiments at ORNL's Spallation Neutron Source and the Rutherford Appleton Laboratory in the United Kingdom, demonstrates features of water under ultra confinement in rocks, soil and cell walls, which scientists predict will be of interest across many disciplines.

"At low temperatures this tunneling water exhibits quantum motion through



An illustration of the dopamine transporter in its outward- (left) and inward-opening (right) state. Note that the inward opening has brought about an outward closing and a change in the number of water molecules (blue and pink spheres) inside and outside the cell. Image courtesy of Cornell University the separating potential walls, which is forbidden in the classical world," said lead author Alexander Kolesnikov of ORNL's Chemical and Engineering Materials Division. "This means that the oxygen and hydrogen atoms of the water molecule are 'delocalized' and therefore simultaneously present in all six symmetrically equivalent positions in the channel. It's one of those phenomena that only occurs in quantum mechanics and has no parallel in our everyday experience."—*Ron Walli*

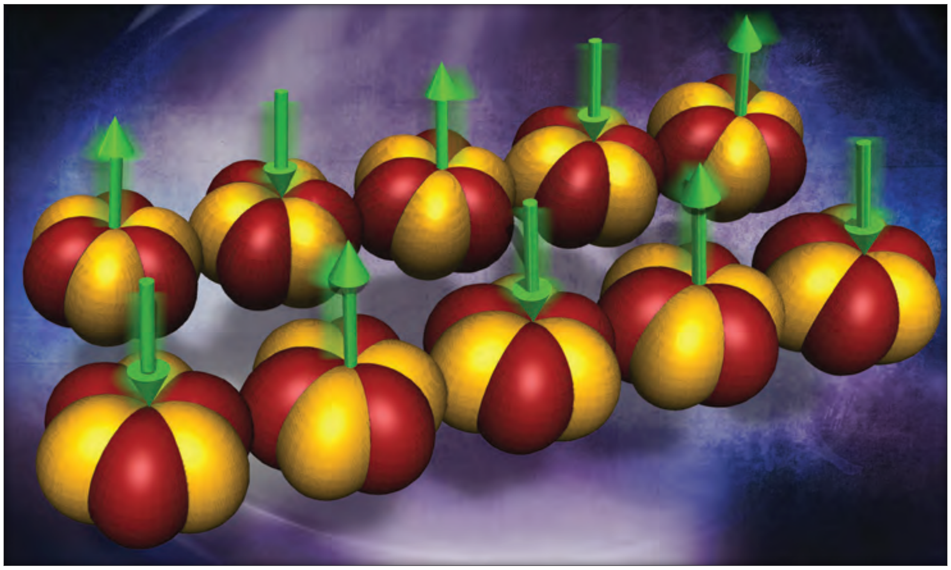
For more information: http://go.usa.gov/chSwe

In the Arctic, dry soils mean more released carbon

A study published in *Nature Climate Change* indicates soil moisture levels will determine how much carbon is released to the atmosphere as rising temperatures thaw Arctic lands.

An international team led by Northern Arizona University scientists analyzed the results of 25 experiments from multiple research groups including ORNL. The researchers had measured the release of greenhouse gases from incubated soil samples, which originated in field sites in Alaska, Canada and Russia, under a temperature increase of 10 degrees Celsius.

ORNL's Kenneth Lowe operates a hydraulic drill to collect frozen soil cores from Barrow for incubation experiments. Image credit: ORNL



This illustration shows the one-dimensional ytterbium ion chain in the quantum magnet Yb_2Pt_2Pb. The ytterbium orbitals are depicted as the iso-surfaces, and the green arrows indicate the antiferromagnetically aligned ytterbium magnetic moments. Image credit: Genevieve Martin, ORNL

Researchers found that soils with plenty of oxygen from air released about 3.4 times more carbon than wetter soils with limited oxygen. Even accounting for the effects of methane—an extremely potent greenhouse gas produced by microbes in saturated, oxygen-free soils—oxygen-rich soils still released comparatively more carbon.

"It tells us that the tipping point is more toward when that soil becomes exposed to oxygen," ORNL coauthor David Graham said. "If the soils were to drain and dry, it would be a significant change that would dramatically alter the carbon flux coming out of the soil."—*Morgan McCorkle*

For more information: http://go.usa.gov/chsuW

Neutrons reveal unexpected magnetism in rare-earth alloy

A new study by a multi-institutional team, led by researchers from Brookhaven National Laboratory and Stony Brook University, has revealed exotic magnetic properties in a rare-earth-based intermetallic compound. Similar studies suggest a better understanding of those types of behaviors could lead to applications in quantum computing and improved storage-device technologies.

ORNL researchers and their collaborators used neutron scattering to uncover magnetic excitations in the metallic compound ytterbium-platinum-lead. Surprisingly, this 3-D material exhibits magnetic properties that one would conventionally expect if the connectivity between magnetic ions were only one-dimensional. Their research is discussed in a paper published in the journal *Science*.

An electron can theoretically be understood as a bound state of three quasiparticles, which collectively carry its identity: spin, charge and orbit. It has been known that the spinon, the entity that carries information about electron spin, can "separate" itself from the others under certain conditions in one-dimensional chains of magnetic ions such as copper in an insulating host. Now the new study reveals that spinons are also present in metallic ytterbium-platinum-lead.

The experimental team included ORNL postdoctoral researcher and lead author Liusuo Wu and Georg Ehlers and Andrey Podlesnyak, instrument scientists at ORNL's Spallation Neutron Source. The team made use of the neutrons' sensitivity to magnetic fluctuations at the atomic scale and the world-leading capabilities of the SNS Cold Neutron Chopper Spectrometer instrument.—*Jeremy Rumsey*

For more information: http://go.usa.gov/xTgaF

Looking to the future of science

ORNL winners of the 2016 Early Career Research Program award from DOE's Office of Science, from left: Melanie Mayes, Travis Humble, Clayton Webster, and Wellington Muchero.
Image credit: Carlos Jones, ORNL

ORNL prepares young researchers to lead

by Leo Williams
williamsjl2@ornl.gov

ORNL's Olga Ovchinnikova saw an opportunity early this year during a one-on-one meeting with Thomas Zacharia.

Zacharia, the lab's deputy for science and technology, makes a point of sitting down with young scientists. Ovchinnikova, a chemical physicist in ORNL's Center for Nanophase Materials Sciences, used the time in part to make the case for advanced microscopy equipment.

She had just been heavily involved in getting one high-tech chemical imaging device up and running—a mass spectrometer that focuses a pulsed ion beam on a sample to obtain detailed surface information—but for years ORNL researchers had been trying to obtain another powerful device: a monochromated aberration-corrected scanning transmission electron microscope. This new tool would visualize vibrational energy and provide insights into magnetic excitations and chemical bonding, and it would complement the lab's strength in neutron scattering.

Olga Ovchinnikova

"I was telling Thomas that we're not really taking full advantage of the instrument," Ovchinnikova explained. "We could be real leaders in chemical imaging and imaging in general, and we could be better at leveraging our technologies. In terms of characterizing and understanding chemical functionality, you can't just have one tool."

Not only did Zacharia listen, he asked Ovchinnikova to shepherd a proposal for the new machine. Working with her colleagues and managers, and integrating years of groundwork done by other imaging scientists into one story, she handed in the document within two weeks, Zacharia agreed with their recommendation, and the new electron microscope is expected in September 2016.

Bringing young scientists into the fold

This story is noteworthy not only because it brought in a device that will greatly strengthen the lab's imaging capabilities, but also because Ovchinnikova has been a staff scientist here for only four years.

"This is an example where early-career scientists are talking to the top level in the lab," said Moe Khaleel, ORNL's director of institutional planning. "They're not making the decisions, but they're influencing the decisions. It's a very nice thing when you realize that, as an early-career scientist, if you have the right thoughts, the right level of energy, things can happen."

Others also see the value in ORNL's young researchers. Four recently received Early Career Research Program awards from DOE's Office of Science (see stories on pages 8, 9, 10 and 11).

ORNL works to mentor its young scientists and engineers, giving both lab staff and postdoctoral researchers the opportunity to share ideas and learn skills they will need in the research world. The strategy can be seen in approaches ranging from regular classroom opportunities in grant and proposal writing to the inclusion of early-career staffers in decision-making committees.

The strategy helps young researchers, certainly, but it also helps ORNL.

"Sixty-seven percent of the laboratory's scientific population has been here less than 10 years," Zacharia explained. "It is their future. Giving them a sense of ownership for the trajectory of the laboratory is very important so they can take great pride 10 years from now, 15 years from now, knowing they shaped how this institution evolved."

One major component of this support is the opportunity to guide and conduct ORNL-funded research under the Laboratory Directed Research and Development program. According to John Neal of the lab's Office of Institutional Planning, early-career researchers are well represented in the program both as principal investigators and within the committees that guide the program.

Neal also noted that the lab's Named Fellowship program, which operates within the LDRD program, gives a limited number of outstanding postdoctoral researchers the opportunity to spend a significant portion of their time conducting research on a topic of their choosing.

These opportunities give young researchers the tools they need to later seek funding outside the lab.

"If you give me an LDRD as an early career, you're using your internal resources to grow me as a principal investigator," Khaleel said. "Then I become more competitive on the outside. It's good for us, and good for the individuals."

As Neal points out, committee posts may offer just as fruitful an experience.

"Not only do they learn the internal process," he said, "but one of the best ways to learn how to write better proposals and give better presentations is to watch a lot of people do so. You can see what works and what does not from the other side of the table."

Postdocs get their due

The mentoring process is important not just for staff researchers. ORNL has also spent the last three years revamping the program for its 300-plus postdoctoral researchers. According to Ian Anderson, ORNL's director of Graduate Education and University Partnerships, the lab wanted to avoid two common pitfalls of postdoc hiring: treating the young researchers as cheap labor without giving them the opportunity to grow in their careers and treating them as permanent postdocs.

"A postdoc is still a training position," Anderson said. "These are not yet full-fledged scientists; they still need that last bit of training to be able to run on their own. And they are not just a cheap pair of hands."

Among changes brought to the program, postdocs are now encouraged to participate in a wide range of professional-development activities that can help them further their careers. They hold postdoctoral positions for two or three years only, and they cannot have had more than one previous postdoctoral appointment.

In addition, they have their own organization. The Oak Ridge National Laboratory Postdoctoral Association sponsors events including a research symposium and a career fair and fills a position on the postdoc program's advisory committee from among the postdoc community.

Encouraging researchers to stay

For ORNL the commitment to helping young scientists and engineers is a way both to retain talented individuals and to generate goodwill. Anderson noted, for instance, that most ORNL postdocs will not stay at the lab; nevertheless, those who have a positive experience will enhance the lab's reputation.

For researchers who stay, the presence of new opportunities and a supportive community may help keep them at the lab.

"What we're trying to do is create a labwide environment to retain them," Khaleel said. "If your colleagues are people who are pushing the envelope on technology and science, you want to be part of that. So what we're trying to do is create these forums where they can dialogue, talk, work together, and so on."

Ultimately, if ORNL does right by its young researchers, they will be in a better position to do right by the lab.

"Today I am closer to the end of my career than to the beginning," Zacharia said. "My biggest priority is to help these early-career staff realize their potential and the promise that they have, because their success is the success of this institution. It's also the promise of a better future. That's why it's very important."

When soils exhale

One thing the earth does very well is recycle—plants, animals, even us. Living things grow and thrive by taking elements from the earth and the sky, and when they die, those elements are returned. As the Book of Common Prayer puts it, "Earth to earth, ashes to ashes, dust to dust."

This recycling job falls to microbes, countless microscopic organisms that break down organic material and return elements to the soil and the atmosphere. How they go about this task is critical not only to the regeneration of life but to the workings of our climate as well.

> *"That's actually something I love about ORNL. ORNL and DOE are mission-driven agencies. What that means is, if there is a need for something to be done, and you have the initiative and the desire to figure out how to do it, you can do it."*
>
> — ORNL researcher **Melanie Mayes**

It is also the focus of the Early Career Research Program award won by ORNL researcher Melanie Mayes.

"Soils store large percentages of carbon here on earth, more than the atmosphere and the biosphere combined," Mayes explained. "They're very significant, but they're also very hard to understand, because they are heterogeneous. We have everything from tropical soils, which have lots of rainfall and are highly leached, to permafrost soils, in which carbon gets stored quite readily, because it's frozen and doesn't decompose."

Mayes's early career award, which comes from DOE's Office of Science, will allow her to spend the next five years increasing our understanding of how microbes do their jobs in wet, tropical regions and how they drive the release of greenhouse gases such as carbon dioxide, nitrous oxide and methane.

The project is timely in part because climate science needs a boost in both: wet soil and the tropics. Eventually the insights coming from this project will be available for use in climate modeling.

When microbes break down plants and animals in the soil, they typically rely on oxygen-burning aerobic processes. In swamps, bogs and other wet soils, however, they must go another route.

"In wet environments, you start to lose the oxygen in your system," she said, "so instead of consuming oxygen to decompose

See SOILS on page 12

Where there's a willow, there's a way

As rising temperatures continue to melt arctic permafrost that has been around for thousands of years, tons of carbon locked within this permafrost are released to the atmosphere in the form of carbon dioxide and methane, threatening to accelerate both the melting and global warming in general.

One potential bright spot in this alarming scenario is the plant life that has been appearing on land uncovered by the receding ice. These plants draw carbon from the atmosphere and have the ability to hold it throughout life spans that can run into decades. They can also be used as feedstock for valuable products such as biofuels and carbon fiber. The challenge, though, is that you need lots and lots of biomass to make these processes economically feasible.

Through an Early Career Research Program award from DOE's Office of Science, ORNL quantitative geneticist Wellington Muchero will be working to understand and enhance the ability of arctic plants to capture carbon for long-term storage and conversion into renewable bioproducts. His work focuses on the genus *Salix*—willows—a widely used bioenergy crop that has emerged as a key species in colonizing land exposed by receding arctic permafrost.

The key to a plant's ability to capture and store carbon can be found in its relationship with soil microbes, Muchero said.

"My interest is in understanding how plants accommodate symbiotic microbes, which help them perform functions that they cannot perform by themselves," he explained.

