OAK RIDGE NATIONAL LABORATORY

Review

Protecting the grid:

Oak Ridge National Laboratory

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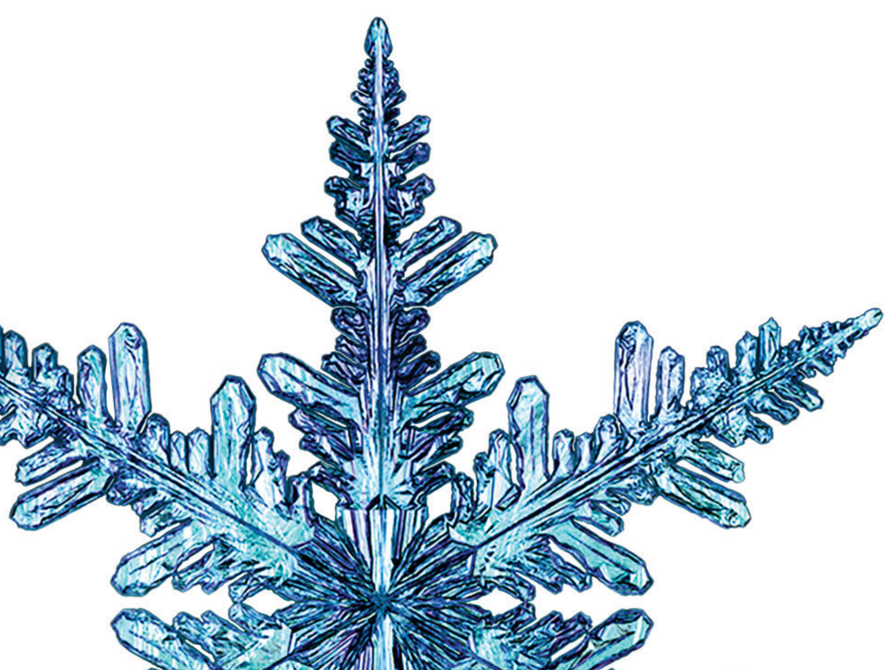


On the Cover
Ben Ollis leads ORNL's work on microgrid controls.
Image credit: Carlos Jones, ORNL

The grand grid challenge

We take for granted that when we flip a switch each morning, the lights will come on, but transporting electricity from power plants to homes and businesses is a monumental task. It involves physical equipment and vast computer networks, private and public operators, planners and regulators, all working together to sustain a system that keeps electrons flowing without interruption.

Outages of even a few hours can disrupt the economy and stop essential services. Long or widespread disruptions can seriously threaten health, public safety and even national security.

For these reasons, it is a national priority to protect the grid against physical threats, cyberattacks and natural disasters. It requires that we develop new, secure technologies and that we implement them without disrupting the existing system.

At Oak Ridge National Laboratory, our researchers are working closely with industry to modernize America's electricity delivery system through the development and deployment of sensors, controls, protective relays and intricate simulations of the grid. We are also analyzing how components such as power plant fuel supply, microgrids with renewable resources, energy storage and smart technologies can contribute to a secure and resilient distribution of electricity.

The genesis of our work dates to the 1980s, when ORNL conducted an experiment to automate the distribution of electricity to 10,000 customers in Athens, Tennessee. The project relied on the technology of the time, including dial-up computer networks and the first generation of smart meters.

Since then, technology has finally caught up to the lab's vision of a fully automated system that constantly monitors the grid, sensing disruption and, in many cases, avoiding it proactively. Advances such as fiber optic communications, high-fidelity sensors, advanced power electronics, control algorithms and supercomputing are making it possible to continually scan for threats and reroute electrons at the speed of light.

In this issue of *ORNL Review*, we highlight our important contributions to grid security and resilience (see "Defending the grid: Solutions for power system vigilance and resilience," page 6). We delve into a new strategy to protect grid controls (see "DarkNet: Lighting up a secure grid communication network," page 10). We learn how our microgrid controls research is being tested in two communities in the Southeast (see "Real communities test ORNL microgrid controller," page 8.) We hear from one of our closest industry partners about how working with ORNL keeps them ahead of the pack in technological innovation (see "Gig City grid: A conversation with EPB's Jim Ingraham," page 12). And we take a look at how the lab's innovations touch nearly every sector of the national power grid (see "ORNL on the grid," page 20).

Elsewhere in the *Review*, we celebrate the International Year of the Periodic Table with a look at ORNL's role in discovering new elements (see "The human element," page 26), we discuss a new electron microscopy technique that may lead to a deeper understanding of proteins (see "Microscopy technique offers an up-close view of proteins," page 18), and we look back at an ORNL contribution to the Apollo 11 mission 50 years ago (see our regular "Time Warp" feature, page 40).

I hope you enjoy learning about ORNL's contributions to the electric grid and other scientific advances in this issue.

Thomas Zacharia

Thomas Zacharia
Laboratory Director

Genetics pioneer Liane Russell dies

Mammalian genetics pioneer Liane B. Russell died Saturday, July 20. She was 95.

Russell arrived in Oak Ridge in 1947 with her husband, William L. Russell, to study radiation-induced health effects using mice, which are genetically similar to humans.

Among her important discoveries at ORNL were the effects of radiation on developing embryos, which led to health precaution guidelines for women of child-bearing age that are still observed today, and in determining through mutations in female mice the Y chromosome's role as the male-determining chromosome in mice. The Russells also studied chemically induced mutations and developed a variety of mutations to serve as models for human genetic disorders.

"Lee Russell's incredible life journey has left us with a legacy of discovery that expanded, through genetics research, our understanding of our world, our lives and our health. The global scientific community will honor her many contributions to science. Our Oak Ridge community will remember her, as well, for her support for early career researchers and her work on behalf of our East Tennessee environment," said ORNL Director Thomas Zacharia.

Russell's Austrian family fled the Nazis in the late 1930s, eventually arriving in the United States. The daughter of a chemist, she became interested in chemistry and biology as a college student. She met Bill Russell while participating in a research assistantship at the Jackson Laboratory in Bar Harbor, Maine.

The Russells chose the Clinton Laboratories—ORNL's Manhattan Project name—as a destination largely because, in contrast to most universities, Lee would be allowed to work alongside Bill. Over the next six decades, their volume of work with mutant mouse strains led to the development of an extensive mouse colony known as the Mouse House and a number of discoveries related to their mammalian genetics research.

Liane and Bill Russell in 1997. Image credit, Curtis Boles, ORNL

Lee Russell was an internationally recognized researcher throughout her career. She was the scientific advisor for the U.S. delegation to the first Atoms for Peace Conference in 1955, received the Roentgen Medal in 1973 and became a member of the National Academy of Sciences in 1986.

In 1994 she received the Department of Energy's Enrico Fermi Award, the agency's highest scientific award. The citation honored her for "her outstanding contributions to genetics and radiation biology including her discovery of the chromosomal basis for sex determination in mammals and her contributions to our knowledge of the effects of radiation on the developing embryo and fetus."

The Russells' Mouse House at the nearby Y-12 National Security Complex, which housed as many as 200,000 mice, was one of ORNL's most famous institutions and made lasting contributions to genetics research. For example, in 2017 winners of the prestigious Crafoord Prize from the Swedish Royal Academy noted the importance of a mutation known as "scurfy," identified by the Russells decades earlier, to their research in autoimmune disease.

Russell experienced many of the career difficulties common to women in science and became an advocate for them. ORNL established the Liane Russell Distinguished Early Career Fellowship in 2013 to attract diverse and promising early-career scientists whose career goals align with DOE missions. Lee personally greeted the first classes of fellows in the program.

The Russells were known for their environmental advocacy. Lee and Bill, who died in 2003, fell in love with the East Tennessee region and were instrumental in founding Tennessee Citizens for Wilderness Planning, establishing the Big South Fork National River and Recreation Area and obtaining National Wild and Scenic River designation for the Obed River.

Russell was a resident of Oak Ridge.—*Bill Cabage*

Soft drink science

ORNL has teamed with Cornell College and the University of Tennessee to study ways to repurpose waste soft drinks for carbon capture that could help cut carbon dioxide emissions.

In a collaborative study, researchers used a simple chemical process on a variety of regular and diet sodas and discovered that regular sodas containing citric acid made the most efficient porous carbon structures for carbon dioxide adsorption. The unconventional approach follows interest in other low-cost feedstocks, such as banana peels and coffee grounds, for adsorbents to capture carbon dioxide emitted by power plants and other fossil-fueled industries.

“Our process is unique in avoiding harsh chemicals typically used to activate carbon, resulting in eco-friendly and easily recyclable adsorbents,” said ORNL’s Shannon Mahurin. Transforming discarded sodas into raw materials could also bring energy and environmental solutions to waste-heavy soft drink production at facilities worldwide.—*Ashley Huff*

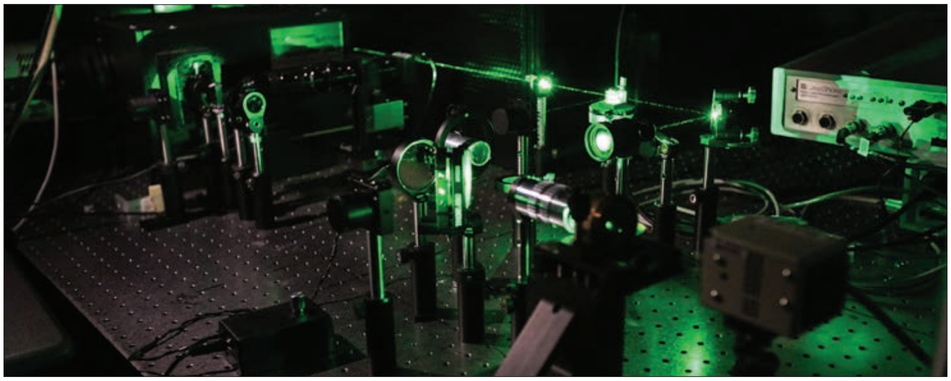
Quantum security for three-way messages

ORNL scientists studying quantum communications have discovered a more practical way to share secret messages among three parties, which could ultimately lead to better cybersecurity for the electric grid and other energy assets.