> *"ORNL has an unparalleled legacy in translating fundamental discoveries into practical solutions, so I'm in the right environment for finding applications for my research."*
>
> — ORNL quantitative geneticist **Wellington Muchero**

Among these microbes are ones that help the plant grab nutrients from its environment. Not only does the process promote the goal of carbon capture, he said, but also helps the plant thrive, much like chemical fertilizers would. The challenge is that plants have a love–hate relationship with soil microbes; they have very strong defenses to ward off those they regard as harmful, but they can relax these defenses for microbes they deem helpful. The choices they make are genetically coded and differ from species to species.

Muchero's goal in this project is to identify plant–microbe combinations that promote carbon capture, identify plant genes

See WILLOW on page 12

Computing by the atom

Computers that grow ever faster require creators who are ever more inventive.

The inventors have done well so far, boosting individual processors by fabricating tinier and tinier components, networking hundreds of thousands of processors together, and commandeering specialized devices such as graphics processing units to act as accelerators.

Each approach works, but each has its limits, and only revolutionary approaches will allow the pace of progress to continue.

One promising strategy is quantum computing, systems that rely on the strange behavior of nature's tiniest particles. ORNL quantum computer scientist Travis Humble is committed to bringing this technology to scientific computing.

Humble is also winner of an Early Career Research Program award from DOE's Office of Science. The award will support his efforts to promote the creation of quantum processing units, GPU-like accelerators based on quantum physics.

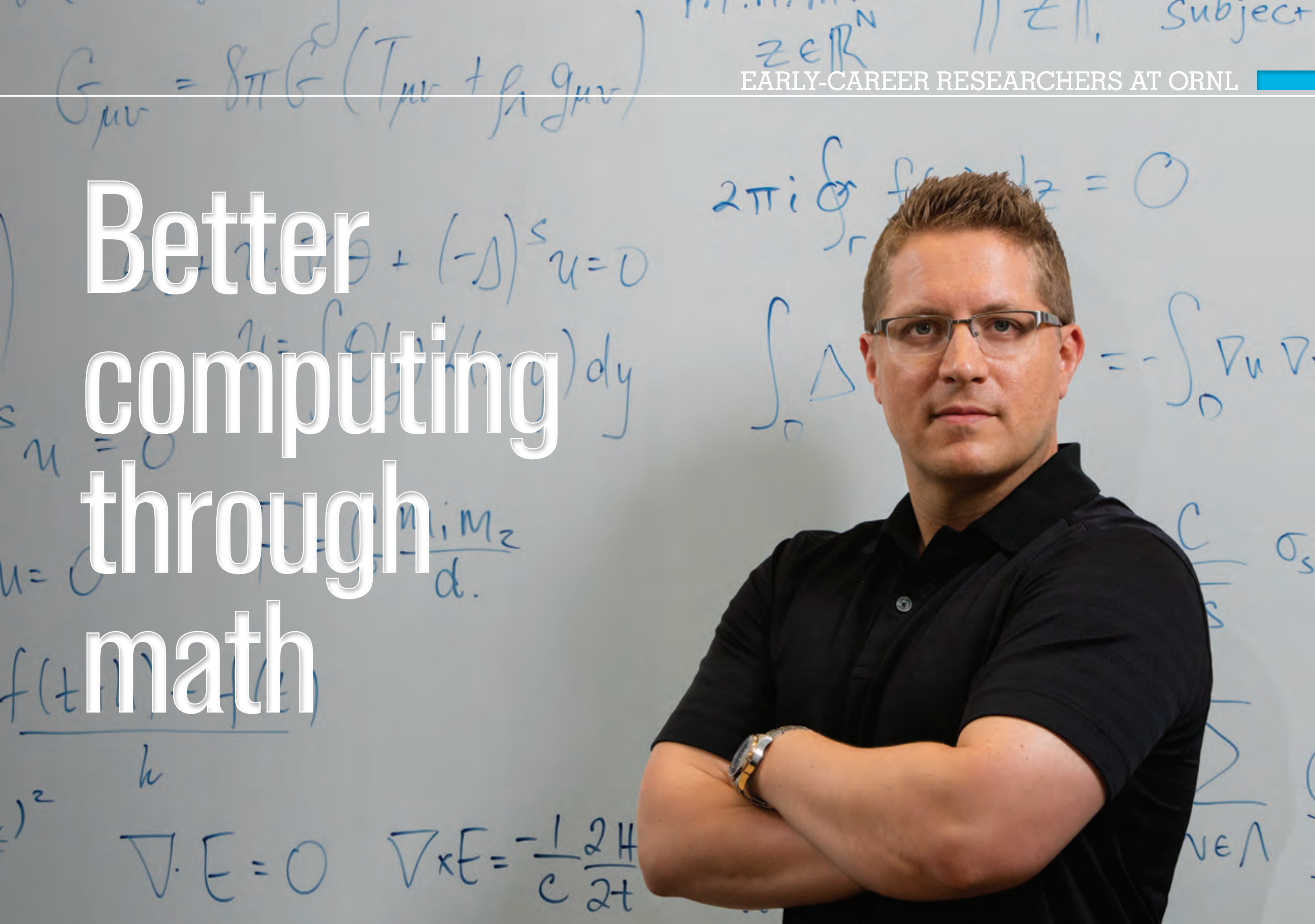
Quantum computing gets its promise from physical properties found only at the nanoscale. One is superposition, which allows a particle to be in more than one contradictory state at the same time (pointing both up and down, for instance). Another is entanglement, in which two or more particles are connected, so changes in one are reflected by the others.

These properties open up enormous possibilities for computing if they can be harnessed. While the fundamental building block of traditional computing, the bit, has only two possible values ("0" or "1"), the building block of quantum computing—known as a quantum bit, or qubit (pronounced "CUE-bit")—can have a value of "0" or "1" or both simultaneously. In addition, multiple qubits can be entangled so a change to one will also change the others.

> *"There is this idea that we can build a computer that basically uses individual atoms to do computation. As soon as you do that, the physics of the atoms makes it possible to do things that you can't do with normal computers."*
>
> — **Travis Humble**, ORNL quantum computer scientist

"When you flip a penny, it can be heads or tails," Humble explained. "But in the quantum world, when you flip a penny, it

See COMPUTING on page 13



Better computing through math

The goal of scientific computing has always been to recreate the physical world, but the physical world is extraordinarily complex. Whether you're simulating a nuclear reactor or something as seemingly simple as the flow of air over a wing, there are more factors—or variables—to consider than even the most powerful systems can handle if you need all the details.

Even physical experiments fall victim to chance.

"Nothing is deterministic," ORNL mathematician Clayton Webster explained. "The air flowing over a wing, normally we would say it flows at some rate, so we fix that. But that's definitely not true. If you've been on an airplane and experienced turbulence, it's simply because of the way that air flows over a wing. It's definitely not a constant rate."

Webster is the winner of an Early Career Research Program award from DOE's Office of Science. He is working to develop more sophisticated means to identify the mathematical underpinnings for complex systems, whether they are associated with a computational simulation or a physical experiment.

His job, finding the important information in mountains of data, is akin to the task of compressing digital images. While the original image has three values for each pixel—corresponding with its red, green and blue levels—developers have been able to identify the data most important to re-creating the image and, possibly more importantly, the information that can be left behind with minimal loss to the image's quality.

> *"Outside of my parents, I was told by everyone else, 'I don't know what you will do with a degree in math.' I pointed out to them that you can do anything with a degree in math. It's been very good to me, but it's also a curse, because a mathematician never stops thinking about their problems. Otherwise, it's my hobby. It's what I do."*
>
> — ORNL mathematician **Clayton Webster**

"The things that we do in some sense mimic that procedure," Webster explained. "The challenge is that now I don't have an image, but I have something very complicated under the hood, and I want to play the same game. I want to look at some complicated

See MATH on page 13

SOILS from page 8

organic matter, you use other products such as nitrate, sulfate, and eventually carbon dioxide. Oxygen-mediated processes yield carbon dioxide as a waste product, while anaerobic processes yield nitrous oxide and methane. Methane and nitrous oxide both have a shorter half-life in the atmosphere than carbon dioxide, but they are more potent greenhouse gases."

> *"I thought, 'Man, I really like this science thing.' Eventually it hit home that I wasn't going to be a journalist, so I went into geology."*
>
> — ORNL researcher **Melanie Mayes**

The project will link specific genes within the soil microbial community to their role in producing specific greenhouse gases. Mayes and her colleagues will work in Puerto Rico and Panama, noting gases released in different seasons, during both wet and dry spells. She will also bring soils back to ORNL for study under more controlled conditions and genetic analyses of the soil microbial community.

Mayes grew up in rural Missouri. She entered the University of Missouri thinking she would pursue a journalism career, largely because she had an aptitude for writing. What she discovered, however, was that she was having a much better time in her science courses.

"I didn't like journalism, but I had taken a geology class, and an anthropology class, and a sociology class. And I thought, 'Man, I really like this science thing.' Eventually it hit home that I wasn't going to be a journalist, so I went into geology."

She has been at ORNL in one capacity or another since shortly after she received her bachelor's degree, completing a master's and Ph.D. at the University of Tennessee. Before working on climate projects, she studied radionuclides and toxic metals in the ground—an interest she maintains with a continuing study of mercury contamination.

Her ability to tackle diverse problems is reflected even in the fluidity of her professional designation. After all, what kind of scientist is she?

"That's a great question. My career hasn't allowed for easy pigeon-holing. My background is in geology, but I've never done any traditional geology—I did hydrology and geochemistry. And now I'm doing soils and climate work, and even microbiology. I'm not really a soil scientist, because I don't have a degree in soil science. Am I a climate scientist? Well, that's a different thing, too.

"That's actually something I love about ORNL. ORNL and DOE are mission-driven agencies. What that means is, if there is a need for something to be done, and you have the initiative and the desire to figure out how to do it, you can do it. People don't stop you; they help you."

WILLOW from page 9

that play nice with those microbes, and use these genes to enhance other willow species. In the project, he is going to work with willow collections at West Virginia University and New York's Cornell University, as well as research sites in the arctic.

The process will be painstaking. First, Muchero and his colleagues must collect samples from each location, identify microbes that interact most closely with individual species, and analyze the genome of each species. Once they identify differences in the genome, they must find those that promote plant–microbe interactions and carbon capture.

"When we look at differences in genomes among willow species, that's where things get very exciting but also very challenging," Muchero said. "Some of the differences will have nothing to do with plant–microbe interactions. They may be responsible for things like differences in leaf shape or whether one species prefers direct sunlight or shade. So, we'll be trying to disentangle those differences that are just random from differences that actually control beneficial interactions."

> *"This was right at the time when I was trying to make long-term career choices after a brief stint working as an administrator in the life insurance industry and realizing that finance wasn't my calling."*
>
> — ORNL quantitative geneticist **Wellington Muchero**

Muchero, who grew up in Zimbabwe, was attracted to science, especially biology, from a very early age. His enthusiasm was stoked when he learned about the world's first cloned animal, Dolly the sheep, born in 1996.

"This was right at the time when I was trying to make long-term career choices after a brief stint working as an administrator in the life insurance industry and realizing that finance wasn't my calling," he said. "It really captured my imagination—that this thing called DNA could be manipulated in such amazing ways to do all these things we could really never conceive of."

From Zimbabwe he moved to California, earning a bachelor's degree at Cal Poly Pomona and a Ph.D. from the University of California at Riverside.

He has been a staff member at ORNL since 2010. As he grows in his career, he would like to find ways for himself and other researchers to more effectively follow through on the insights of their research.

"I would really love to find an avenue where we see more of our findings actually making a difference in the real world," he explained, "and DOE missions are typically directed at that more so than those of academic institutions. ORNL has an unparalleled legacy in translating fundamental discoveries into practical solutions, so I'm in the right environment for finding applications for my research."

COMPUTING from page 10

can be heads, tails, or a superposition of these states. Extending to the case of two pennies, they can again each be heads or tails. But a pair of quantum pennies can be entangled, so they will stay correlated even when flipped again and again.

> *"In 20 years I see myself solving problems using quantum computers as opposed to solving the problem of quantum computers. That's what I think would be ideal. I'm willing to put my money on that, because I believe it's worth it."*
>
> — **Travis Humble**, ORNL quantum computer scientist

"There is this idea that we can build a computer that basically uses individual atoms to do computation. As soon as you do that, the physics of the atoms makes it possible to do things that you can't do with normal computers. My job is to try to figure out how to make that work."

Humble's road to quantum computing began when he left the premed track, after realizing he didn't like the sight of blood. ("That was an important point," he joked.) Instead, he focused on theoretical chemistry, earning a bachelor's degree from the University of North Carolina at Wilmington and a Ph.D. from the University of Oregon.

He came to ORNL in 2005 as an Intelligence Community Postdoctoral Research Fellow and eventually joined ORNL's staff in the Computer Science and Mathematics Division.

"At the moment I'm focused on pulling together everybody at the lab that I can find to work on quantum computing, because I really think it's the type of goal that the lab is made for. It has so many disciplines that are required, and ORNL is one of the best places that I know of to find that diversity."

Eventually, he said, quantum computers will be an everyday reality, and he will be able to go back to focusing on theoretical chemistry.

"In 20 years I see myself solving problems using quantum computers as opposed to solving the problem of quantum computers. That's what I think would be ideal. I'm willing to put my money on that, because I believe it's worth it."

MATH from page 11

problem—it can be air flow over a wing or a reactor—and I want to understand some behavior of that complex object, but I want to do it in some reduced form where I can still get back all the features I want, but with minimal information."

If it's done right, the process will allow even the most powerful supercomputers to handle problems potentially thousands of times more complex than they otherwise could.

Webster, who leads the lab's Computational and Applied Mathematics Group, is a math person to the core and always has been.

"I was in gifted math classes starting in the second grade," he said. "That and baseball were all I ever wanted to do. I was lucky that I found what I wanted to do very early, because I pretty much am not good at anything else."

Webster grew up in Branford, Ontario—"the home of Wayne Gretzky and Alexander Graham Bell"—earning bachelor's and master's degrees from McMaster University before moving on to Florida State University for a Ph.D. Before coming to ORNL, he was a John von Neumann Fellow at Sandia National Laboratories and also worked in commodities trading, another math-intensive activity.

> *"I was in gifted math classes starting in the second grade. That and baseball were all I ever wanted to do. I was lucky that I found what I wanted to do very early, because I pretty much am not good at anything else."*
>
> — ORNL mathematician **Clayton Webster**

To the apparent surprise of many people he has encountered, Webster has not found his obsession with math to be limiting.