Current protocols such as quantum key distribution, a prevailing approach in cybersecurity research, are designed for only two parties and require a pair of light particles called entangled photons. Securely extending quantum cryptography to three parties usually requires the difficult step of creating a three-photon entangled state.

“In our experiment, we were able to add the laser source as a third active participant while only needing to produce one pair of photons,” said ORNL’s Brian Williams, lead author of the study published in *Physical Review A*. “Our method removes the need for producing a third photon, which dramatically improves operation efficiency.”

This finding could inspire improved security for existing and future computer networks.—*Sara Shoemaker*



A new study by ORNL has revealed a more practical way to share secret messages among three parties by including the laser source as a third active participant in quantum communications. The approach could lead to better cybersecurity for the electric grid and other energy assets.
Image credit: Genevieve Martin, ORNL

Marcel Demarteau heads ORNL Physics Division

ORNL has named Marcel Demarteau as Physics Division director.

“Marcel brings a keen sense of physics research to the Physics Division and will help in shaping its future in the areas of heavy-ion collisions, fundamental symmetries, neutrino physics, nuclear structure and astrophysics, and stable isotope production and research,” said David Dean, associate laboratory director for physical sciences.

An expert in particle collider physics and a fellow of the American Physical Society, Demarteau leads research in the structure and evolution of the universe. He chairs several advisory committees through which the particle physics community takes stock of past progress and charts future enterprises.

He comes to ORNL from DOE’s Argonne National Laboratory, where he directed the High Energy Physics Division with a program ranging from studies at CERN’s Large Hadron Collider in Switzerland to investigations of the afterglow of the Big Bang using the South Pole Telescope in Antarctica.

At Argonne since 2010, Demarteau conducted research and development in fundamental physics; advocated for investments in advanced instrumentation, building on the multidisciplinary nature of the laboratory; organized the first DOE workshop on quantum sensing for particle physics; and championed astrophysics and cosmology initiatives.

Marcel Demarteau

He earned a doctorate in particle physics from the University of Amsterdam in 1986. After a postdoctoral fellowship at the State University of New York at Stony Brook, he joined Fermilab as a Wilson Fellow in 1992.—*Dawn Levy*

Evaluating performance of building envelopes

An online tool developed by ORNL researchers provides architects and engineers with a fast and efficient way to assess the performance of a building’s envelope design before construction begins.

The Building Science Advisor allows builders to evaluate the moisture durability of the envelope, or exterior, of residential buildings.

“Most building envelope issues are associated with moisture problems,” ORNL’s Andre Desjarlais said. “With BSA, we’re guiding builders through the design process by identifying features that impact durability.”

The tool helps builders make better-informed decisions for energy efficiency through two pathways—expert or educational. “The expert pathway gives builders the ability to input construction plan information uninterrupted, and the educational path guides users through each step of the material selection process, providing feedback so that the user can adjust plans in real time,” Desjarlais said.

The BSA will be expanded to include roofing systems, retrofits and commercial envelopes evaluation.—*Jennifer Burke*

ORNL's Dennis Youchison is the director of DOE's Innovation Network for Fusion Energy program. Image credit: Carlos Jones, ORNL

ORNL leads fusion partnership program

DOE has established the Innovation Network for Fusion Energy program, or INFUSE, to encourage private-public research partnerships for overcoming challenges in fusion energy development.

The program, sponsored by the Office of Fusion Energy Sciences within DOE's Office of Science, focuses on accelerating fusion energy development through research collaborations between industry and DOE's national laboratory complex, with its scientific expertise and facilities. The program is currently soliciting proposals and plans to select projects for awards between $50,000 and $200,000 each, with a 20 percent project cost share for industry partners.

"We believe there is a real potential for synergy between industry- and government-sponsored research efforts in fusion," said James Van Dam, DOE associate director of science for Fusion Energy Sciences. "This innovative program will advance progress toward fusion energy by drawing on the combined expertise of researchers from both sectors."

ORNL will manage the new program with Princeton Plasma Physics Laboratory. ORNL's Dennis Youchison, a fusion engineer with extensive experience in plasma-facing components, will serve as the director, and PPPL's Ahmed Diallo, a physicist with expertise in laser diagnostics, will serve as deputy director.

"I am excited about the potential of INFUSE and believe this step will instill a new vitality to the entire fusion community," Youchison said. "With growing interest in developing cost-effective sources of fusion energy, INFUSE will help focus current research. Multiple private companies in the United States are pursuing fusion energy systems, and we want to contribute scientific solutions that help make fusion a reality."

Through INFUSE, companies can gain access to DOE's world-leading facilities and researchers for tackling basic research challenges in developing fusion energy systems.

INFUSE will help address enabling technologies, such as new and improved magnets; materials science, including engineered materials, testing and qualification; plasma diagnostic development; modeling and simulation; and magnetic fusion experimental capabilities.—*Jason Ellis*

Controlling fuel tests with smaller samples

For the first time, ORNL has completed testing of nuclear fuels using MiniFuel, an irradiation vehicle that allows for rapid experimentation.

The compact experiment, which was irradiated at ORNL's High Flux Isotope Reactor and then examined to see how the fuel responded, comprises a miniature target that holds pinhead-size fuel kernels. Conventional fuel tests use pellets with volumes more than 1,000 times larger.

MiniFuel's small size helps researchers better control variables and accelerate burnup conditions during irradiation.

"Fuel performance testing is extremely complex, and it is difficult to interpret the data because so much is happening across the fuel pellet," said ORNL's Chris Petrie, who developed the concept. "With MiniFuel, we can isolate conditions, test specific fuel phenomena and acquire performance data much faster."

The ORNL-designed MiniFuel significantly decreases the size of fuel specimens and capsules that are irradiated in ORNL's High Flux Isotope Reactor. The smaller experiments allow researchers to better control conditions during irradiation and improve interpretation of data during post-irradiation examination. Image credit: Carlos Jones, ORNL

The first tests are focused on uranium nitride fuel for light water reactors—a fuel type lacking performance data.—*Jason Ellis*

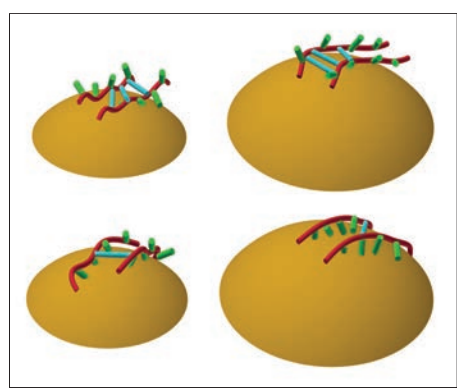
Designed polymers for next-generation batteries

ORNL researchers have demonstrated that designed synthetic polymers can serve as high-performance binding material during charging and discharging of next-generation lithium-ion batteries.

Binders serve a critical role in battery performance by maintaining the electrochemical balance of materials and extending battery life span.

The team discovered that stronger adhesion strength alone does not always improve binder performance. Rather, performance is significantly influenced by several factors working together during the battery's operation.

"Our results indicate that rational design of polymer binders is a key enabler



This illustration shows how polymers perform as a binding agent during the charging and discharging states of lithium-ion batteries. Image credit: Tomonori Saito, ORNL for high-capacity anodes in next-generation batteries," ORNL's Tomonori Saito said. The results, published in *ACS Energy Letters*, could impact batteries in future consumer electronics and electric vehicles.—*Jennifer Burke*

New 3D printing method for big metal parts

A novel additive manufacturing method developed by ORNL researchers could be a promising alternative for low-cost, high-quality production of large-scale metal parts with less material waste.

Researchers printed thin metal walls using a closed-loop, feedback-controlled technique to provide uniform flat beads and layers at a desired height. The system automatically regulates the printing process, creating stable properties within the metal deposit and producing a high-quality build throughout the part.

"We achieved a precise geometry for the components by using real-time feedback sensors to correct for abnormalities," ORNL's Andrzej Nycz said. "Because metal printed walls represent the basic building blocks of parts manufactured with big area additive manufacturing, we expect the same stable properties to hold for parts printed with complex geometries."

The large-scale metal additive manufacturing method deposits materials at high rates, which allows for multiple metal feedstocks. The team's results were published in *Applied Sciences*.—*Jennifer Burke*

Error-checking health care data

An ORNL-led study explored the interface between the Department of Veterans Affairs' health care data system and the data itself to detect the likelihood of errors, leading to the design of an auto-surveillance tool to help improve overall quality and safety.

The team's computing method can scan data for more than a million patients and push system error alerts for the VA to review and address.

An ORNL-developed computing method can scan data for more than a million patients and push system error alerts for the Department of Veterans Affairs to review and address.
Image credit: Genevieve Martin, ORNL

"Similar surveillance tools can detect human errors, but our major focus is rooting out machine-generated errors that could lead to unintended consequences in health IT," said ORNL's Olufemi Omitaomu, coauthor of the published study.

Feedback from the VA's reviews informs improvements to the surveillance tool. The next phase will involve machine learning techniques for smarter, faster error detection. Over time, the VA's platform will run more smoothly, accurately and efficiently in real time, enabling a quicker response to potentially unsafe conditions in or functionality of health IT.—*Sara Shoemaker*

Controlling heat in thermoelectrics

Scientists have discovered a way to alter heat transport in thermoelectric materials, a finding that may improve energy efficiency as the materials convert heat flow into electricity.

Caltech theorists simulating the thermoelectric material lead selenide saw something surprising—a thermal wave that did not propagate. They determined the trick to potentially increasing energy efficiency in this material was to stop heat-carrying vibrational waves without thwarting electricity-bearing electrons.

To verify the discovery, they called on experimentalists to probe a real crystal.

"Vibrational waves stop propagating in a perfect crystal because of nonlinear interactions between phonons," said ORNL's Michael Manley.