"Outside of my parents, I was told by everyone else, 'I don't know what you will do with a degree in math.' I pointed out to them that you can do anything with a degree in math," Webster said.

"It's been very good to me, but it's also a curse, because a mathematician never stops thinking about their problems. Otherwise, it's my hobby. It's what I do."

Printed components

benefit from manufacturing–computing collaboration

by Miki Nolin
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Mike Matheson of the Advanced Data and Workflow Group (front) and Vincent Paquit of the Manufacturing Demonstration Facility demonstrate 3-D visualization and real-time rendering of additive manufacturing data. Image credit: ORNL

Additive manufacturing—commonly known as 3-D printing—is transforming manufacturing by allowing the design and development of highly complex objects that would be impossible to create with traditional manufacturing methods.

Additive manufacturing is now at the tipping point of being broadly adopted by industry. The missing piece is certification and validation—in a nutshell, ensuring that printed objects are within their design specifications and have the material properties required for their final use.

To advance this technology—and to address certification requirements in particular—ORNL's Manufacturing Demonstration Facility is developing a data analytics framework for manufacturing. By integrating scientific knowledge from researchers focusing on material development, method optimizations, and data analytics, this framework aims to provide a better understanding of the material properties of additively manufactured components.

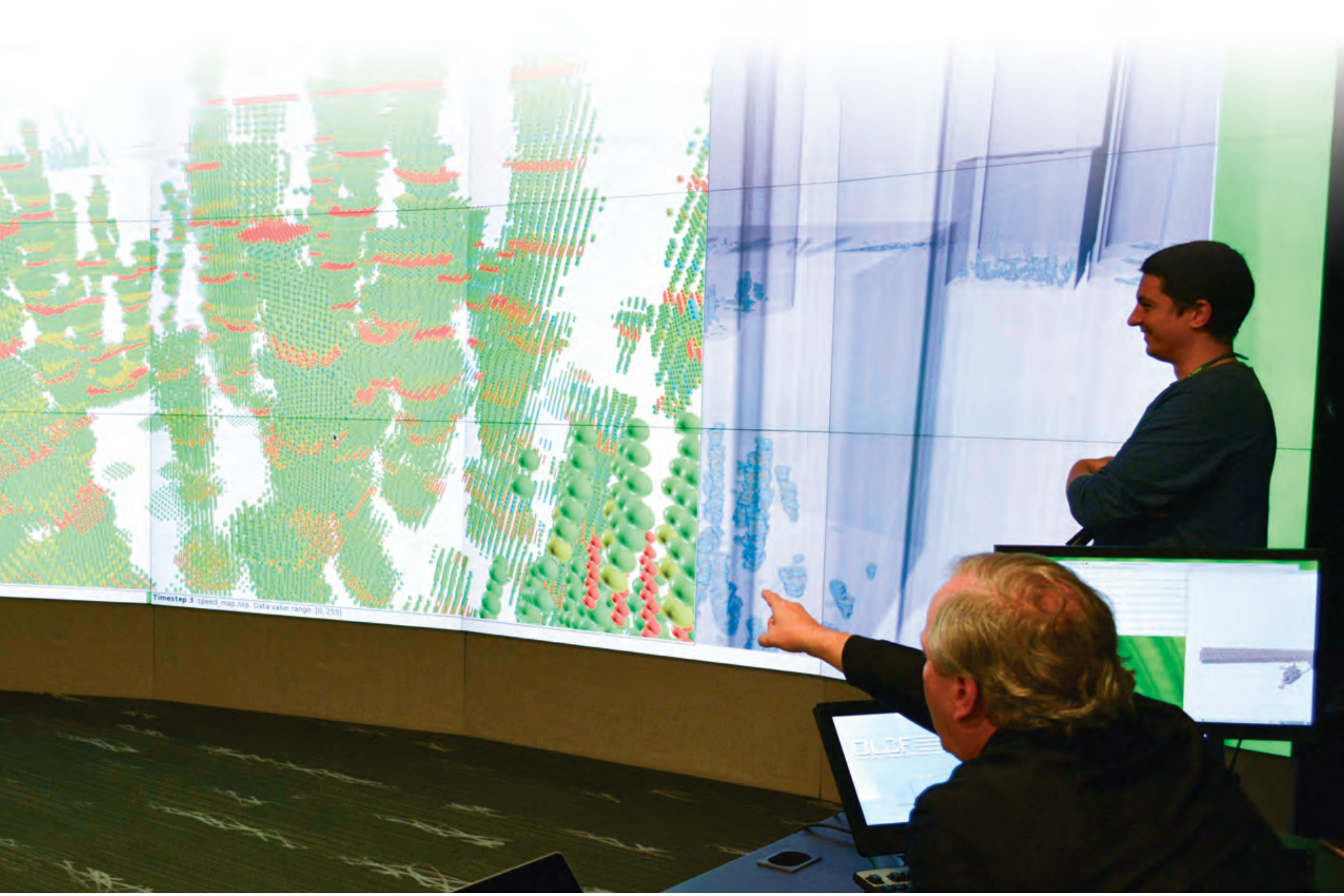
For materials scientists the ability to visualize this information in 3-D provides new insight into object quality and spatial information. The MDF reached out to the Oak Ridge Leadership Computing Facility's Advanced Data and Workflow Group to support such an effort.

The project began last fall after MDF staff realized they needed access to high-performance computing resources and visualization expertise to study variables related to additive manufacturing at a terabyte scale with extremely high resolution.

"We have experts who can help us do this at ORNL, so it made perfect sense to reach out to the Advanced Data and Workflow Group and leverage its expertise in the field," MDF researcher Vincent Paquit said. "We can gain greater understanding of the manufacturing process just by visualizing the data and manipulating the variables—something that the group is great at."

Testing 3-D printed objects begins with building the same part with several different parameters. The printing process can produce defects such as porosities—gaps in the material structure that can lead to part failure—so MDF researchers must understand what printing parameters lead to these defects and which processes ensure the highest-quality products.

"Currently, 3-D printing is at a stage where it's not mature enough to have set parameters that guarantee a product with no



defects," said Sreenivas Rangan Sukumar, group leader for the Advanced Data and Workflow Group. "By visualizing the object, the MDF can determine what is and isn't causing the defects."

To study its printed objects, the MDF requires high-quality images generated at interactive frame rates on large data-sets containing many variables. Off-the-shelf visualization tools cannot handle such demands, but the OLCF's EVEREST visualization facility, with its custom software and the necessary computing systems, can.

"We can gain greater understanding of the manufacturing process just by visualizing the data and manipulating the variables—something that the group is great at."

— **Vincent Paquit**, MDF researcher

The visualization workflow developed by Sukumar's group pulls data in real time from the MDF to the OLCF, including input from the computer-aided design model, image data, and immediate measurements from the printer. The data can then be retrieved by EVEREST, so MDF staff can visually determine how printing parameters and processes influence the printed component's porosity, malleability, and other structural characteristics, according to Mike Matheson, a member of Sukumar's group and the primary workflow developer.

The MDF is currently the main user of this workflow, but Sukumar's group began working to expand the service after additional OLCF users expressed interest in 3-D visualization.

Moving forward Sukumar's group plans to develop a mechanism that will allow the MDF to remotely view its 3-D artifacts. Facility staff will be able to wear a virtual-reality headset and walk through the 3-D models from anywhere.

By helping to ensure products get certified for quality, the visualization work is moving 3-D printing one step closer to transforming how high-quality commercial parts are made.

"Certification is the ultimate goal," Sukumar said. "We must certify that the 3-D printed object is what we set out to build and that it is built correctly."

Plug-free wireless charging demonstrated at ORNL

20-kilowatt wireless charging system for vehicles.
Image credit: Jason Richards, ORNL

by Ron Walli
wallira@ornl.gov

Electric vehicles are becoming increasingly convenient. Before long you won't even have to plug them in.

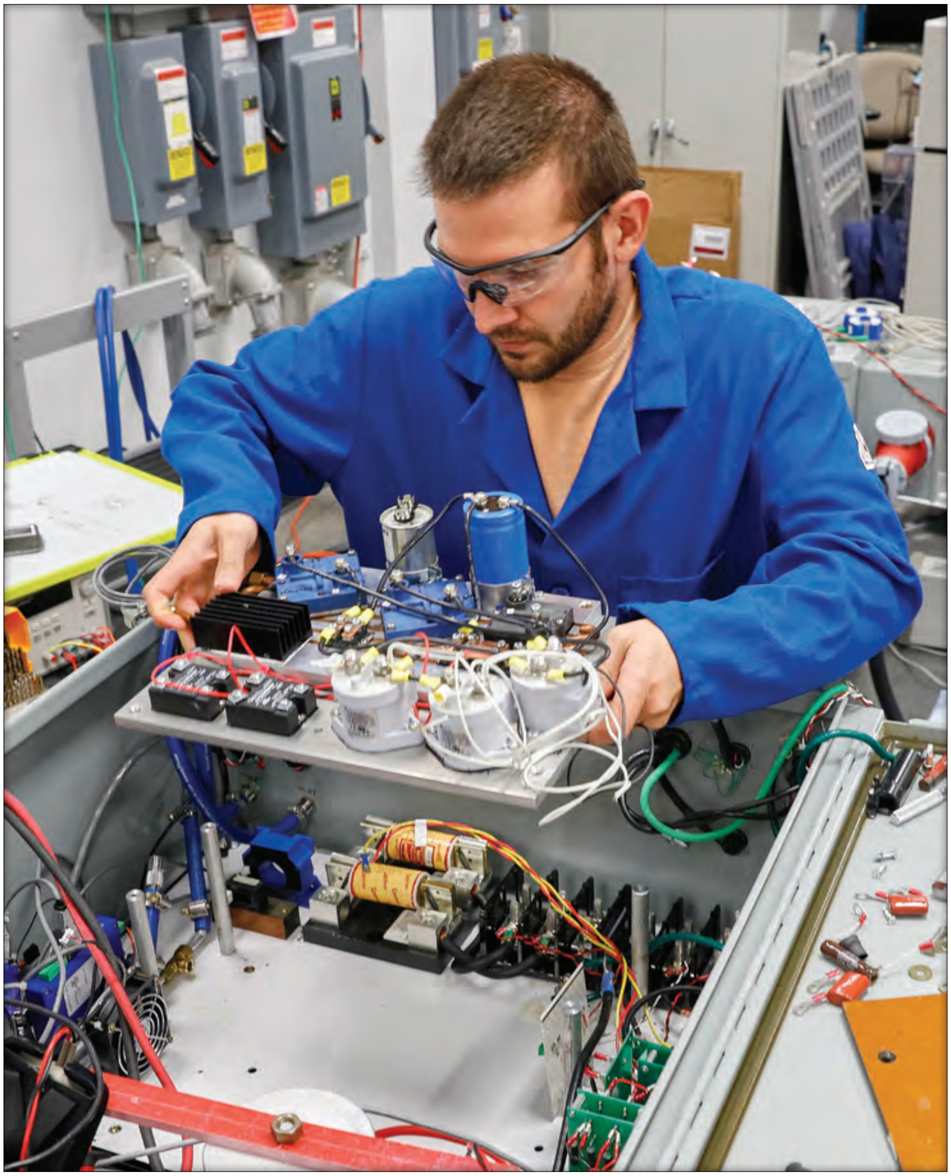
A 20-kilowatt wireless charging system demonstrated at ORNL has achieved 90 percent efficiency at three times the rate of the plug-in systems commonly used for electric vehicles today.

This ability can help accelerate the adoption and increase the convenience of electric vehicles. Industry partners from Toyota, Cisco Systems, Evatran, and Clemson University International Center for Automotive Research contributed to development of the technology.

"We have made tremendous progress from the lab proof-of-concept experiments a few years ago," said Madhu Chinthavali, ORNL Power Electronics Team lead. "We have set a path forward that started with solid engineering, design, scale-up and integration into several Toyota vehicles. We now have a technology that is moving closer to being ready for the market."

ORNL's Power Electronics Team achieved this world's-first 20-kilowatt wireless charging system for passenger cars by developing a unique architecture that included an ORNL-built inverter, isolation transformer, vehicle-side electronics and coupling technologies in fewer than three years. For the demonstration, researchers integrated the single-converter system into an electric Toyota RAV4 equipped with an additional 10-kilowatt-hour battery.

The researchers are already looking ahead to their next target of 50-kilowatt wireless charging, which would match the power levels of commercially available plug-in quick chargers. Providing the



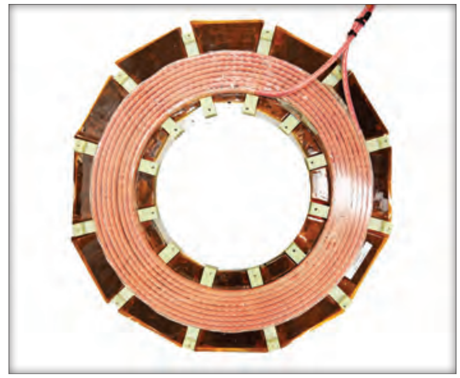
ORNL's Steven Campbell works with the electronics that enable wireless controls and communications between the grid and the wireless charging coils. Image credit: Carlos Jones, ORNL

> *"Wireless power transfer is a paradigm shift in electric vehicle charging that offers the consumer an autonomous, safe, efficient and convenient option to plug-in charging."*
>
> — **David Smith**, ORNL vehicle systems program manager

same speed with the convenience of wireless charging could increase consumer acceptance of electric vehicles and is considered a key enabler for hands-free, autonomous vehicles. Higher power levels are also essential for powering larger vehicles such as trucks and buses.

As the researchers advance their system to higher power levels, one of their chief considerations is safety.

"The high-frequency magnetic fields employed in power transfer across a large air gap are focused and shielded," Chinthavali said. "This means that magnetic fringe fields decrease rapidly to levels



Wireless power transfer coils. Image credit: Jason Richards, ORNL

well below limits set by international standards, including inside the vehicle, to ensure personal safety."

Convenience and simplicity are at the heart of the ORNL system, which places a strong emphasis on radio communications in the power-regulation feedback channel augmented by software-control algorithms. The result is minimization of vehicle onboard complexity as ORNL and partners pursue the long-range goal of connected vehicles, wireless communications and in-motion charging. While the team's initial focus has been static, or motionless, wireless charging, the researchers also evaluated and demonstrated the system's dynamic charging capabilities.

The Vehicle Technologies Office in DOE's Energy Efficiency and Renewable Energy Program provided funding for this competitively selected project as part of a broad portfolio in support of DOE's EV Everywhere Grand Challenge, which aims to make plug-in electric vehicles as affordable to own and operate as today's gasoline-powered vehicles by 2022.

"Wireless power transfer is a paradigm shift in electric vehicle charging that offers the consumer an autonomous, safe, efficient and convenient option to plug-in charging," said David Smith, vehicle systems program manager at ORNL. "The technology demonstrated today at ORNL is a stepping stone toward electrified roadways where vehicles could charge on the go."

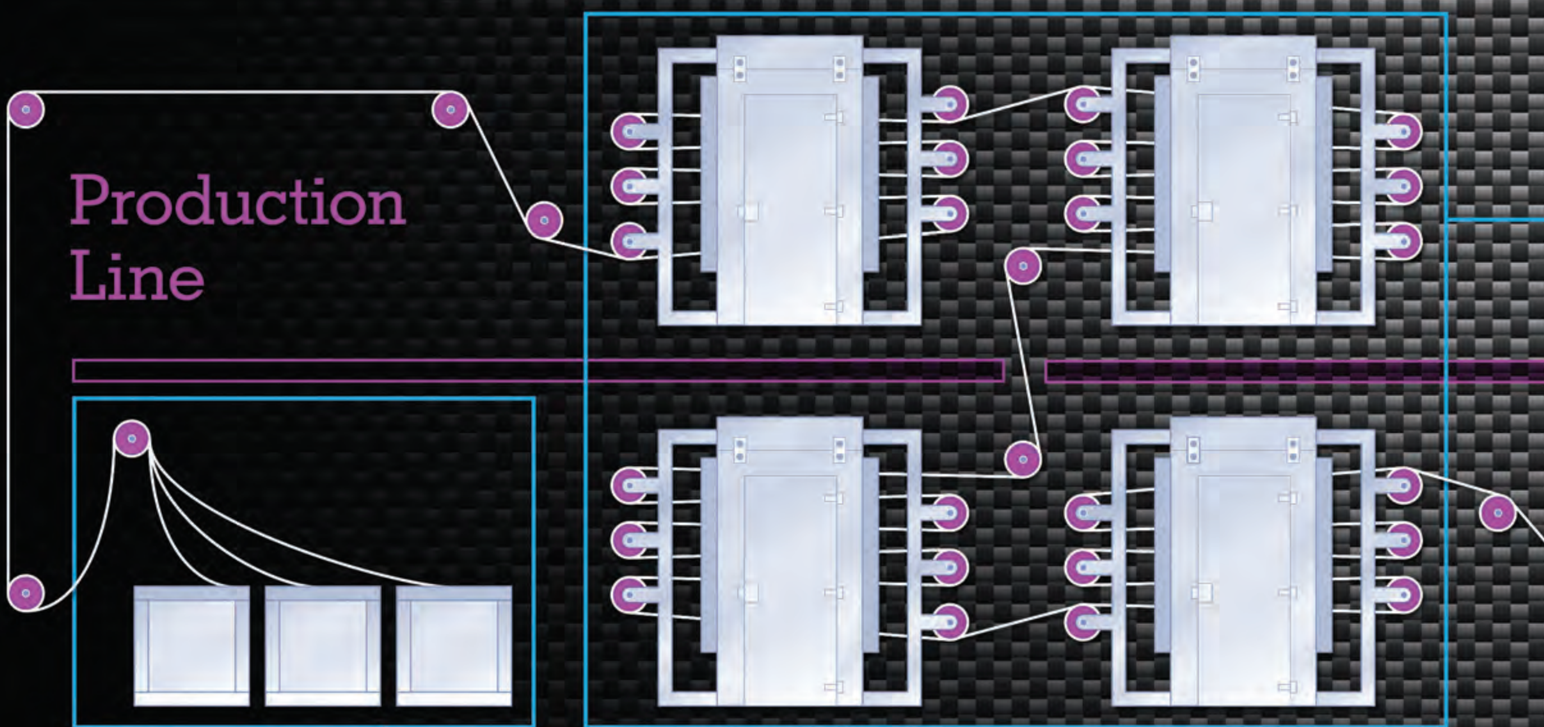
Toyota provided several vehicles for the research, including RAV4s, a Scion and a plug-in Prius.

Carbon Fiber Technology Facility

The CFTF is designed to produce up to 25 metric tons (about 26 U.S. tons) of carbon fiber each year, enough to develop and demonstrate new manufacturing processes. New production technology from ORNL allows the CFTF to run at up to three times its design capacity, although that is still far below the capacity of a typical commercial plant (1,500 metric tons, or about 1,650 U.S. tons).

Purposes of CFTF

- Demonstrate technology that can reduce the production cost of carbon fiber by at least half, enabling widespread use in vehicles and other high-volume energy applications. Strong and lightweight carbon fiber components improve fuel economy by reducing vehicle weight.
- Produce enough low-cost carbon fiber for manufacturers to use in manufacturing process evaluations and prototyping.
- Demonstrate scalability of novel carbon fiber production technologies.
- Function as training facility for carbon fiber production workers.



① Tow Feed Station

Production begins with a line (tow) that can contain more than 100,000 individual fibers.

- Specialty acrylic fiber: Expensive, intended for high-performance uses such as spacecraft and aircraft. *Currently used in nearly all commercial production.*
- Textile acrylic fiber: Much less expensive, used primarily in textiles (e.g., clothing, carpets). *ORNL researchers have used it to produce low-cost carbon fiber appropriate for the auto industry.*

② Ovens

The line runs 1–2 hours through four ovens at 200–300°C (roughly 400–600°F).

- The fiber oxidizes, preparing it for high-temperature furnaces later on.
- Air blows over fibers to aid in oxidation.

③ Furnaces

The line runs 2–5 minutes through a two-step carbonization process that turns it into carbon fiber.

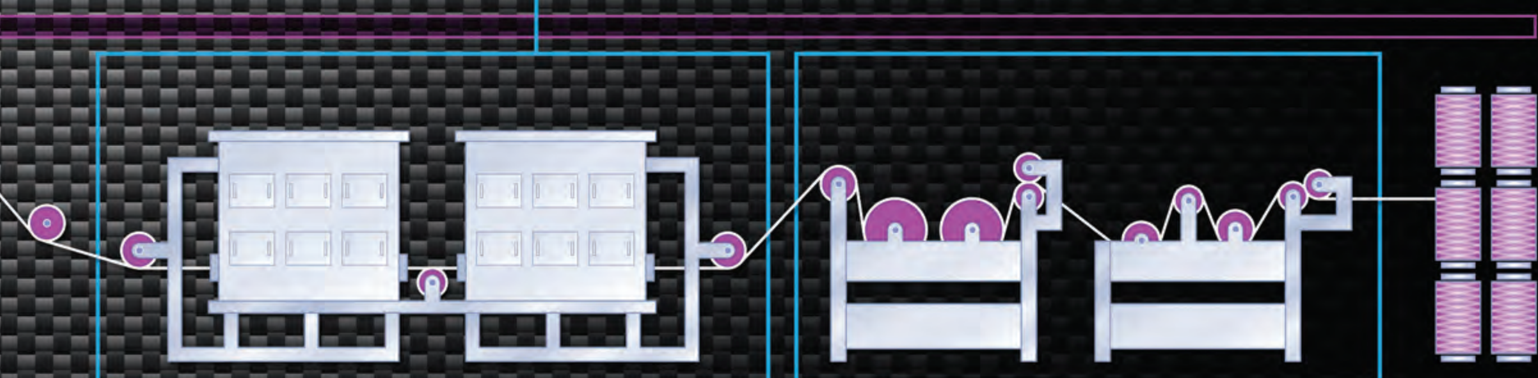
Furnace 1

- Rated to 1,000°C (about 1,800°F).
- Vaporizes about half the fiber mass, including nearly all the noncarbon material, which enters the pollution-control system.
- Begins developing the carbon fiber grain structure.

Furnace 2

- Rated to 2,000°C (about 3,600°F).
- Completes developing the carbon fiber grain structure.

Image credit: Brett Hopwood, ORNL



④ Posttreatment

- The fiber is plated with oxygen-containing chemical groups in an electrolysis bath, improving its ability to bond with resin to make effective composites.
- A polymer coating, or sizing, protects the fiber and aids in handling.

Broadening the bilayer

by Eric Gedenk
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Scientists studying cells once thought the cellular membrane was just a scaffold where proteins reside, passively allowing materials in and out.

However, as experimental methods and computational power advanced, many researchers started to see that lipids and proteins making up a cell membrane may actually have a more functional role than previously thought.

> *"Without having access to high-speed computing and neutron experiments, this study would be impossible."*
>
> — **Xiaolin Cheng**, ORNL researcher

With the help of two world-class ORNL research tools, the Titan supercomputer and the Spallation Neutron Source, researchers are studying the processes that govern lipid raft formation—a phenomenon with broad implications for research ranging from how cells regulate proteins to how viruses invade healthy cells.

"Without having access to high-speed computing and neutron experiments, this study would be impossible," said ORNL researcher Xiaolin Cheng. Cheng, ORNL researcher John Katsaras, and their respective research groups are collaborating to understand membrane organization and how it affects biology.

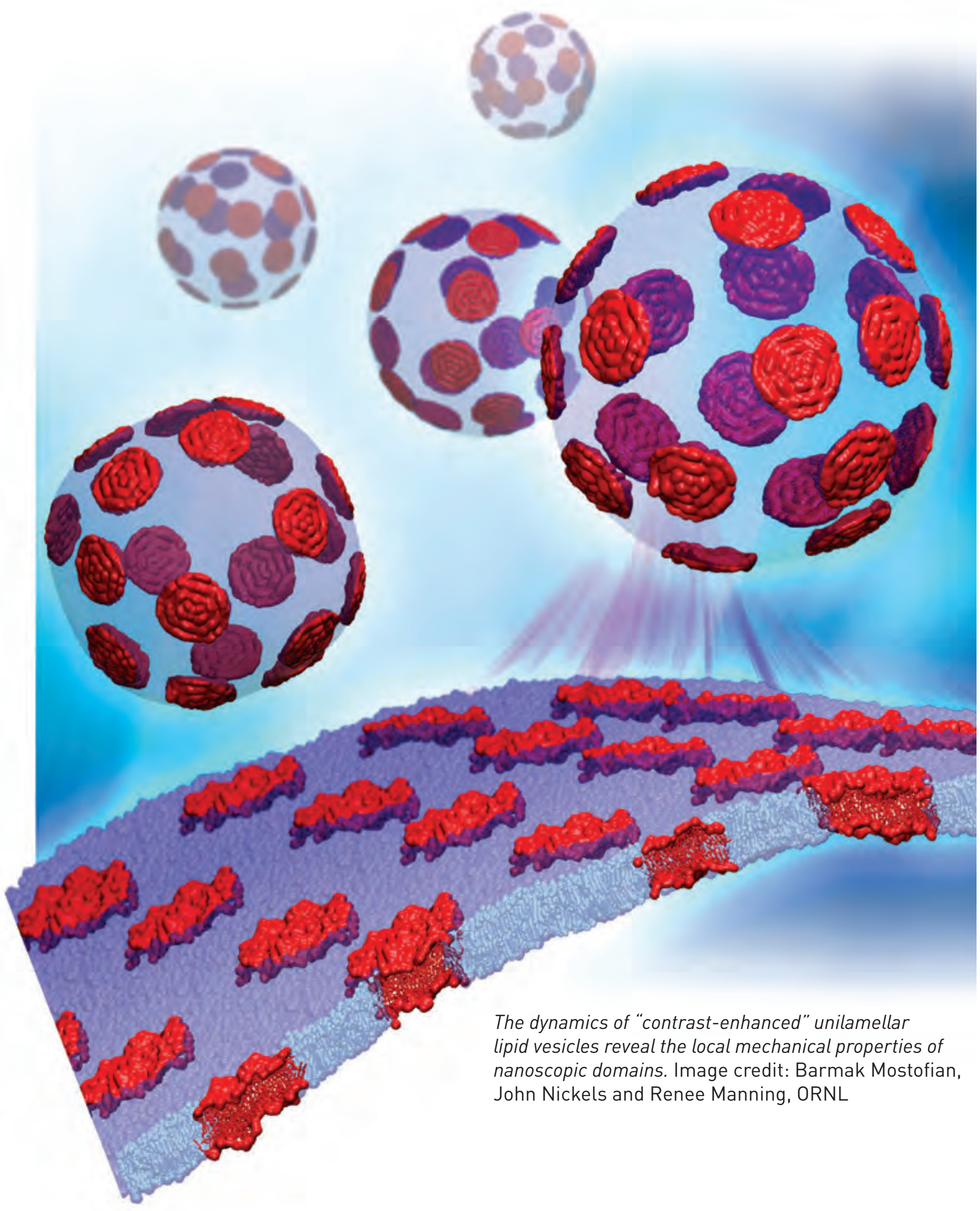
In the near term, the larger team seeks to determine the presence or absence of lipid rafts.

Despite efforts over 40 years, no experiment has conclusively shown the existence of lipid rafts in a living system because the rafts are very small and highly dynamic.