The experiment used neutron scattering at ORNL's Spallation Neutron Source and the National Institute of Standards and Technology's Center for Neutron Research, as well as X-ray scattering at Argonne National Laboratory's Advanced Photon Source. The discovery improves understanding of thermoelectric performance and may enable unconventional heat transport in future materials.—*Dawn Levy*

ORNL's Moyer honored with Seaborg Award

Bruce Moyer, leader of the Chemical Separations group in ORNL's Chemical Sciences Division, has won the 2019 Glenn T. Seaborg Award from the Actinide Separations Board.

The award recognizes "U.S. scientists and engineers who have made outstanding and lasting contributions to the development and application of actinide separations process and methodology."

Bruce Moyer

Moyer was cited for "outstanding accomplishment and meritorious achievement in actinide separations science."

Moyer is an ORNL Corporate Fellow with nearly 40 years of experience in separations science and technology, especially in applying fundamental principles to waste treatment, nuclear fuel recycle and critical materials recovery. He led the Sigma Team for Advanced Actinide Recycle for the DOE Office of Nuclear Energy from 2009 to 2018.

The winner of two R&D 100 Awards, Moyer now leads a focus area on diversifying critical materials supply for clean energy for DOE's Critical Materials Institute, as well as an Office of Science program on chemical recognition and transport in extractive separations.—*Bill Cabage*

Defending the grid:

Solutions for power system vigilance and resilience

by Stephanie Seay
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Electricity powers so much of modern life that it's hard to imagine a world without it. From keeping the lights on to energizing phones and laptops to controlling indoor climate and fueling transportation, a reliable flow of electricity is essential to daily living.

ORNL researchers have long been engaged in research to protect the critical infrastructure that generates and delivers electricity. Today the work has a new sense of urgency as grid-focused cyberattacks are on the rise and utilities tackle the challenge of integrating intermittent renewable energy with traditional power plants.

It is not an easy task. Over time, the grid has been stitched together out of disparate, individually owned generation, transmission and local distribution equipment.

"There was no original blueprint of what the future grid would look like," said Tom King, director of ORNL's Sustainable Electricity Program. "So now the challenge is how to add new intelligent technologies and integrate them into these older legacy systems.

"Historically we've used a Band-Aid approach, building add-ons to protect the network. But what we need is to have security and resilience designed into the system as we modernize the grid."

ORNL's grid work largely falls into four areas: monitoring, modeling, controls and advanced components.

Monitoring

The first—monitoring—relies heavily on the lab's history in sensors and measurements. ORNL has developed sensors that can monitor the essential elements of the grid, from the first generation of electricity to its end use in businesses and homes.

For example, ORNL scientists have developed low-cost sensors that monitor dissolved gases in transformers. An excess of acetylene gas in a transformer's insulation oil may indicate electrical arcing. With this knowledge, operators can better assess equipment and reroute power before faults occur and cascade into blackouts. The lab is also developing sensors printed on flexible substrates that can measure current and voltage on electrical equipment ranging from high-voltage transmission lines to heating, ventilation and cooling systems at businesses and homes.

"Historically we've used a Band-Aid approach, building add-ons to protect the network. But what we need is to have security and resilience designed into the system as we modernize the grid."

— ORNL Sustainable Electricity Program Director **Tom King**

In perhaps the lab's most ambitious monitoring program, researchers led by UT-ORNL Governor's Chair Yilu Liu have developed a low-cost sensing system, GridEye, consisting of frequency disturbance recorders plugged into 120-volt outlets. The compact recorders transmit real-time data on the grid's electrical frequency and voltage angle, monitoring the wide-area grid in much the way that an electrocardiogram monitors the cardiac system.

The sensors have been installed at 250 locations in North America. The system was recently refined as a mobile device, with an app known as the Mobile Grid Analyzer that enables operators to monitor the grid in the field using smart phones and tablets.

"It's the only system in the U.S. that gives a complete view of what's happening across the grid in North America," Liu said.

See DEFENDING THE GRID, page 14

ORNL's Sustainable Electricity Program Director Tom King.
Image credit: Carlos Jones, ORNL

Real communities

test ORNL microgrid controller

by Jennifer Burke
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When the power goes out unexpectedly in the United States, the cause inevitably points to one of two culprits—nature or man. Fortunately, the electrical grid is robust and, barring catastrophic events from either source, can rebound quickly when outages occur.

Nevertheless, recent natural disasters and the increasing threat of cyberattacks have spurred research to ensure the grid remains secure and adaptable.

ORNL engineer Ben Ollis has spent the past few years researching grid resilience. Recently, Ollis has led the deployment of a microgrid governed by an ORNL-developed open source controller—called CSEISMIC, for Complete System-level Efficient and Interoperable Solution for Microgrid Integrated Controls—in Alabama Power's Smart Neighborhood located in Hoover, Alabama. The Smart Neighborhood comprises 62 energy-efficient homes connected to a residential microgrid capable of serving as the community's main power source, independent from the main grid.

"The microgrid in Alabama includes natural gas generators, solar panels and a battery pack, so it can generate and store power, operating independently from the main grid or in conjunction with the grid," Ollis said. "For this to happen, though, there's a lot of back-and-forth communication that has to occur between the microgrid, the controller and the homes."

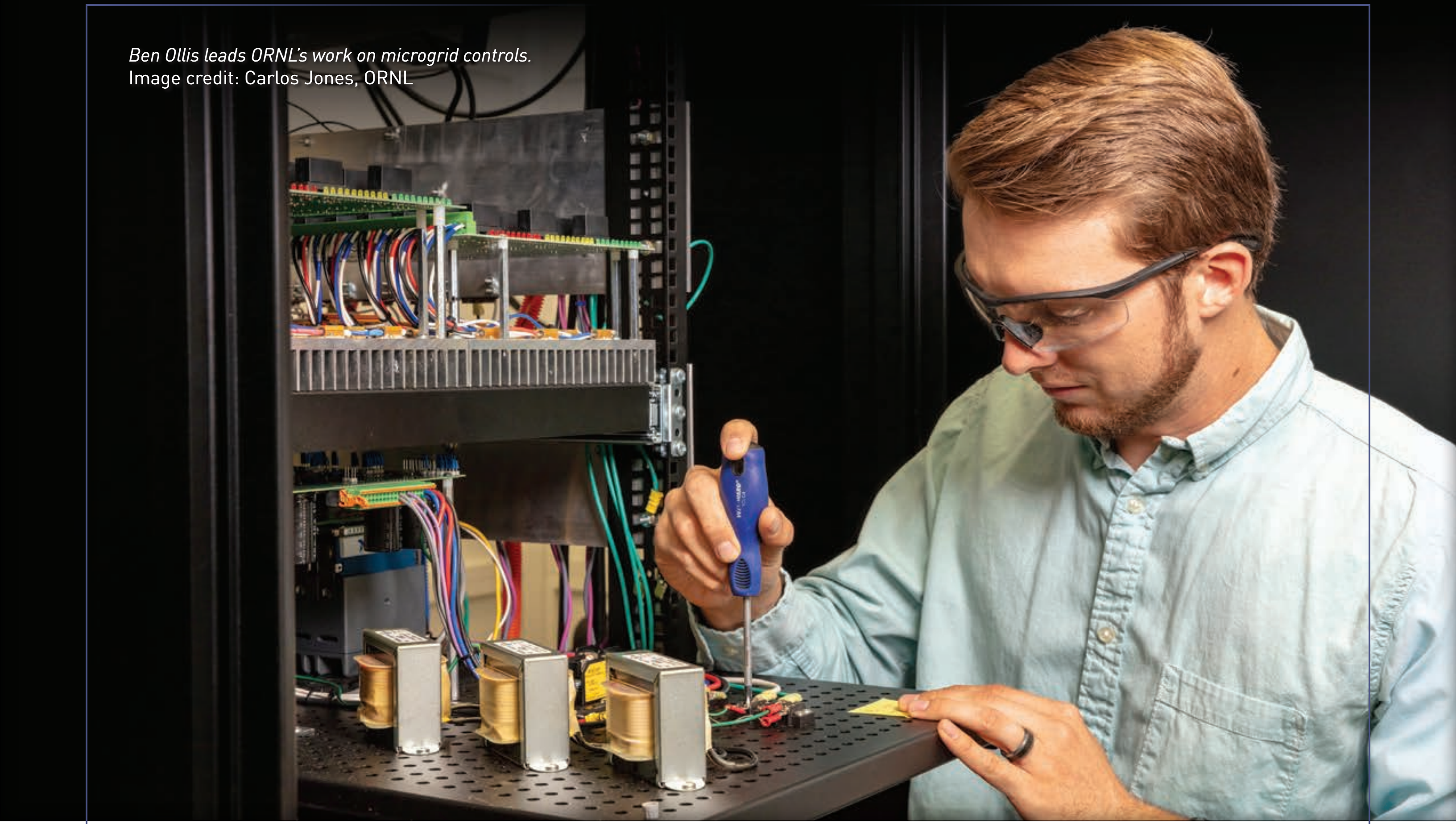
Determining whether all parties are working and communicating as they should happens only when an outage triggers power disruption.

CSEISMIC integrates seamlessly with the home's energy management system, which directs heating, cooling and smart appliance loads, with the controllers sending signals back and forth as conditions like temperature and occupancy change. The researchers successfully tested the ability to "island" the microgrid, simulating a power outage during which the local generators are called upon to serve the neighborhood's full power load.

"Because events are normally unexpected, we caused our own disruption to the neighborhood and performed intentional islanding with the microgrid," Ollis said. "On a perfect

The microgrid for the Smart Neighborhood in Hoover, Alabama, consists of solar panels and a battery pack and allows homes to disconnect from the main power grid. Image credit: Southern Company

The Smart Neighborhood in Hoover, Alabama, a 62-home development connected to a microgrid operated by ORNL's open source controller. Image credit: Southern Company



Ben Ollis leads ORNL's work on microgrid controls.
Image credit: Carlos Jones, ORNL

weather day, we shifted power to the microgrid as if a fault had occurred. And each time, there was no visible disruption to the homeowner. CSEISMIC switched power to the microgrid within milliseconds, performing exactly as it should."