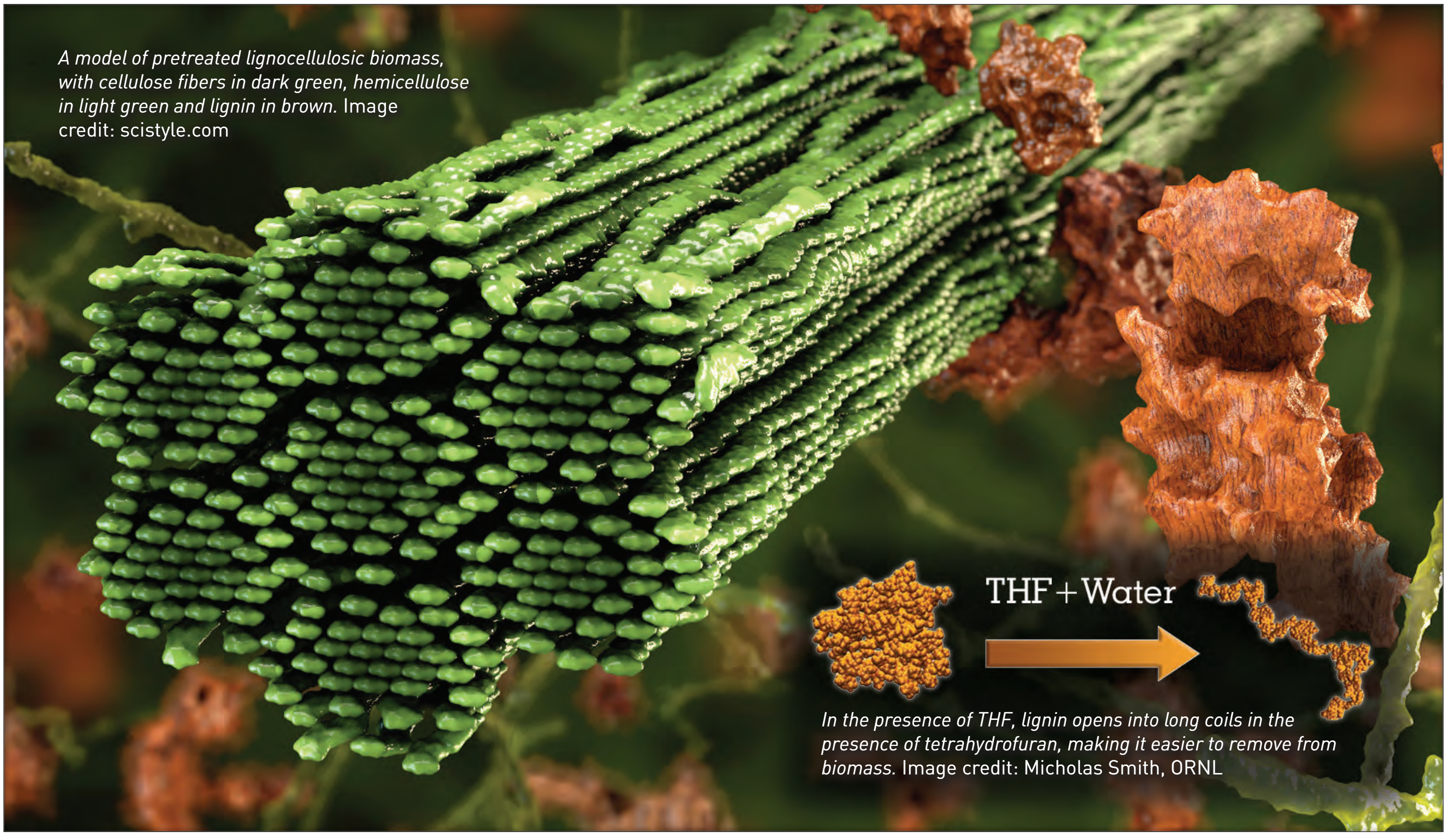
Access to SNS has allowed the Katsaras group to perform neutron spin echo experiments to observe the bending properties of the lipid patches that populate the membrane. "The neutron spin echo experiments allowed us, for the first time, to measure the mechanical properties of isolated, individual patches of lipids," Cheng said. "No other technique can do this. We basically measured the mechanical properties of this tiny patch by probing the undulation motion of the bilayer."

By introducing Titan, the researchers were able to simulate how the atoms' motions contribute to the signal. In essence, supercomputing was the only method for the team to verify its world-class experiments.

For more information: http://go.usa.gov/cttRP



The dynamics of "contrast-enhanced" unilamellar lipid vesicles reveal the local mechanical properties of nanoscopic domains. Image credit: Barmak Mostofian, John Nickels and Renee Manning, ORNL



A model of pretreated lignocellulosic biomass, with cellulose fibers in dark green, hemicellulose in light green and lignin in brown. Image credit: scistyle.com

In the presence of THF, lignin opens into long coils in the presence of tetrahydrofuran, making it easier to remove from biomass. Image credit: Micholas Smith, ORNL

Biofuel researchers

use Titan to probe 'lignin shield'

by Jonathan Hines
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When the Ford Motor Company's first automobile, the Model T, debuted in 1908, it ran on a corn-derived biofuel called ethanol, a substance Henry Ford dubbed "the fuel of the future."

Cheap fossil fuels undermined Ford's vision of wide-scale renewable transportation fuel, but recent advancements in biofuel research, including research conducted on the Titan supercomputer at ORNL, have rekindled the dream of economically viable ethanol.

Today, a major focus of biofuel research is cellulosic ethanol—alcohol made from woody plants, grasses, and waste biomass. Breaking down these plant materials into simple sugars is a costly and complex process, requiring large quantities of acid, water, and heat. Experimental pretreatments, however, hold the promise of driving down these costs by making more biomass available for fermentation by enzymes.

To better understand why these experimental pretreatments work, a team led by Jeremy Smith, the director of ORNL's Center for Molecular Biophysics, used Titan to study an effective solvent called cosolvent enhanced lignocellulose fractionation, or CELF.

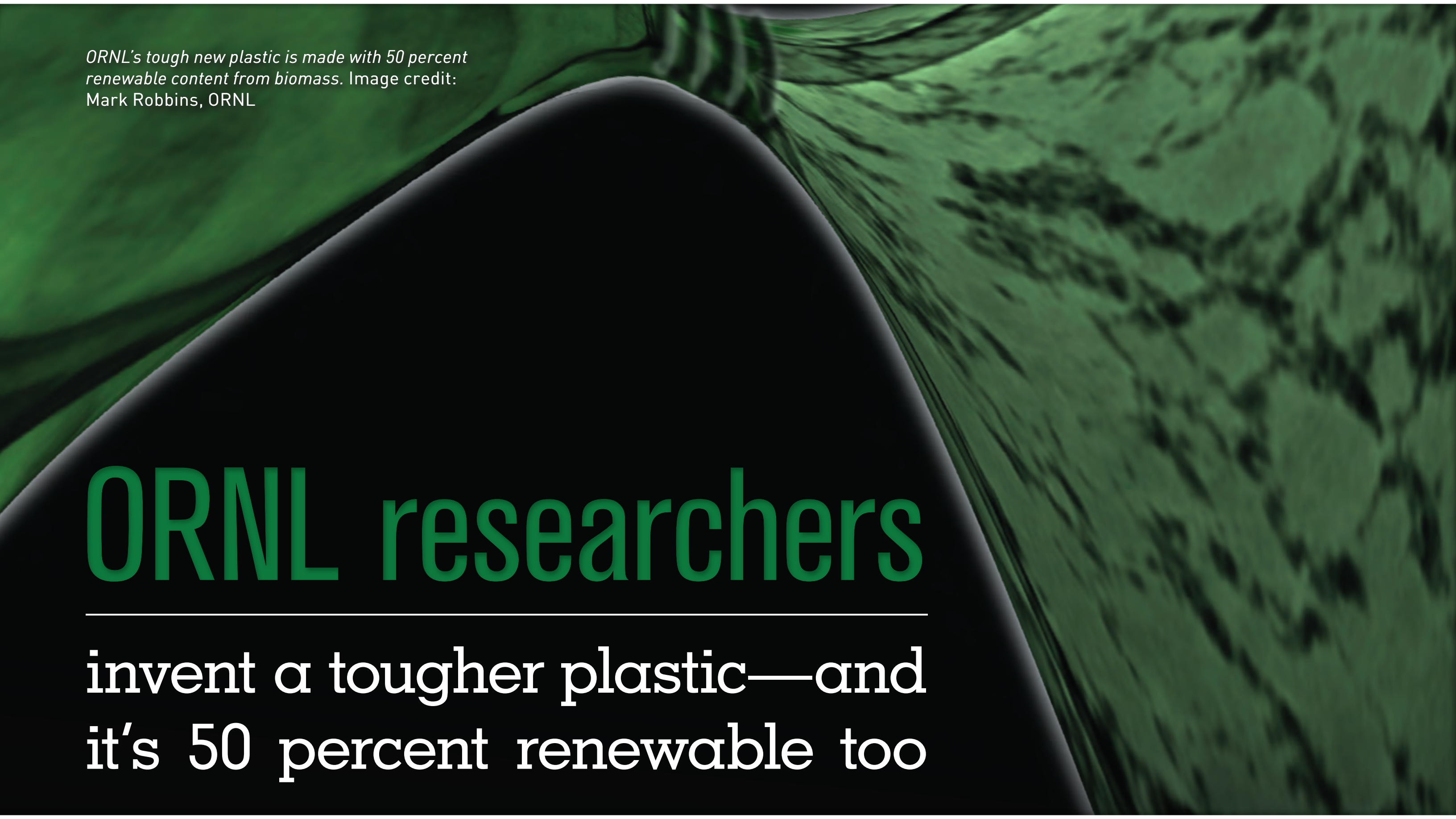
Developed by DOE BioEnergy Science Center researchers in California, CELF is a two-part solvent consisting of water and an industrial chemical called tetrahydrofuran, or THF. Studies have shown CELF to be more than three times as effective as conventional dilute acid pretreatment in freeing up cellulose, the substance that is converted to ethanol.

As the team's 250,000-atom simulation revealed, much of the improvement can be attributed to how CELF interacts with water and lignin, a problematic molecule for ethanol production. The simulation demonstrated that THF acts like a shield for lignin, protecting it from water and making lignin easier to remove during biofuel processing.

"With conventional pretreatment, lignin clumps up and binds to cellulose because it wants to limit its interaction with water," said ORNL staff scientist Loukas Petridis. "In the presence of THF, however, lignin opens into long coils, which can be more easily removed when the biomass is washed."

Scientists can use these insights to refine techniques for processing biofuels and developing new ones, Petridis said.

For more information: http://go.usa.gov/ctzDB



ORNL's tough new plastic is made with 50 percent renewable content from biomass. Image credit: Mark Robbins, ORNL

ORNL researchers

invent a tougher plastic—and it's 50 percent renewable too

by Dawn Levy
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Your car's bumper is probably made of a plastic polymer called ABS, shorthand for its acrylonitrile, butadiene and styrene components. Light, strong and tough, it is also the stuff of ventilation pipes, protective headgear, kitchen appliances, Lego bricks and many other consumer products. Useful as it is, one of its drawbacks is that it is made using chemicals derived from petroleum.

Now, ORNL researchers have made a better plastic by replacing styrene with lignin, a brittle, rigid polymer that forms the woody cell walls of plants, along with cellulose. In doing so they have invented a solvent-free production process that combines nanoscale powdered lignin and synthetic nitrile rubber. The result is a meltable, moldable material that's at least 10 times tougher than ABS and 50 percent renewable. Called ABL—for acrylonitrile, butadiene, lignin—the material is also recyclable, as it can be melted three times and still perform well.

"The new ORNL thermoplastic has better performance than commodity plastics like ABS," said Amit Naskar in ORNL's Materials Science and Technology Division. He and co-inventor Chau Tran filed a patent application for the process to make the new material, which team members Jihua Chen and Jong Keum helped characterize. "We can call it a green product because 50 percent of its content is renewable, and technology to enable its commercial exploitation would reduce the need for petrochemicals," Naskar added.

The technology could use the lignin-rich byproducts of biorefineries and paper mills instead of petroleum.

"Lignin is a very brittle natural polymer, so it needs to be toughened," explained Naskar. In a heated chamber with two rotors, the researchers "kneaded" a molten mixture of equal parts powdered lignin and nitrile rubber. The result was a material with properties of neither lignin nor rubber but something in between—a combination of lignin's stiffness and nitrile rubber's elasticity.

For more information: http://go.usa.gov/cSpRw

> *"We can call it a green product because 50 percent of its content is renewable, and technology to enable its commercial exploitation would reduce the need for petrochemicals."*
>
> — ORNL researcher **Amit Naskar**

Halogen atom competition

leads researchers toward better solar films

by Ashanti B. Washington
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A team of ORNL researchers is taking a peek at sunlight-absorbing materials, revealing a path for improvements in solar cell efficiency with a combination of high-powered imaging techniques.

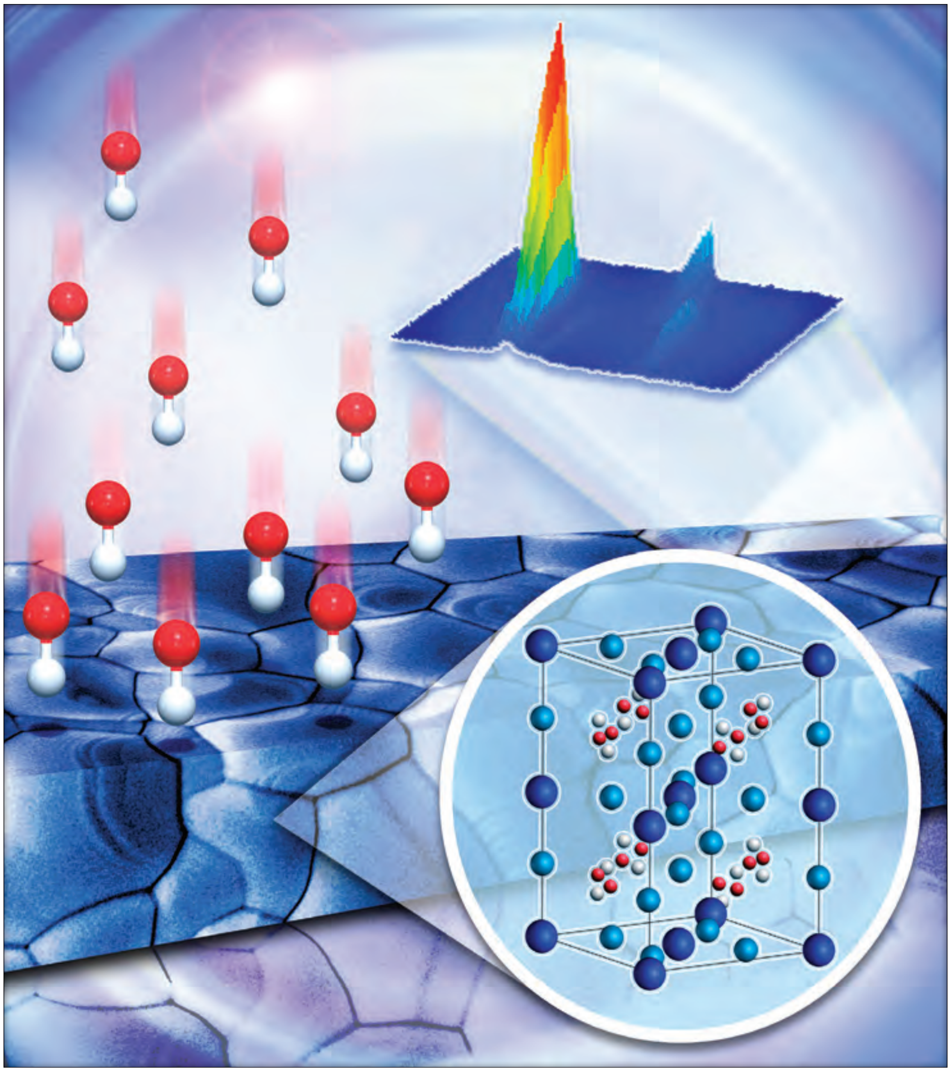
Photovoltaic cells that convert sunlight directly into electricity are becoming increasingly prominent in the world's renewable energy mix. ORNL researchers tracked the outcome of halogen atom competition during the synthesis of perovskites, a promising material less expensive and more efficient than conventional silicon, yet hindered by unanswered questions.

"To take that first step and maximize solar cell technology made with organometallic halide perovskites, we need to know how to grow high-quality light-absorbing material and establish optimal film growth processes," said Bin Yang, an ORNL postdoctoral researcher and the study's lead author.

Halogen ions, jockeying for a position in the growing structure, can affect the movement of charges through the solar crystals and subsequently impact the efficiency of sunlight's conversion to electricity.

As described in a study published in the Journal of the American Chemical Society, organometallic perovskites were imaged with both X-ray diffraction and ion mass spectrometry to provide information about molecular activity on the crystals' surfaces as well as chlorine's eventual distribution in the grain boundaries, or crevices, of perovskite films.

Researchers discovered that while bromine, chlorine and iodine ions facilitate growth in a developing organometallic perovskite structure, only iodine gets a spot in the final crystal.



ORNL scientists combined imaging techniques to measure crystallization kinetics of perovskite films following exposure to a mixed halide vapor. Over time, extra halide reactants settle in the film's grain boundaries, demonstrating atomic competition in crystal growth. Image credit: Jill Hemman, ORNL

However, though they are left out of the final structure, the sidelined molecules build "team morale" because they help promote overall crystal growth.

"The kinetic activity found in halide perovskites poses significant challenges for advancing high-efficiency optoelectronic materials and devices," said Kai Xiao, study co-author and ORNL staff scientist. "Identifying the chemical phenomenon of halide competition in hybrid perovskites will help in engineering large-grain perovskite films for better, cheaper solar devices."

For more information: http://go.usa.gov/ch26J

Neutron 'splashes'

reveal signature of exotic particles

by Katie Bethea
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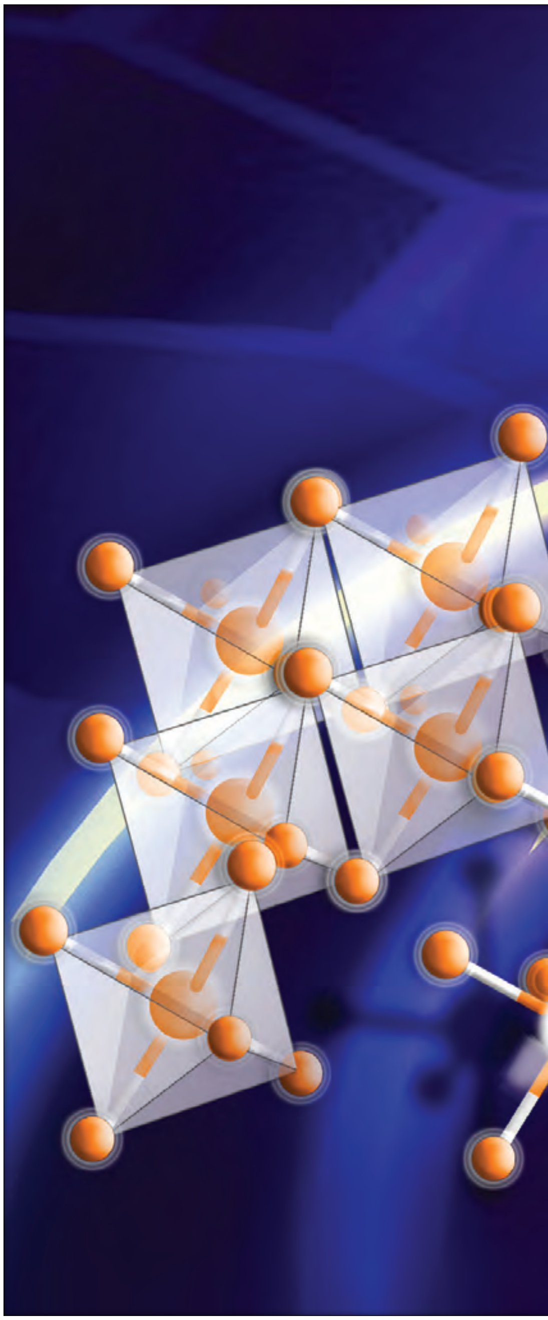


ORNL researchers have used neutrons to uncover novel behavior in materials that holds promise for quantum computing. The findings, published in *Nature Materials*, provide evidence for long-sought phenomena in a 2-D magnet.

In 2006 physicist Alexei Kitaev developed a theoretical model of microscopic magnets ("spins") that interact in a fashion that leads to a disordered state called a quantum spin liquid. This "Kitaev quantum spin liquid" supports magnetic excitations equivalent to Majorana fermions—particles that are unusual in that they are their own antiparticles.

The presence of Majorana fermions is of great interest because of their potential use as the basis for a qubit, the essential building block of quantum computers.

Familiar magnetic materials exhibit magnetic excitations called spin-waves that occur in quantized lumps, but in the Kitaev quantum spin liquid, the lumps are split and the Majorana excitations are therefore termed "fractionalized."

Scientists have theorized that Kitaev interactions exist in nature in certain materials containing magnetic ions that exhibit strong coupling between the electron spin and orbital angular momentum. Arnab Banerjee, the study's lead author and a postdoctoral researcher at ORNL, explained that one way to observe spin liquid physics in such a material is to "splash" or excite the liquid using neutron scattering.

Banerjee and colleagues from ORNL and the University of Tennessee, working with collaborators from the Max Planck Institute in Dresden, Germany, and Cambridge University in the United Kingdom, used the splash technique to investigate a 2-D graphene-like material, alpha-ruthenium trichloride. Neutrons shining onto and scattering from this material can deposit small amounts of energy that create magnetic excitations.

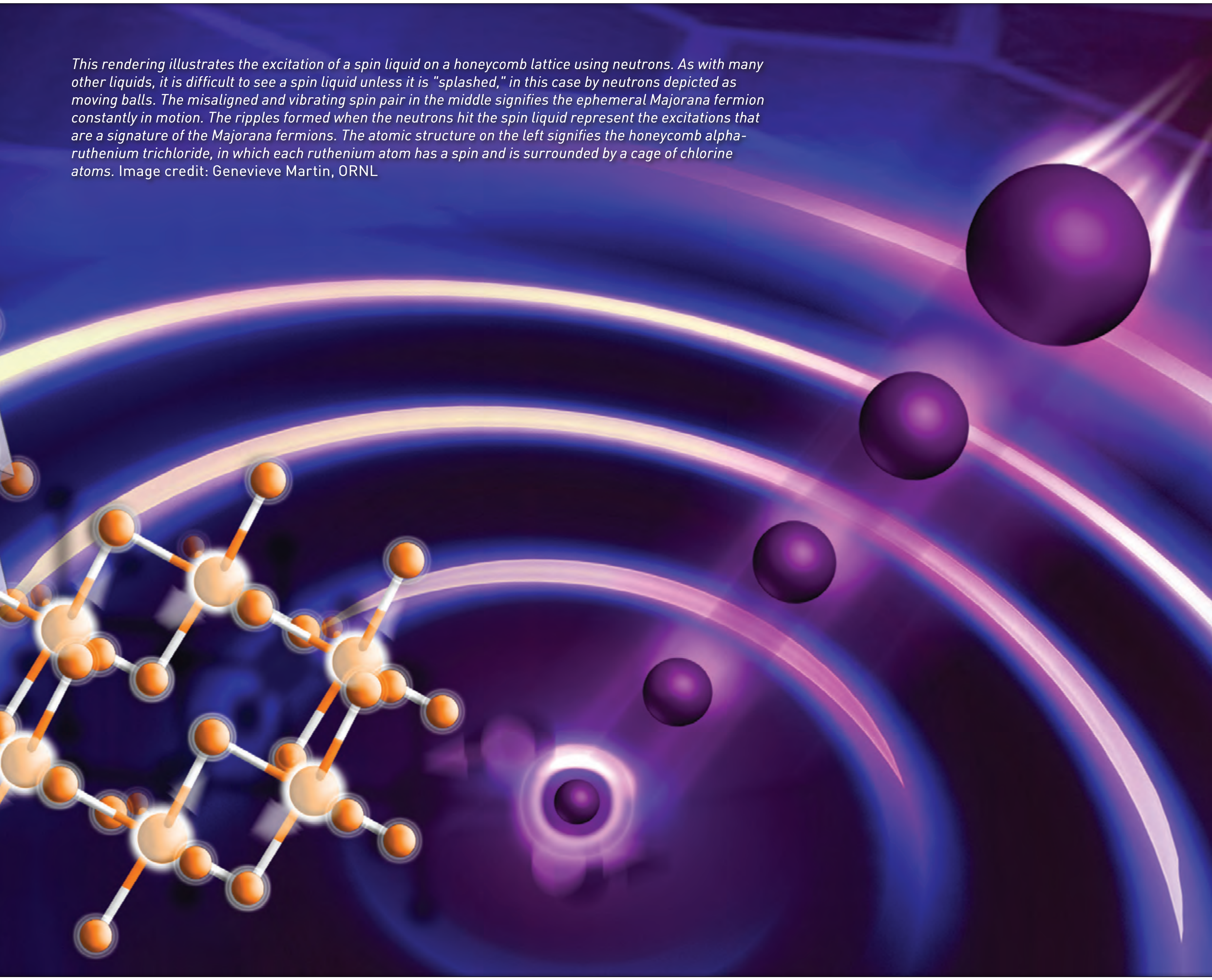
> "Neutron scattering not only provided the splash we needed to see them but also directly measured the resulting magnetic excitations."
> — ORNL physicist **Arnab Banerjee**

The form of magnetic excitations created in alpha-ruthenium trichloride was found to be different from spin waves seen in ordinary magnets but was very well-matched to the spectrum predicted for the Majorana fermions expected in the Kitaev quantum spin liquid.

"The concept of Majorana fermions originated in fundamental high-energy particle physics, but we saw their signatures in a solid-state material at modest temperatures," Banerjee said. "Neutron scattering not only provided the splash we needed to see them but also directly measured the resulting magnetic excitations."

The Spallation Neutron Source's SEQUOIA instrument is best suited for this research because the range of energy and momentum one can access with the instrument perfectly matches the regime in which Majorana fermions show up.

"The observation of these fractionalized excitations is truly remarkable," said Steve Nagler, director of the Quantum



This rendering illustrates the excitation of a spin liquid on a honeycomb lattice using neutrons. As with many other liquids, it is difficult to see a spin liquid unless it is "splashed," in this case by neutrons depicted as moving balls. The misaligned and vibrating spin pair in the middle signifies the ephemeral Majorana fermion constantly in motion. The ripples formed when the neutrons hit the spin liquid represent the excitations that are a signature of the Majorana fermions. The atomic structure on the left signifies the honeycomb alpha-ruthenium trichloride, in which each ruthenium atom has a spin and is surrounded by a cage of chlorine atoms. Image credit: Genevieve Martin, ORNL

Condensed Matter Division at ORNL and co-corresponding author of the paper. "There has been a huge push recently to see if Kitaev quantum spin liquid physics can be found in materials. Time will tell whether this represents a first step on the road to a new qubit technology."

The experiment required extremely pure samples that were prepared by Banerjee and Craig Bridges of ORNL. The interpretation of the experiments was helped by theoretical predictions of team members Roderich Moessner of the Max Planck Institute, Johannes Knolle of Cambridge, and their colleagues.

"This study proved that the proper honeycomb lattice materials can have the exotic excitations long sought by the scientific community, potentially bringing us closer to realizing Kitaev's vision of topologically protected quantum information," said Alan Tennant, chief scientist for Neutron Sciences at ORNL and a co-author on the paper.

The research team also included Jiaqiang Yan, Adam Aczel, Matthew Stone, Garrett Granroth, and Mark Lumsden from ORNL; David Mandrus, a joint faculty member from the University of Tennessee and ORNL; Ling Li and Yuen Yiu from the University of Tennessee; Dmitry Kovrizhin from Cambridge; and Subhro Bhattacharjee from the Max Planck Institute. The paper was published as "Proximate Kitaev quantum spin liquid behaviour in a honeycomb magnet."

For more information: http://go.usa.gov/che8F

Charmed half-life:

Target used to discover element 117 took a circuitous route to Russia

by Bill Cabage
cabagewh@ornl.gov

ORNL physicist Krzysztof Rykaczewski's role in the discovery of element 117 included the nerve-wracking task of getting the radioactive targets from Oak Ridge to Russia. Image credit: Carlos Jones, ORNL

The discovery of element 117—tennessine, as it has been provisionally named—was made possible by a collaboration of researchers in the United States and Russia. ORNL provided the radioisotope berkelium-249, which was bombarded with a beam of calcium-48 at Russia's Joint Institute for Nuclear Research in Dubna until atoms of element 117 appeared.

The achievement was a long time coming. As the stars aligned in 2009 toward the search for the theorized element, ORNL's Jim Roberto knew he needed someone to help manage what would certainly be a complex international effort. The discovery of this synthetic element was going to be a race against time.

Roberto, who helped organize the international search, asked the Physics Division's Krzysztof Rykaczewski to work behind the scenes to make sure the Russian team had everything it needed from ORNL to run the experiment.

"It's good to have a nuclear spectroscopist on the team," says Rykaczewski, an American Physical Society fellow and veteran of nuclear decay spectroscopy research at ORNL's Holifield Radioactive Ion Beam Facility.

It was good because the Holifield studies have identified about 10 new alpha and proton radioactive nuclei and led to the investigation of "superheavies"—exotic radioactive nuclei packed with protons and neutrons and often very short-lived. The experience ORNL and University of Tennessee physicists gained in studying even shorter-lived alpha and proton decays of exotic nuclei provided the Russian experiment with much insight into superheavies' behavior and detection.