The system was also tested during an unplanned disruption caused by nature.

"Unfortunately, a squirrel caused a temporary fault in the system, and the microgrid immediately opened and started feeding the neighborhood for about 30 minutes," he said. "When the main grid was stable again, we closed the microgrid back and reconnected. It did exactly what it was supposed to do in this unexpected scenario."

Balancing act

In February, Ollis demonstrated another capability of the microgrid and CSEISMIC—the ability to balance load control for cost-effectiveness and efficiency.

"We're now doing real energy load control on the homes," Ollis said. "From the energy usage home data, we know what electricity price we can offer every 15 to 20 minutes or so. Then, based on that price, the home can try to optimize to the homeowner's comfort while minimizing electricity consumption."

Energy data is securely sent from the controller to DOE's cloud-based VOLTTRON platform, which supports applications for end-use energy loads.

> *"The home adjusts its settings based on the data; there's no action on the homeowner's part."*
>
> — ORNL engineer **Ben Ollis**

Using algorithms developed by ORNL, the VOLTTRON system can forecast and optimize home energy use in response to signals from the microgrid controller. The integration of CSEISMIC with ORNL's transactive controls allows for efficient management of energy resources from generation to storage to end-use. Homeowners gain multiple opportunities for cost savings, while grid operators benefit from more precisely controlled load-balancing.

Ollis said this all happens seamlessly for the homeowner. "The home adjusts its settings based on the data; there's no action on the homeowner's part," he said.

See REAL COMMUNITIES, page 13

DarkNet:

Lighting up a secure grid communication network

by Stephanie Seay
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How do you defend the world's largest machine? This is the question scientists and engineers have faced as the power grid presents an increasingly attractive target for hackers bent on societal disruption.

For ORNL researchers, one answer lies in the way grid equipment communicates. The lab's scientists are focused on a new architecture for transferring the grid's data using "dark," or underutilized, optical fiber to build a private, secure communication network.

DarkNet represents "foundational research, from which other cybersecurity solutions will flow."

— ORNL physicist **Peter Fuhr**

The DarkNet program was conceived several years ago as ORNL physicist Peter Fuhr discussed with DOE officials the idea of getting grid communication off the public internet. Fuhr and his colleagues at ORNL then spoke with electric utilities and service companies who were intrigued by the idea and who, more importantly, had enough fiber optics sitting near major power plants, transmission and distribution systems, and other grid assets to make the project work.

Today, DarkNet researchers are developing a private network architecture that grid operators can scale up and use to quickly and accurately control power generation and transmission equipment that may sit hundreds or thousands of miles away from a central operational control center—without fear of cyberintrusion.

The scientists are testing the architecture on ORNL's own grid equipment; next they will demonstrate communication on a regional scale and, later, on a national scale.

DarkNet represents "foundational research, from which other cybersecurity solutions will flow," Fuhr said, emphasizing that the project is more than just the creation of a secure, private network. The researchers are taking on other tasks as well, such as creating a best practices guide for grid operators to follow as they modernize, and developing high-fidelity sensor suites that will give operators an unprecedented real-time view of grid operations.

The deployment of high-fidelity sensors is another step toward hardening the grid against disruption—whether manmade or natural, Fuhr noted. Advanced sensors measuring voltage, current, frequency and ambient conditions like sunlight and temperature give operators an in-depth awareness of what's going on at any moment and can even predict disruption and reroute around it for seamless reliability.

"You end up with a system that is cognizant of what is going on both operationally and on the IT side of the street," Fuhr said. The sensors function at what's known as the "grid edge"—on the outer edges of the network. They report to the command center, but they can also be given the ability to communicate with each other.

Combining a secure, fast, fiber optic-based communications network with sensors and other protective

Marissa Morales Rodriguez of ORNL's Sensors and Embedded Systems Group. Image credit: Carlos Jones, ORNL

elements "becomes the backbone of DarkNet," said ORNL's Mark Buckner.

"It creates a connected ecosystem," he said. "If you have verified data that says, 'This happened, this happened, and this happened,' and you know other things like your electrical load, then it tells you what you need to do" to respond to and even prevent outages.

Buckner said such a real-time, self-aware system is an essential building block for a smoothly functioning grid with automated controls. "That's the only way we're going to get to a truly resilient grid," he said, "because a lot of dynamics happen at a time scale where human operators can't operate."

That kind of decentralized architecture, in which devices operate in an interconnected manner on the grid edge, also introduces redundancy into the system, which could likewise deter outages, said ORNL's Marissa Morales Rodriguez.

"If you lose one device, it's already communicated its data to the other devices at the edge of the system," she said. "So instead of having a single data repository, you have many, and there's not a single point of failure."

To further protect operational data, ORNL researchers are examining the use of quantum key distribution, or QKD, which harnesses the randomness of quantum mechanics to authenticate and encrypt information. Scientists from ORNL and Los Alamos National Laboratory in New Mexico earlier this year demonstrated metro-scale QKD on the Chattanooga Electric Power Board system. The project demonstrated that two different systems could send and receive signals using QKD. Demonstrating the interoperability of two disparate systems was a key milestone for the research, since utilities often use a mix of components, and no two power distribution systems are alike.

The digital record-keeping technology known as blockchain also holds promise as a form of encryption. Blockchain verifies digital transactions, including the time of data transfer and identity of the users, and assigns those transactions with a unique identifying code.

The system, which updates in real time, could be applied to grid transactions such as those between power generators and consumers. Once data is in a blockchain platform, it cannot be altered, the scientists explained. ORNL is performing preliminary research into the feasibility of using blockchain to authenticate grid transactions, and depending on the outcome, the researchers could build a larger test bed, Fuhr said.

Gig City grid:

A conversation with EPB's Jim Ingraham

by Stephanie Seay
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Ten years into its program to create an automated smart grid supported by an all-fiber-optic communications network, the Electric Power Board of Chattanooga, Tennessee, has seen tremendous benefits. Power outages are down by 60 percent, and operational costs have fallen by some $60 million a year for the municipal utility operating in the town nicknamed America's first Gig City.

EPB's grid also serves as a living laboratory for researchers at ORNL, just over an hour's drive north. Since 2014, the lab has tested a wide range of technologies on the EPB system, such as

- sensor arrays at substations,
- microgrid controls and advanced power electronics to integrate energy storage and solar installations into the grid,
- drones that can speed infrastructure inspection and maintenance, and
- an energy use model for every building in EPB's territory to explore efficiency improvements.

Most recently, EPB teamed with ORNL and Los Alamos National Laboratory in New Mexico to perform one of the first real-world demonstrations of the use of quantum mechanics to authenticate and encrypt vital utility communications data.

Jim Ingraham, vice president of strategic research at EPB, guides the utility's business development and oversees its relationship with ORNL. We talked with Ingraham about what it's been like to partner with a national laboratory.

Jim Ingraham is vice president of strategic research at the Chattanooga Electric Power Board. Image credit: Chattanooga EPB

1. Did you have any qualms about allowing ORNL scientists to test their technologies on the EPB system? Why even allow it?

The challenges that DOE and its national labs are taking on are our challenges. Those challenges come in the rise of renewable energy and distributed energy resources, in the rise of cyber threats, in the rise of electric and autonomous vehicles and their impact on the grid, and in our desire to be able to use the trillion points a year of data we're already receiving from our system to give our customers the very best service.

We provide a rich research environment, with the stipulation that nothing be tested in a way that could disrupt service. We developed a program that gave ORNL researchers in-depth training on how our system operated before they began their work. We're confident that the basic and applied science being explored here will benefit the nation as a whole.

2. Why is grid modernization important?

Automating the grid enhances quality and reliability of service for our customers. In the circumstances of the 21st century, if your electricity and broadband aren't working, you're not working.

For instance, we had a storm in 2011 that spawned multiple tornadoes and knocked power out to about 70 percent of our system. It took us 10 days to rebuild. Now imagine if 60 percent of cars on our grid are electric. So you don't have electricity at your house and you can't go anywhere in your car. These are the kind of problems DOE is exploring, and we think a modern grid can help solve those challenges.

3. What have been the benefits of your collaboration with ORNL?

It's my job to make sure we have the most efficient and reliable system possible. Getting to be the first to test the new technologies coming out of Oak Ridge gives us direct knowledge that helps guide future investment decisions.

There's another benefit, too. Our employees love working with ORNL scientists and engineers. It's the cool, Buck Rogers stuff that has helped us retain talented, smart people and keep them engaged, to get them to think outside the box as we continue to innovate. That's what I tell people when they ask about our partnership with ORNL. We learn new stuff, but the thing that is just as valuable is the give and take with the Oak Ridge people. Oak Ridge's involvement is a point of pride in this town. It raises our profile as a technically advanced community and helps us grow our talent and our economy.

> *"Our employees love working with ORNL scientists and engineers. It's the cool, Buck Rogers stuff that has helped us retain talented, smart people and keep them engaged."*
>
> — **Jim Ingraham,** vice president of strategic research, Chattanooga Electric Power Board

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The edge and beyond

With the Alabama project progressing as planned, Ollis' work next focuses on a new Smart Neighborhood with Georgia Power in the Atlanta area. This time, the 40-plus residential dwellings are four-story town homes. The project will differ significantly in that each home will contain its own microgrid—solar panels and a battery pack—rather than be part of a large, centralized power system serving the neighborhood.

"Given the Georgia neighborhood is residential-scale energy generation instead of grid-scale, we won't have as much data to report, but we're still looking at how these homes operating independently of each other can interact with the main grid," he said.

Ollis said the Georgia neighborhood will be a test of how the edge of the grid responds and adapts to energy sources such as solar and batteries.