"We knew perfectly what was involved because of our earlier discoveries of new alpha emitters and proton emitters in experiments at the Holifield Facility," Rykaczewski says.

The superheavies also hold clues to the "island of stability," even heavier isotopes that now exist only in theory. Rykaczewski deems progress toward these long-lived synthetic nuclei more important than adding elements to the periodic table, because they could open new realms of physics and chemistry.

Rykaczewski oversaw the development of detectors and instruments loaned to the Russian facility. But ORNL's key contribution to the project was the production and delivery of 22 milligrams of the isotope berkelium-249, a byproduct of the production of californium-252, for which ORNL is one of the world's only sources.

Krzysztof Rykaczewski. Image credit: Carlos Jones, ORNL

The most nerve-wracking part of the element-117 discovery was getting the berkelium-249 to Dubna under an oppressive time constraint.

Berkelium-249 has a 330-day half-life. That's nearly a year, but the radioisotope has to decay three months after emerging from ORNL's High Flux Isotope Reactor before it can be processed. Then come three months of chemical separations. Half the year ticks away up front before it's ready to fly to Russia.

Under Rykaczewski's watch, the radioisotope was carefully packaged, divided into five heavily shielded parcels and documented. Airline pilots have to approve their cargo, however, and the first pilot balked. After a week, another pilot agreed to take it on board.

"I am happy," Rykaczewski remembers.

His happiness, like the superheavies, was short-lived. A day later the package was back in New York. There was an oversight, it seems.

"The cargo was marked by all labels known to man as dangerous goods, and it arrived in Moscow without any shipping papers," he says.

No matter. Two days later it flew the Atlantic again, and a day later it was again back in New York. "We were expecting a fax before the plane arrived" was the reason offered by dutiful officials at the destination airport.

Third time's a charm: The shipment, replete with fax, was accepted.

"Then some junior official kept it for a week, just to show us. All the time it's decaying. This was my life in 2009," Rykaczewski says.

"The cargo was marked by all labels known to man as dangerous goods, and it arrived in Moscow without any shipping papers."

— **Krzysztof Rykaczewski**, ORNL researcher

The precious shipment finally arrived at the Research Institute of Atomic Reactors at Dmitrovgrad, where the berkelium-249 was hand-painted onto a target. From there it traveled to JINR. Six months of continuous bombardment and data acquisition yielded a half-dozen atoms of element 117. Follow-up experiments confirmed the discovery.

"The Russians were impressed by the purity of the berkelium samples," Rykaczewski says. "ORNL's High Flux Isotope Reactor irradiated the seed material, and our Radiochemical Engineering Development Center contributed the processing, and it was just really great work."

Building better geothermal models

by Jim Pearce
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The ingredients that make geothermal energy suitable for electricity production are simple: heat, permeability (usually fractured rock) and water. Until recently the trick has been finding all in the same place and in the right amounts.

Enormous heat energy is available between 3 and 10 kilometers below the surface of the U.S., notes Yarom Polsky, an engineer in ORNL's Energy and Environmental Sciences Directorate, but researchers haven't yet determined how to extract it. Current thinking suggests we will need to develop enhanced or engineered geothermal systems. These are systems that lack at least one of the ingredients—usually water or fractured rock.

To create an enhanced geothermal system—or EGS—an energy producer would drill a well down to where the rocks are hot enough (in the range of 250–300 degrees Celsius or roughly 500–550 degrees Fahrenheit) and then hydraulically fracture the rock to create permeability.

In the oil and gas industry this permeability allows oil and gas to be recovered. In EGS wells, permeability allows water pumped down the well to flow through the fractures and absorb heat from the surrounding rock. The heated water will then be pumped out of the ground at a second well that intersects the fracture network and be used to generate electricity by powering a steam turbine.

Polsky and his colleagues hope to improve energy producers' ability to analyze proposed EGSs before drilling begins by producing more accurate computer models of how water flows through these systems under a variety of conditions.

Traditionally, energy producers wanting to estimate the rate of flow through a proposed EGS have had to rely on idealized models of fluid flow—models that are often inaccurate. To address this shortcoming, Polsky and his colleagues are using neutrons generated by ORNL's High Flux Isotope Reactor to develop a more sophisticated way to visualize the flow of fluid through the complex fractures that occur in real geological samples.

Image credit: Mircea Podar, ORNL

"We're developing a way to visualize the flow through more complicated systems so we can use that as a basis for calibrating flow models," Polsky said.

Typically, researchers experimentally measuring flow through complex geometries have had to use materials they could see through, usually machined plastics, which limited both the complexity of the systems and the pressures they could use. For Polsky and his colleagues, the compelling thing about visualizing flow with neutrons is that rock samples are transparent to neutrons, while water is not, enabling researchers to see the water inside actual rock samples rather than through plastic surrogates.

Because Polsky and his colleagues were using neutrons to image continuously moving flows, they had to develop methods that used contrast agents that could be tracked. In this case they injected small bubbles of a fluid called Fluorinert that looks different from water to the neutrons. Then they captured neutron radiographs of the rock sample about once every 10 milliseconds. By doing this they could visualize the motion of the fluid.

"If we can calculate the velocity fields within actual complex fracture geometries, then we can validate computational fluid dynamics models that help predict how fluid will flow through the system," Polsky said. "This becomes the basis for estimating the system's heat production."

Not only are rocks transparent to neutrons, but so is the pressure vessel that holds the rock, meaning Polsky and his colleagues can match the conditions of the sample being studied to those of the rocks in the proposed EGS. This is true for pressures up to 10,000 pounds per square inch and temperatures up to 350 degrees Celsius, or about 660 degrees Fahrenheit.

"The problem with studying subsurface systems is that we never really know what we have down there," Polsky said. "However, we can come up with a range of possibilities. I've done a lot of modeling and simulation work, and we always get an answer. Whether or not the answer reflects reality is another question."

"We need a way to validate the results of our simulations—either with field experiments or with laboratory experiments. That's what we're providing with this research."

"The problem with studying subsurface systems is that we never really know what we have down there. However, we can come up with a range of possibilities. I've done a lot of modeling and simulation work, and we always get an answer. Whether or not the answer reflects reality is another question."

— **Yarom Polsky**, ORNL researcher

ORNL refrigerator

cools with magnetism, not Freon

by Leo Williams
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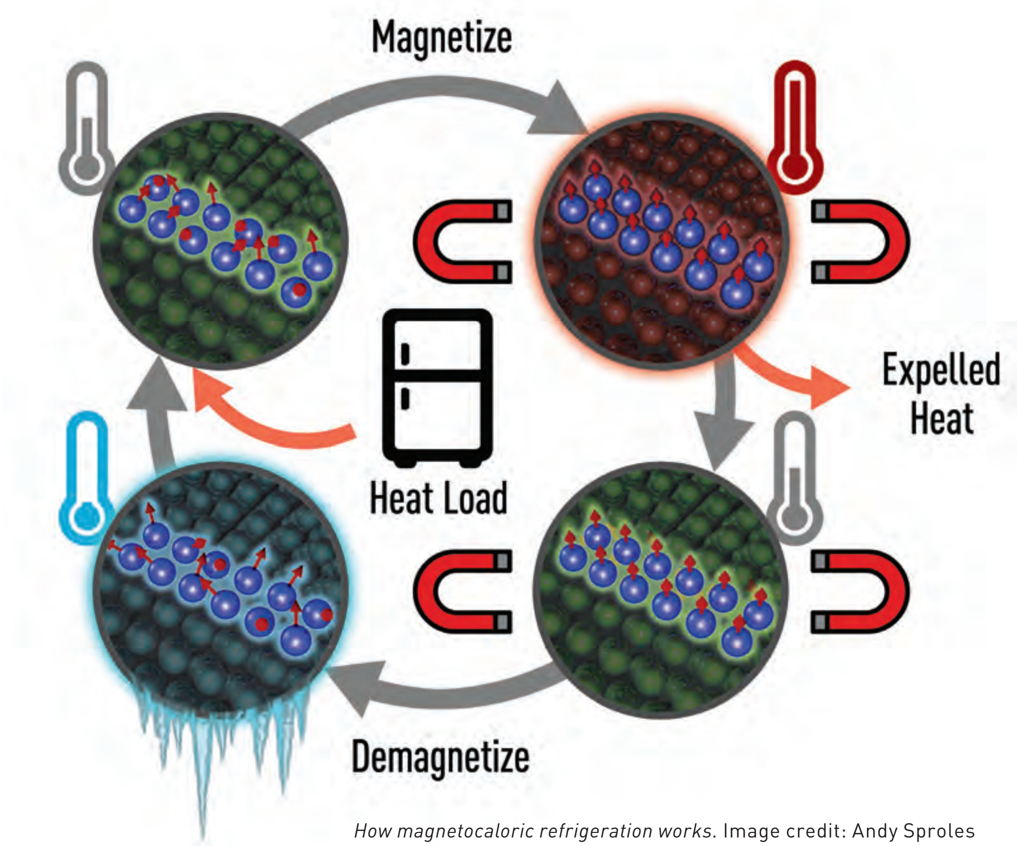
Some metals do a remarkable thing when they're placed within a magnetic field: They heat up. Remove the magnetic field, and they grow cold.

It's not difficult to see how this heating and cooling, known as the magnetocaloric effect, might be put to good use. Refrigerators and air conditioners could not only become more energy efficient but also be freed from century-old technology that relies on environmentally harmful refrigerants.

Researchers with ORNL's Building Equipment Research Group are working with General Electric Appliances to produce a refrigerator based on the magnetocaloric effect. The ORNL team is also developing an air conditioner based on the same principle.

Their efforts so far suggest such products will be not only greener but also 25 percent more energy efficient than conventional appliances.



How magnetocaloric refrigeration works. Image credit: Andy Sproles

"Right now emissions that arise from heating, ventilating, air conditioning, and refrigeration equipment are receiving a lot of scrutiny," said mechanical engineer Omar Abdelaziz, leader of the ORNL BER Group. "In the U.S., this equipment consumes about 20 percent of the nation's energy."

In addition, he noted, common refrigerants are powerful greenhouse gases. The global warming potential for the most common refrigerator refrigerant, for instance, is 1,400 times higher than that of carbon dioxide. The global warming potential of the most common air conditioning refrigerant is 2,000 times higher, and that of the most common commercial refrigerant is 4,000 times higher.

The researchers are experimenting with alloys of lanthanum, iron, silicon, cobalt, and sometimes hydrogen, using the magnetocaloric properties of different recipes to create a practical appliance. Magnetocaloric materials lose their magnetism above a specific temperature, known as their Curie temperature. By fine-tuning the alloy composition, the team can create materials with progressively lower Curie temperatures, allowing them to arrange the alloys to amplify cooling.

Magnetocaloric materials are very touchy, though, so researchers had to overcome some serious practical challenges to take advantage of this oddity of physics.

For instance, a magnetocaloric refrigerator uses a water-based liquid to transfer heat and cool the compartment. If that liquid is simply pushed through the powdered alloy, however, the benefits are offset by the work needed to push the liquid.

One solution is to run the liquid through tiny channels in the material. But to produce those channels, the alloy must be finely ground, which presents the first challenge.

"Any conventional manufacturing processes where we make microchannels requires very fine powder," ORNL mechanical engineer Ayyoub Momen said. "But as soon as you crush these materials to such a powder, let's say 5 micrometers, they become so reactive in some cases that they can even become explosive."

The second challenge, he said, is that the alloys are very brittle, meaning they're unsuited to conventional manufacturing processes. And, finally, they are heat sensitive.

"In most cases these particles hate heat," Momen explained. "As soon as you heat them up, they lose their magnetocaloric properties."

The research team came up with a solution that involves 3-D printing the materials and holding them together with an epoxy. With this process, developed at ORNL's National Transportation Research Center, they can create channels as small as 100 micrometers.

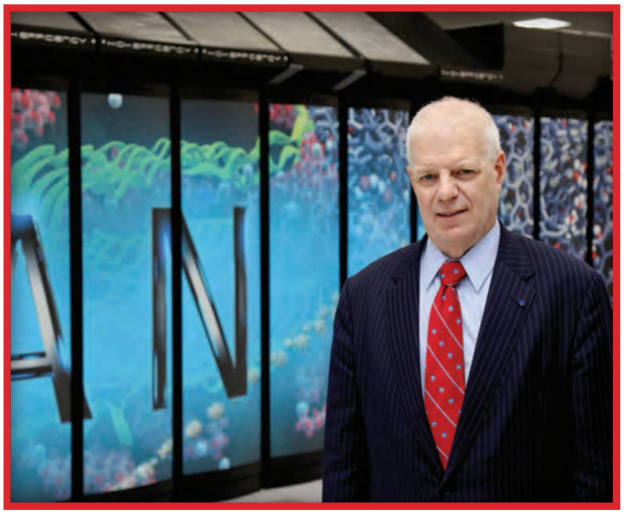
They also developed the means to heat—or "sinter"—the material to make it stronger without destroying its magnetocaloric properties.

The team is developing a process that uses magnetic fields to cause the powder—and channels within it—to line up automatically, much like the patterns created by iron filings on a piece of paper placed over a magnet.

The researchers have two papers pending that describe their work. Plans call for a magnetocaloric refrigerator to be commercially available by 2020.

Ayyoub Momen works on a magnetocaloric proof-of-concept refrigeration prototype. Image credit: Jason Richards, ORNL

Distinguished



Alton Romig Jr.

1. How have the challenges of nonproliferation changed over the years?

First off, let me open with a comment. What I'm about to say is the opinion of Al Romig. It's not an official opinion rendered by the National Academies or any other entity. But in my own perspective, I think that over the last few decades proliferation has gone down several different paths. In the early days all we worried about was the proliferation of nuclear weapons. Since that time there has been worry over proliferation of biological materials. Same thing with chemicals. Same thing with missile technology. So there are many more things with which we concern ourselves that are proliferants than we have in the past. And secondarily, whether it's just nuclear things or all of the other issues that I just mentioned, there are more and more countries that are now entering and developing technology in those fields, so it's broadened the base both with respect to technologies that might proliferate as well as the countries—or even potentially non-state actors—that might be the proliferants of whatever that technology might be.

2. How do you see these challenges changing in the foreseeable future?

Unfortunately, I think they will just continue down the path of more and more complexity. I think there'll be more and more countries that desire to get in the game. One of the interesting things about proliferation is that once somebody in a neighborhood, so to speak, gets in the game, then their local neighbors want to get into it. So my concern is that the entire proliferation regime could change over the course of the coming decades. That a few more countries will become proliferants of missiles or nuclear weapons or whatever it might be, and that will cause local proliferation races in that region of the world.

Lecturers

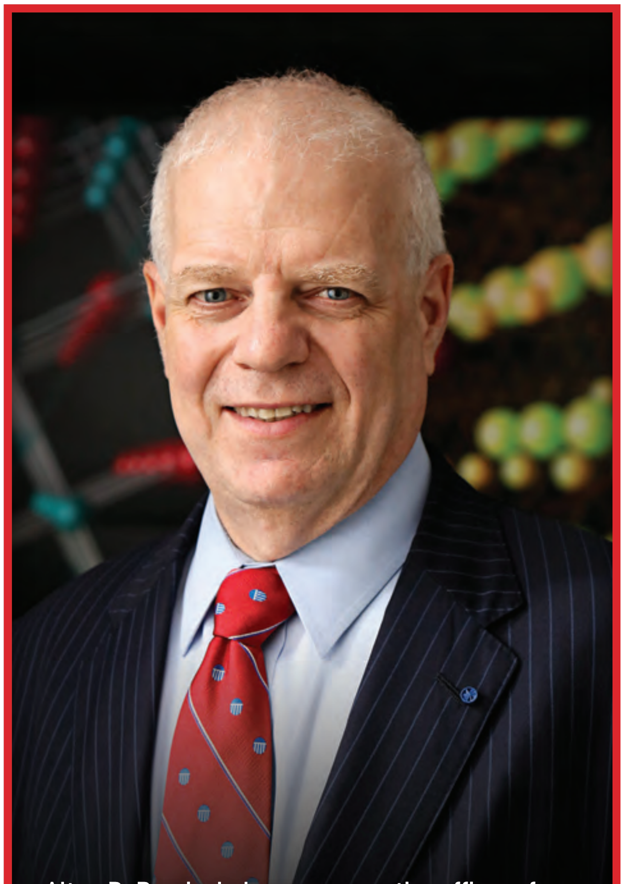
3. What role does the National Academy of Engineering play in America's nonproliferation efforts?

The National Academies were created from the very beginning, all the way back by Lincoln in 1863, to be independent, educated, knowledgeable, unbiased advisors to the government on matters of science and technology—in fact of all of human creation, all arts. So I believe as the whole issue of proliferation continues to grow in complexity, the government will likely turn more and more frequently to the academy to render objective advice to the government on what are the appropriate policies we need and actions we need to take in order to deal with those proliferation matters.

4. Why was it important to visit ORNL, meet with researchers here, and participate in the Wigner Lecture Series?

My career began in 1979 when I left graduate school. And during the 1980s, early '90s, and then again in the early part of the 2000s, I had lots of reason to interact with people in Oak Ridge, both at the national laboratory and at Y-12 [the Y-12 National Security Complex]. And so, in part, I was coming back to visit old friends. It's been some number of years since I've been here—I think about eight, as near as I could count—and so I wanted to come back and see how the laboratory had changed.

On my last visit here, the Spallation Neutron Source was just about to come on line; I wanted to see how that had evolved. So it was a personal interest for me to come. And secondarily, I think as more and more young people enter the workforce, anything I could do to help them understand the rich history and heritage of where they work and what a facility like Oak Ridge means to the country was very important to do. And so, as an old Cold Warrior who is closer to the end of his career than to the beginning, I think it's important to share that message with those who will replace us.



Alton D. Romig Jr. became executive officer of the National Academy of Engineering after a long career at Sandia National Laboratories. Romig holds a Ph.D. in materials science from Lehigh University and is a fellow of professional societies including ASM International (formerly the American Society for Metals) and the American Association for the Advancement of Science. He was elected to the National Academy of Engineering in 2003 and the Council on Foreign Relations in 2008.

Romig delivered the Eugene Wigner Distinguished Lecture June 23, 2016, on the topic "The National Academies and Nuclear Nonproliferation: Yesterday, Today, and Tomorrow." This is an edited transcript of our conversation following his lecture.

The Eugene P. Wigner Distinguished Lecture Series in Science, Technology, and Policy gives scientists, business leaders and policy makers 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 scientists and engineers, 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.

Pranab Roy Chowdhury

Graduate student, Geographical Information Science and Technology Group
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Kolkata, India

What are you working on at ORNL?

My research revolves around the application of geospatial data-driven methodologies to study how population dynamics affect energy demand over space and time. Currently, I am developing a method to use satellite images to distinguish between various classes of residential energy use.

What would you like to do in your career?

I would like to continue working to better understand population dynamics and how they affect energy and resource scenarios, with a goal to address planning and policy issues surrounding sustainable energy security. I am also interested in science administration, which is my long-term career goal.

Why did you choose a career in science?

Science enables me to comprehend the world around me! I love the process of making an abstract idea into a workable solution to solve real-world problems. My journey so far has been truly rewarding and has contributed immensely to my intellectual and personal growth.

Guinevere Shaw

Graduate student, Fusion and Materials for Nuclear Systems Division
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Rocky Mount, Virginia

What are you working on at ORNL?

I am currently collaborating with researchers from the University of Tennessee and ORNL on the ability to quantify fuel-retention mechanisms in tungsten using laser-based characterization techniques.

What would you like to do in your career?

I am interested in staying in the fusion science and technology community after I receive my Ph.D. I plan to apply to the Fusion Energy Sciences Postdoctoral Research Program.

Why did you choose a career in science?

I chose a career in science for my innate curiosity for something much bigger than myself.

Andrew Miskowiec

Postdoc, Nuclear Security and Isotope Technology Division
Ph.D., Condensed Matter Physics, University of Missouri at Columbia
Hometown: Milwaukee, Wisconsin

What are you working on at ORNL?

As part of a Laboratory Directed Research and Development project, I led the fabrication of a unique sample cell that allows us to apply particular humidity conditions during neutron spectroscopy measurements at the Spallation Neutron Source. We have used this setup to study fuel-cycle uranium compounds.

What would you like to do in your career?

ORNL's science mission is diverse and spread across many divisions. I'm interested in developing programs and collaborations that combine experience and capabilities across divisions. We work on a lot of different projects here, but we don't often take advantage of our neighbors' expertise.

Why did you choose a career in science?

Science is about discovering the underlying fabric of reality. That's just about the most interesting thing I can imagine, so of course I'm interested in pursuing that goal.

Kyle Sander

Graduate student, Biosciences Division
Ph.D. student, Chemical and Biomolecular Engineering, University of Tennessee (Bredesen Center)
Hometown: Portland, Oregon

What are you working on at ORNL?

I characterize and engineer transcription factors from a bacterium (*Caldicellulosiruptor bescii*) to improve its ability to make ethanol from lignocellulosic feedstocks. Transcription factors are proteins that regulate the expression of other genes. I work as part of the BioEnergy Science Center.

What would you like to do in your career?

I hope to conduct/lead and otherwise take part in research addressing problems broad in scope that necessitate interdisciplinary research teams. A publicly funded national laboratory seems to me the best place for this, so I want to someday be a staff scientist at a national laboratory,

Why did you choose a career in science?

I was (and continue to be) amazed at how researchers approach problems, continually learn and make breakthroughs. I was drawn to the idea nurtured within science that there are no limits to how we solve problems or what problems we can solve; we are limited by what we can conceive.

Kathleen Buckley

Postdoc, Global Security Directorate
Ph.D., Cellular Biology and Anatomy, Augusta University, Augusta, Georgia
Hometown: Bonita Springs, Florida

What are you working on at ORNL?

I am working in bionuclear forensics. The goal is to effectively integrate biological systems for use in nuclear forensic applications. My background includes EPA and FDA regulatory work, and I hope to apply that knowledge and skill set to my work here at ORNL.

What would you like to do in your career?

I have had a diversified career to date, spanning from environmental chemistry to cancer and stroke research and teaching medical students. I enjoy tackling new problems and growing as a scientist, while using my knowledge to try to help improve this world for others.

Why did you choose a career in science?

I chose to build my career first in environmental chemistry, then in biological chemistry, because I can strive to understand complex systems while working to help others. As a scientist, you are constantly learning and challenging yourself, and this career allows you a unique opportunity to do that.

Adam Witt

Postdoc, Environmental Sciences Division
Ph.D., Civil Engineering, University of Minnesota
Hometown: Champlin, Minnesota

What are you working on at ORNL?

I am part of the Energy-Water Resource Systems Group, which works to advance innovative water power technologies. My research seeks to characterize the technological and environmental limitations, functional requirements and economic feasibility of modular hydropower and pumped storage concepts. I am also developing a forecasting tool to help mitigate the environmental impacts of hydropower on the mid-Columbia River.

What would you like to do in your career?

I very much appreciate the complex and codependent relationship between energy and water. This relationship is evolving faster than ever before, and I hope to continue contributing to our common understanding of the many important challenges we face with respect to water and energy sustainability, security, consumption and availability.

Why did you choose a career in science?

While working at an intellectually unfulfilling job after college, I made a conscious decision to alter my career trajectory and focus on big problems that involve our human relationship with nature. I desired a career where I could curiously and rigorously contemplate the "why" and the "how." Hence, science!

The short life of a neutron

by Tim Gawne
gawnetj@ornl.gov

Although the neutron is a senior citizen of sorts, whose existence was predicted in 1920 and confirmed in 1932, it's still not fully understood.

It was James Chadwick of Cambridge's Cavendish Laboratory who, after nearly a decade of experimentation, devised a method to detect these particles, which have essentially the same mass as the proton but no electrical charge. Not only did Chadwick's triumph earn him the Nobel Prize in Physics three years later, it also gave him and the physics community a new particle to play with.

The discovery of the neutron allowed scientists to conceive of the possibility of nuclear chain reactions and explain isotopes—versions of an element that contain the same number of protons but different numbers of neutrons. Neutrons also provided a versatile tool for exploring the structure and dynamics of materials, including soft matter.

Despite the attention it has received, however, the neutron is still in some ways a mystery. For instance, what is the half-life of an unbound neutron?

Like most social beings, neutrons don't do well on their own. Put them inside a stable nucleus and they last indefinitely, but take them out and their time is limited. Attempts before World War II to determine the neutron's half-life were hobbled by the lack of intense neutron sources.

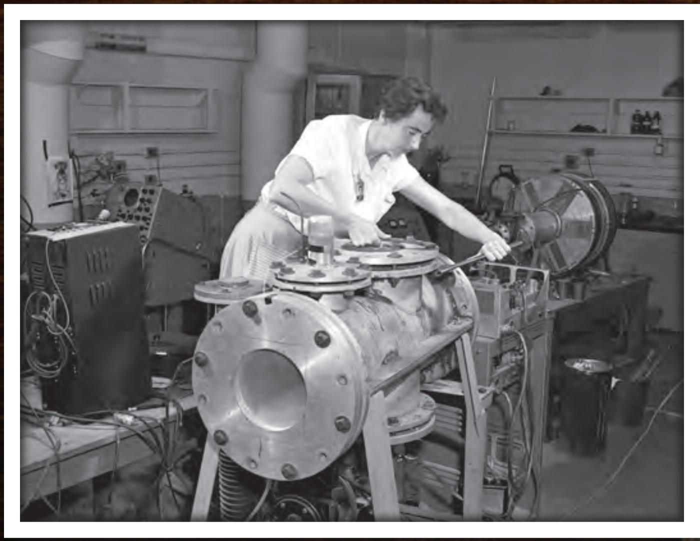
Enter the Oak Ridge Graphite Reactor, the world's first permanent nuclear reactor.

Soon after the war ended, Arthur Snell and Leonard Miller of ORNL's predecessor, Clinton Laboratories, built a vessel that allowed them to focus a beam of neutrons from the Graphite Reactor. When a neutron decays, it emits a proton, an electron and an antineutrino, and the device was able to detect the proton and electron. The two researchers observed this neutron decay, and Snell presented their findings in April 1948 to a meeting of the American Physical Society in Washington. (Miller had died in a vehicle collision.)

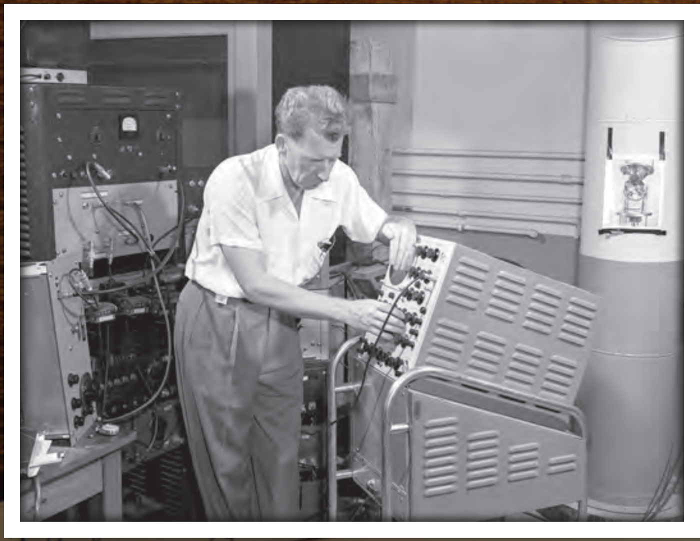
Observing the decay was one thing, but measuring it was going to take a more refined instrument. After Miller's passing, Snell had the help of Physics Division colleagues Frances Pleasonton and Rube McCord in perfecting a device to deliver more precise counts of decay products in the neutron beam.

By this time nuclear reactors were becoming more common, and British physicist John Robson tackled the same problem using the NRX reactor at Canada's Chalk River Laboratories. In 1950 Robson's and Snell's teams published their work simultaneously in *The Physical Review*, with Snell's team coming up with a neutron half-life of 10 to 30 minutes and Robson's reporting a half-life of 9 to 25 minutes.

Physicists have been repeating their experiments for going on seven decades but have yet to land on a specific neutron decay time. Both Snell's and Robson's time ranges for neutron half-life span the currently estimated value, somewhere around 10.2 minutes, but the hunt continues. ORNL—through the Spallation Neutron Source's Fundamental Physics Beam Line—is one of more than a dozen institutions around the world working to pin down this elusive number.



Frances Pleasonton



Dr. A. H. Snell

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