"What happens at the edge of the grid? How can we make adjustments and integrate new systems into a system that has parts more than a century old?" he said. "That's what we're working to figure out, and microgrid projects such as the Smart Neighborhoods provide an excellent platform for grid edge research."

Ollis said that industry has indicated interest in CSEISMIC, paving the way for future commercialization, which could in turn expand the use of microgrids.

ORNL is also working on technology to dynamically network microgrids, so an entire neighborhood or even region's distributed energy resources could communicate about their operations, back up one another and eventually support the larger bulk power system efficiently and effectively.

"People will continue to want more control and flexibility in how they receive electricity," he said. "We'll see microgrids become more commonplace in the future. Growth may be slow initially, but if usage goes from 5 to 10 percent in the next decade, that 10 percent is significant.

"Our job with research is to lay the basic foundation for understanding what works; we've shown you can operate the grid more efficiently by integrating solar and energy storage," Ollis added. "What we're demonstrating now paves the way for maximizing the grid edge in the future."

DEFENDING THE GRID, page 6

"It's important to be able to see all areas of the grid, not just one region. What may happen in Florida will affect systems as far away as the Dakotas."

"These next-generation sensors create situational awareness," King said. "Operators can track and catch trends about the condition of their assets and can take action more quickly."

> *"We want a system that's not necessarily reactive, but proactive. We want to build capabilities so that we can move ahead of where the threat of disruption might be as the operating environment changes."*
>
> — ORNL Electrical and Electronics Systems Research Division Director **Rick Raines**

Wide-area situational awareness is also important as more renewable generation sources such as solar panels and wind turbines are added to the grid, because of their intermittent nature, Liu added.

The data can be fed into simulations of the grid that can help industry better prepare for events such as storm damage or cyber-intrusion as well as long-term trends like shifts in supply and demand. That's the second area of ORNL's grid work: modeling and simulation.

Modeling

As more smart devices such as high-fidelity sensors are installed on the grid, the data flowing back to operators will grow exponentially.

"You'll be able to see events like transients on the system that indicate anomalies, or better understand the condition of grid components so you can make better predictions," King explained. "That's the value proposition for operators."

ORNL's expertise in mathematics and computer simulation has driven modeling work that can, for instance, guide industry in how best to deploy new protection relays, which can automatically reroute power around faults like downed power lines.

Modeling can also give a wider view of the grid to help electric system coordinating agencies, industry and the government gain a better understanding of the grid's interdependencies. ORNL and other national labs are working to model all the underpinnings of the connected grid, analyzing elements like fuel supply (such as the natural gas pipeline network), telecommunications systems, the placement and health of transmission and generation assets, and the placement of microgrids where they can be networked to support the bulk power system.

ORNL has used two of its own inventions to aid modeling and simulation work. A low-voltage test bed called SI-GRID safely tests hardware and software components intended for high-voltage systems. A digital twin of the grid—a simulation fed by real-time information on the grid state—has also been developed to test cybersecurity solutions.

GridEye sensor. Image credit: Carlos Jones, ORNL

Eventually, as more intelligence is built into the grid, sensors will feed into a system that provides real-time control so that outages are not just dealt with quickly but are prevented entirely.

That's where the third thrust of ORNL's grid work enters the picture: software and intelligent hardware controls to introduce more automation on the grid.

Controls

Controls research includes a unique, open-source microgrid controller developed at ORNL and successfully deployed by a partner utility in two residential neighborhoods. ORNL researchers have also developed transactive controls that use advanced algorithms to communicate information about power availability and market price between a consumer and the grid operator to efficiently control energy use in homes and buildings. More precise control of energy generating and consuming equipment can result in customer savings and a more resilient electricity network.

The microgrid controller helps resolve a big issue for the grid: the growing amount of electricity produced by decentralized, distributed generation sources such as solar and wind that must be integrated into the system. Using intermittent renewable generation poses a challenge for utilities accustomed to big power plants and only one-way electricity flows.

"We're developing creative ways to integrate these local power assets and get as much benefit from them as we possibly can," said Ben Ollis, who leads the lab's microgrids research.

ORNL's microgrid controller can help keep the larger grid balanced by selling its excess electricity or by supplying local customers with 100 percent of their power needs. That could happen involuntarily during a grid blackout or voluntarily in a scenario known as demand response. In times of peak demand, the utility will signal the microgrid controller with a price offer. If that offer is accepted, the microgrid will island itself in a practice known as load shedding, Ollis explained.

"Microgrid controls are about taking everything you have to consider on the larger grid and shrinking it," Ollis said. "You have to consider demand as well as supply and be able to serve your local users on a moment's notice" if the microgrid is islanded.

See DEFENDING THE GRID, page 16

Wenxuan Yao of the ORNL Power and Energy Systems Group helped design the mobile app for the Mobile Grid Analyzer sensor system.
Image credit: Carlos Jones, ORNL

DEFENDING THE GRID, page 15

In addition, the transactive controls being developed at ORNL could harness the energy consumption of a fleet of buildings to help balance a grid's electrical loads by, for example, preheating or precooling work and living spaces during off-peak hours without sacrificing occupant comfort.

"We want a system that's not necessarily reactive, but proactive," said Rick Raines, director of the Electrical and Electronics Systems Research Division at ORNL. "We want to build capabilities so that we can move ahead of where the threat of disruption might be as the operating environment changes."

To encourage the most resilient grid possible, ORNL researchers are looking at ways to embed computing power at the grid edge. In this approach, grid controls are decentralized so that devices like protective relays and sensors can continue to function even if parts of the network are compromised and the devices cannot communicate with a control center.

"When you have these distributed, disparate and integrated networks, if you wait until something is communicated to a central location to act, you've already lost the battle," Raines said.

Such a future will rely on artificial intelligence so that the trillions of data points flowing into the control system can be swiftly analyzed and addressed.

"We can use machine learning initially as forensics to analyze past events," explained Mark Buckner, leader of the Power and Energy Systems Group at ORNL. "Then, as the system learns, it creates a predictive model that says, 'This is what I'm expecting to see if I do this,' and when that bears out, it builds confidence in the model. If you extend that model into smart automated controls, you have a system that understands precursors based on past events—so that the system can be proactive when those same events happen in the future."

King added, "Artificial intelligence and machine learning will be important for the operational and controls side, but also for the cybersecurity piece of protecting the grid. We want to get to a system that can immediately determine whether an event is due to a nefarious actor attempting to disrupt the system, or that a car struck a power pole."

One of ORNL's largest grid projects seeks to secure the underpinning for these controls. The DarkNet project creates an architecture with underused optical fiber to construct a private, secure network for grid communication. The key objective is to get grid controls and data transfer off the public internet.

Advanced components

The fourth thrust of ORNL's grid research focuses on supporting the grid of the future with devices such as power electronics, energy storage, intelligent relays and other advanced components that will enable a smart, resilient and secure system. These devices receive signals from the controls side and take action.

For instance, energy storage is a vital element for the grid. Storing energy for later use is essential to the integration of intermittent renewable power sources and to provide resilience if the grid is compromised. ORNL scientists have developed several technologies in this area: a system that stores electricity mechanically in pressurized water vessels; components for a low-cost reduction-oxidation—or redox—flow battery that stores a large amount of electricity in a cross between a conventional battery and a fuel cell; and a system that deploys used electric vehicle batteries for grid-level energy storage.

Power electronics enable the integration of energy storage, solar panels, vehicle chargers and other essential elements into the grid while ensuring reliability of service. ORNL scientists are creating inverters using heat-tolerant silicon carbide materials and low-cost 3D printing methods for both high-voltage transmission systems and lower-voltage local utility systems. These electronics accommodate the multidirectional power flow required for distributed energy and can mimic the operation of conventional power plants to maintain grid frequency—what operators refer to as the balance between electricity supply and demand.

Changes to generation sources also mean that the grid must respond rapidly to frequency fluctuations. ORNL's protective relay research is focused on developing intelligent relays that can monitor and automatically respond to grid frequency changes, clearing faults faster to ensure a stable grid. This is a change from past industry practice, in which relays were often installed in the field with a static setting—referred to as "set-it-and-forget-it."

To prepare for these changes, electric industry partners have increasingly turned to the national labs, working hand in hand to ensure that technological solutions are thoughtfully designed and with a low enough cost to be adopted broadly for the best system-wide outcome. The interdependent grid, after all, is just that—disruption of one part of the network can affect end-users hundreds or thousands of miles away.

"You cannot just implement all these changes quickly. There are already huge hardware investments on the grid," Liu said. "It is our biggest challenge today to make the system resilient without

"You cannot just implement all these changes quickly. There are already huge hardware investments on the grid. It is our biggest challenge today to make the system resilient without adding another $5 trillion on. We need to figure out a way to make the grid resilient without gold-plating it."

— University of Tennessee-ORNL Governor's Chair **Yilu Liu**

University of Tennessee-ORNL Governor's Chair Yilu Liu has developed a low-cost sensing system that records the power grid's electrical frequency and voltage angle. Image credit: Carlos Jones, ORNL

adding another $5 trillion on. We need to figure out a way to make the grid resilient without gold-plating it."

That's where industry partnerships come in. Partners who can help guide research for the best outcome are essential for success.

Partners

ORNL has worked with multiple utilities, equipment vendors, industry research organizations and academic partners to test new technologies. Many of the sensing and control technologies developed by ORNL, for instance, have been tested on the system of the Electric Power Board of Chattanooga, Tennessee. EPB's all-fiber-optic network provides an ideal living laboratory to test smart grid technologies—including a recent test of quantum key distribution. QKD leverages the inherent randomness of quantum mechanics to authenticate and encrypt information, potentially creating a system of grid communication that cannot be hacked.

Southern Company, one of the largest utility operators in the nation, worked directly with ORNL scientists to successfully test microgrid controls in two residential neighborhoods in Alabama and Georgia. The Tennessee Valley Authority has also been a long-standing partner to ORNL in developing generation and transmission technologies, in addition to supplying the bulk of the lab's own power.

Some of ORNL's advancements in monitoring have been accomplished in collaboration with another local partner, CURENT, a National Science Foundation engineering research center at the University of Tennessee. CURENT—the Center for Ultra-Wide-Area Resilient Electric Energy Transmission Networks—was the first engineering research center to be cofunded by the NSF and DOE. ORNL and UT, through CURENT, codeveloped the GridEye and Mobile Grid Analyzer. CURENT likewise works closely with industry partners to help direct its research efforts.

"If we don't have industry partners, our research will go nowhere," King said. "Developing key partnerships with utility companies and vendors is critical to getting these ideas to the marketplace."

Microscopy technique

offers an up-close view of proteins

by Sara Shoemaker
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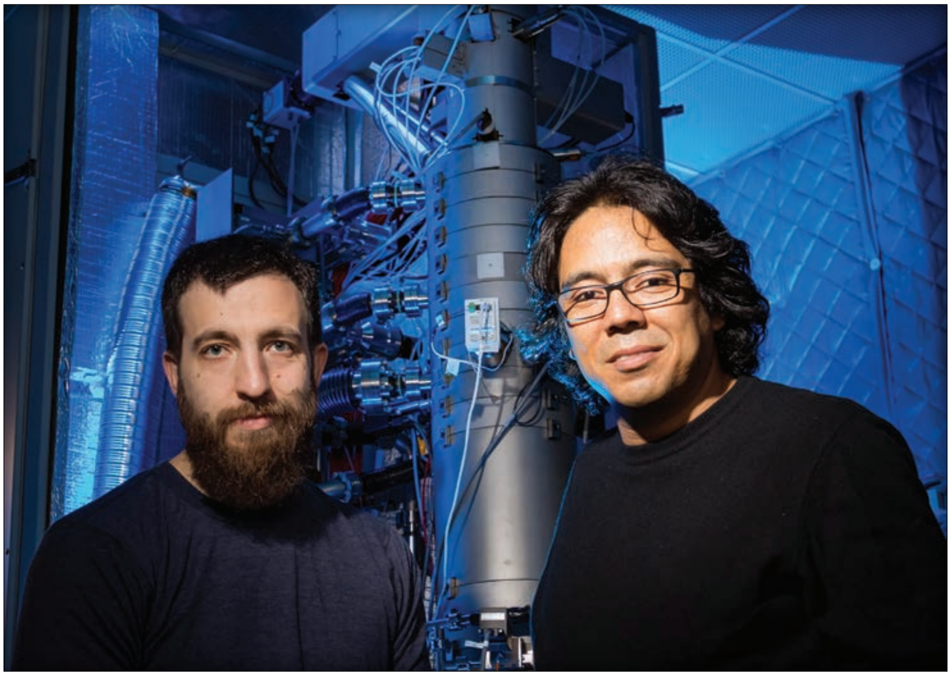
A new electron microscopy technique that detects subtle changes in proteins without damaging them could open the way to deeper, more comprehensive studies of the building blocks of life.

Developed by ORNL scientists, the technique allows researchers to identify a chemical reaction by detecting minute changes in the weights of proteins—down to a single neutron added to or detracted from one of a protein's constituent amino acids.

With this technique, the ORNL researchers became the first to use an electron microscope to directly identify isotopes in amino acids without damaging them. They described their achievement in the journal *Science*.

When an atom of carbon or some other element gains or loses a neutron, it becomes a different isotope of that element. These isotopes are commonly used to label molecules and proteins, because the shifting of atomic weight can be detected by a technique called mass spectrometry—the most common scientific method to measure a sample's mass.

Mass spectrometry is the hallmark in biological research, yet the process destroys samples that could have more information to reveal. Instead of breaking molecules apart, ORNL's electron microscope can identify almost exactly where the mass changes take place based on the molecule's vibrations. The strength of the vibrations directly relates to the molecule's atomic weight.



ORNL scientists Jordan Hachtel, left, and Juan Carlos Idrobo used a monochromated, aberration-corrected scanning transmission electron microscope technique that detects subtle changes in the weight of proteins at the nanoscale—while keeping the sample intact. Image credit: Carlos Jones, ORNL

> *"Isotopic labels are typically seen on the macroscopic level using mass spectrometry, a scientific tool that reveals a sample's atomic weight and isotopic composition."*
>
> — ORNL physicist **Juan Carlos Idrobo**

Because the technique does not destroy the amino acids, it creates a foundation for scientific discoveries ranging from simple to complex biological structures.

"The way we understand the progression of diseases, human metabolism and other complicated biological phenomena is based on interactions between proteins," said lead author and ORNL electron microscopist Jordan Hachtel. "We study these interactions by labeling a specific protein with an isotope and then tracking it through a chemical reaction to see where it went and what it did."

The team's novel experiment, which took place at ORNL's Center for Nanophase Materials Sciences, used a technique called monochromated electron energy-loss spectroscopy in a scanning transmission electron microscope. The technique is sensitive enough to distinguish between molecules that differ by a single neutron on a single atom.

"Isotopic labels are typically seen on the macroscopic level using mass spectrometry, a scientific tool that reveals a sample's atomic weight and isotopic composition," said ORNL physicist and corresponding author Juan Carlos Idrobo.

A mass spectrometer uses an electron beam to break a molecule apart into charged fragments that are then characterized by their mass-to-charge ratio. Observing the sample at the scale of molecules, scientists must use statistics to infer what chemical bonds were likely to have existed in the sample, which is destroyed during the experiment, leaving valuable information undiscovered.

The new electron microscopy technique, as applied by the ORNL team, offers a gentler approach. By positioning the electron beam extremely close to the sample—but without directly touching it—scientists use the electrons to excite and detect the vibrations without destroying the sample, allowing observations of biological samples at room temperature over longer periods of time.

The team's result constitutes a breakthrough for electron microscopy, since the negatively charged electron beam is typically sensitive only to the protons, not the neutrons. "However, the frequency of the molecular vibrations is dependent on the atomic weight, and the accurate measurement of these vibrational frequencies opens the first direct channel to measure isotopes in the electron microscope," Idrobo said.

The ORNL-led research team expects its potentially game-changing technology will complement rather than replace mass spectrometry and other conventional optical and neutron-based techniques currently used to detect isotopic labels.

"Our technique is the perfect complement to a macroscale mass spectrometry experiment," Hachtel said.

Beyond the life sciences, the technique could be applied to other soft matter such as polymers and potentially in quantum materials, where measuring molecular vibrations can play a key role in controlling superconductivity.

The interdisciplinary ORNL research team that brought damage-free isotopic labeling to the nanoscale in the electron microscope includes, from left, Jacek Jakowski, Santa Jansone-Popova, Juan Carlos Idrobo, Jingsong Huang, Jong Keum, Jordan Hachtel and Ilja Popovs, all of ORNL. Not pictured, Tracy C. Lovejoy, Niklas Dellby and Ondrej L. Krivanek of Nion Co. Image credit: Carlos Jones, ORNL

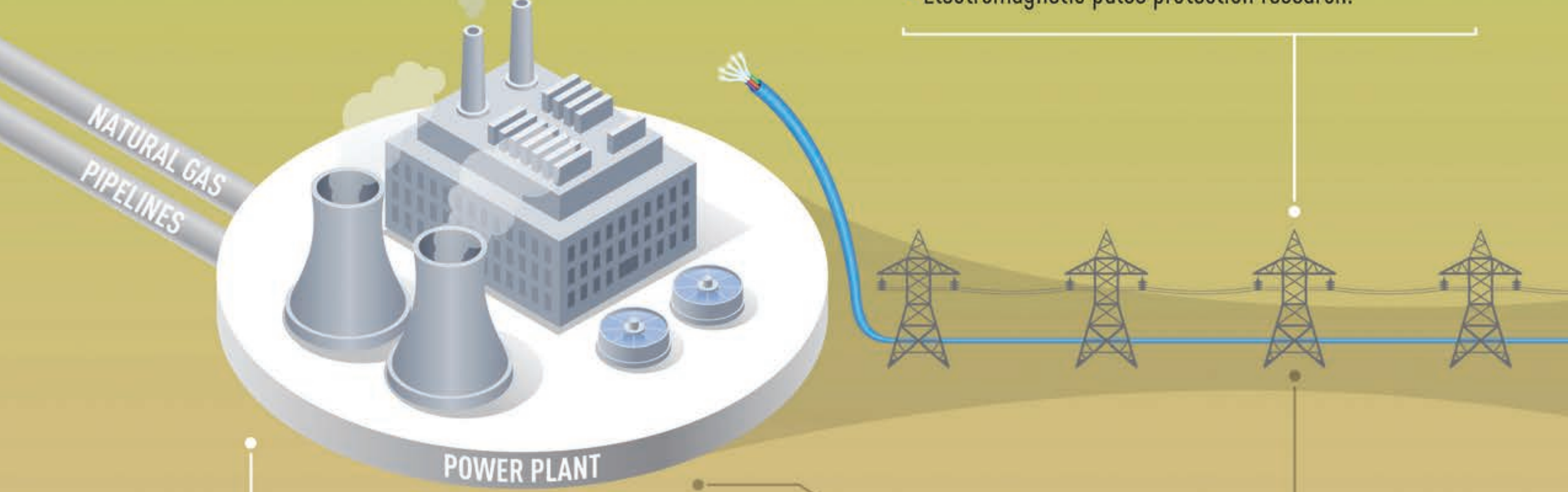
ORNL on the grid

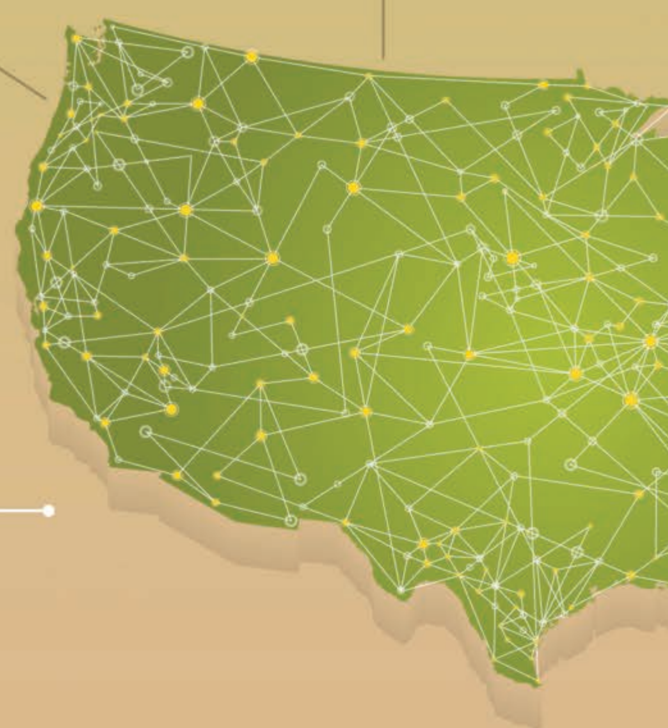
ORNL's research touches nearly every facet of the nation's electricity delivery system from generation to end use.

A modern, secure grid is the goal of ORNL's work targeting innovations in monitoring, modeling, automation and cyber physical security.

Power transmission

- Real-time monitoring of equipment health, current, voltage and other indicators.
- Protective power relays that adapt to system conditions, allowing faster fault response.
- Electromagnetic pulse protection research.





Baseload generation

- Equipment sensors, materials for more efficient power plants and modeling of the interconnected energy grid, including generation plants and fuel supply network.

Modeling and situational awareness

- Surveying and capturing information on power flows and infrastructure health across the nation.
- Eagle-I web portal for energy outage monitoring.
- GridEye system to sense wide-area power fluctuations.
- Nationwide resilience modeling to analyze energy interdependencies and plan for contingencies.

Grid security: DarkNet

- Using optical fiber to create a private, secure grid communication network.
- Quantum key distribution and blockchain to authenticate and secure data transfer.

End use and distributed energy resources

- Power electronics to seamlessly integrate renewable energy and energy storage into the grid and facilitate two-way power flows.
- Open-source microgrid controller, integrated with transactive controls for home energy management and grid load balancing.
- Integration of electric vehicle extreme-fast charging.
- Building modeling to evaluate energy efficiency retrofits.

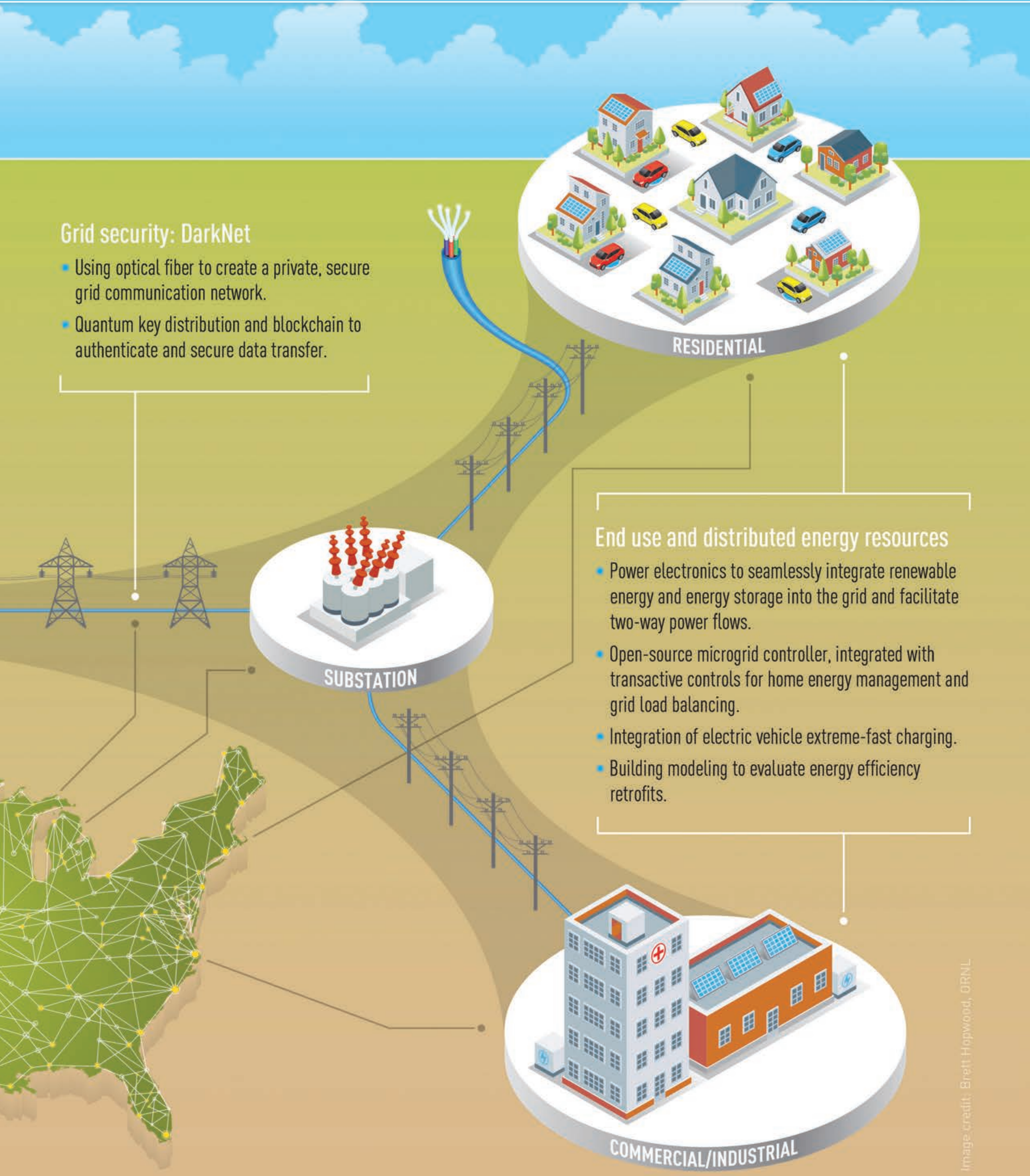


Image credit: Brett Hopwood, ORNL

Low-temp catalysis

promises huge energy savings

by Paul Boisvert
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In catalysis, a chemical reaction is aided by the addition of a substance that itself remains unchanged by the reaction. This may be why the Chinese character for "catalyst" is the same as for "marriage broker": because both facilitate reactions between partners.

The chemical industry uses catalysts to facilitate reactions between "chemical partners" in about 90 percent of all chemical manufacturing processes as a means of optimizing energy use and reducing greenhouse gas emissions.

Chemical production contributes over $5 trillion to the global economy and supports more than 110 million jobs worldwide. Not surprisingly, the chemical industry is also a large energy consumer, accounting for approximately 10 percent of all global energy demand worldwide. The sheer scope of the industry suggests that reductions in energy consumption for certain chemical processes would offer substantial economic and environmental impacts.

Scientists from Louisiana State University are using neutrons at ORNL to promote this goal by studying the use of an alternating electromagnetic field to produce low-temperature catalytic reactions.

The process involves heating iron oxide nanoparticles that have hydrocarbon molecules attached to their surface. The researchers use a radio frequency generator to stimulate the nanoparticles, with the heat transferring to the individual hydrocarbon molecules, changing their chemical bonds to produce new products.

"We want to significantly reduce energy consumption and increase catalytic reaction efficiencies by isolating heat generation to the location of the hydrocarbon molecule, instead of heating the entire reactor to extremely high temperatures," said James Dorman of LSU's Department of Chemical Engineering. "Lowering overall process temperatures during hydrocarbon catalysis also reduces the formation of coke and

Louisiana State University researchers James Dorman and Natalia da Silva Moura used RF fields to heat iron oxide nanoparticles attached to hydrocarbon molecules to achieve more energy efficient catalytic reactions. Image Credit: Genevieve Martin, ORNL

unwanted by-products, such as greenhouse gas emissions."

A 2013 report by the International Energy Agency estimated that energy-saving catalytic processes could reduce energy use in 2050 by 13 exajoules—an amount equivalent to the annual energy use of Germany. At the same time, greenhouse gas emissions could drop by the equivalent of 1.1 billion tons of CO_2, or the amount produced by more than 200 million passenger vehicles.

The LSU team exposed its samples to an RF field in a laboratory chamber, immersed them afterward in liquid nitrogen to freeze everything in place, and then observed the results using neutron-based vibrational spectroscopy at the VISION beamline at ORNL's Spallation Neutron Source. Neutron scattering combined with vibrational spectroscopy is an ideal method to study energy transfer across inorganic-organic interfaces.

> *"The neutron data enables us to see how each shape interacts with our target molecules and then improve the design to maximize the efficiency of the localized heating and reactions."*
>
> — Louisiana State University graduate student **Natalia da Silva Moura**

Currently, the researchers are developing advanced methods of synthesizing iron oxide nanoparticles and modifying their shape to control the surface sites of a sample involved in adsorption and surface reactions. Various particle forms, including spheres, cubes and hexagons, can be produced to optimize their use in different catalytic applications.

"One of our biggest challenges is to control the process of synthesizing nanoparticles and optimizing their morphology at the same time," said Natalia da Silva Moura, a graduate student in Dorman's group at LSU. "The neutron data enables us to see how each shape interacts with our target molecules and then improve the design to maximize the efficiency of the localized heating and reactions."

Part of the experiment includes pulsing the RF field to limit the reaction and prevent the formation of coke on the surface. Of particular interest is the amount of energy transfer caused during heating as a function of the magnetic field's frequency and strength.

Once this relationship is understood, the scientists plan to develop new catalysts to drive reactions down alternative pathways to increase selectivity and yield without the need to apply high temperatures.

Study of exotic ice questions water theory

by Sara Shoemaker
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Much is known about water and its most common solid form—ice. But under very low temperatures and extreme pressure—similar to conditions within massive planets—the super-cold state of water can be pushed into phases far beyond the ice cubes found in our freezer.

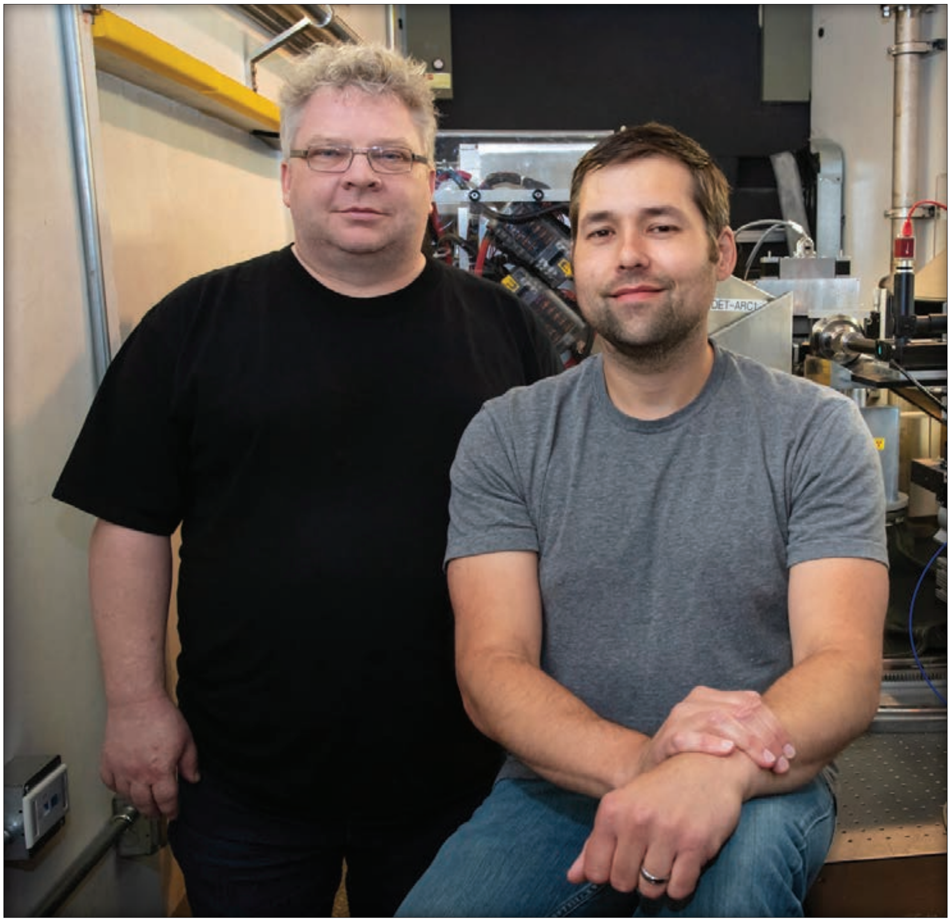
In fact, scientists have discovered up to 17 phases of ice thought to exist beyond Earth's limits. Each is characterized by a unique, dense crystalline structure of water's hydrogen and oxygen atoms.

ORNL researchers studying some of these ice phases collected puzzling data, a finding that challenges accepted theories but will lead to better understanding of super-cooled water.

"As ice changes phases, it's similar to water going from a gas to a liquid to a solid, except at low temperatures and high pressure—the ice transforms between various different solid forms," said Chris Tulk, an ORNL physicist who specializes in neutron scattering at the Spallation Neutron Source, where these experiments took place.

On Earth, when water molecules reach zero degrees Celsius, they enter a low-energy state and settle into a stable, 3D crystalline shape. This frozen form is ice Ih, the most common phase of solid water found on Earth.

Among the forms of solid water found in the universe and created in the laboratory is a formless, non-crystalline phase known as amorphous ice. Tulk and colleagues froze about half a drop of specially treated water to well below zero and applied tens of thousands of pressure units called atmospheres, enough to force super-cold water molecules into a solid, non-crystalline amorphous structure. Their goal was to observe the molecules as they recrystallized into various phases of ice as the pressure increased.



ORNL scientists Chris Tulk, left, and Jamie Molaison were part of a team that discovered a pathway to the unexpected formation of dense, crystalline phases of ice thought to exist beyond Earth's limits. They used the unique neutron scattering capability of ORNL's Spallation Neutron Source for the experiment. Image credit: Genevieve Martin, ORNL

When they observed the neutron scattering data, the scientists discovered they had indeed made ice phases known as ice IX, ice XV and ice VIII. But the expected evidence of amorphous ice was missing.

"I've made many of these samples, always by compressing ice at low temperature," said co-author Dennis Klug from the National Research Council of Canada, the lab that discovered the pressure-induced amorphization of ice in 1984. "I've never previously seen this pressure-temperature path result in a series of crystalline forms like this."

At first, the team thought its observation was the result of a contaminated sample.

Three more experiments with fresh, carefully handled samples produced identical results, confirming the sequence of ice phase changes and no amorphous ice.

"The key was the slow rate of pressure increase and collection of data at a lower pressure that allowed the ice structure to relax and become the stable ice IX form," Tulk said. Previous experiments had quickly passed over the ice IX structure without a point where the molecules relaxed, resulting in the amorphous phase.

"If the data from our experiment was true, it would mean that amorphous ice is not related to liquid water but is rather an interrupted transformation between two crystalline phases, a major departure from widely accepted theory," Klug said.

For 35 years, scientists have been researching the properties of super-cold water and looking for what's known as the second critical point, which is buried within the solid ice phases. But these results question its very existence.

Yet this discovery, reported in the journal *Nature*, will also lead to better understanding of ice and its various phases that could exist on other planets, moons and elsewhere in space.

ORNL scientists studying super-cold states of water discovered a pathway to the unexpected formation of dense, crystalline phases of ice thought to exist beyond Earth's limits. Their findings, reported in Nature, *challenge accepted theories and could lead to better understanding of ice found on other planets, moons and elsewhere in space.* Image credit: Jill Hemman, ORNL

The human element

by Morgan McCorkle
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If it's a been a few years—or decades—since you last opened your high school chemistry textbook, its periodic table, that guiding force for chemists worldwide, is almost certainly out of date. Scientists are constantly pushing the boundaries of chemistry and physics in their search for new elements, a quest that ORNL staff and facilities have supported since the lab's inception in the 1940s.

The United Nations declared 2019 as the International Year of the Periodic Table, recognizing the scientific significance of the chemical categorization system and celebrating a century and a half of scientific discovery since Dmitri Mendeleev first organized elements into the format we know today. Every atom is a specific element depending on the number of protons in its nucleus.

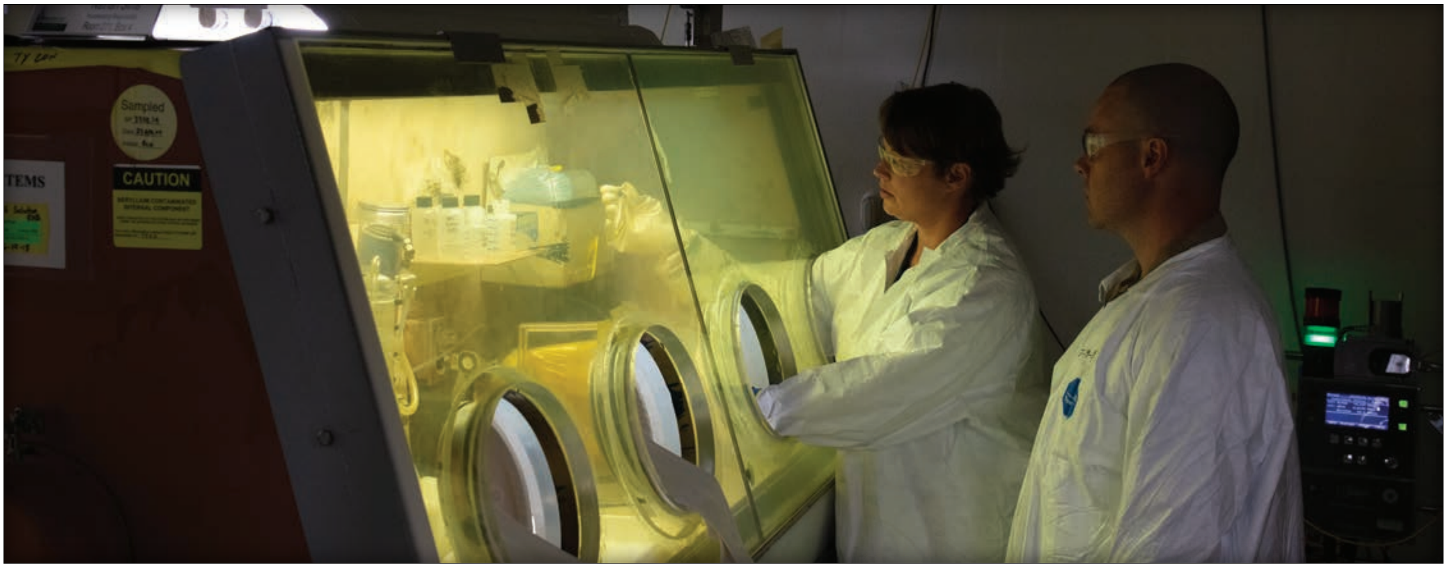
"When you look at any element on the periodic table, you are looking at a building block of the known universe," said James Roberto, retired ORNL associate laboratory director. "The beauty of the table is that the position of an atom in the table helps you describe its properties. But looking closer, there's actually a story behind each one—a story of discovery."

ORNL's story in element discovery began in secret during the Manhattan Project, as scientists analyzed fission products from the X-10 Graphite Reactor. At that time, the periodic table had gaps, places where radioactive elements were anticipated to exist but where they hadn't yet been confirmed because of their relatively short half-lives. ORNL chemists filled one of the gaps in 1945 by separating the missing element 61 from irradiated uranium fuel. They named it promethium, born of fire in the world's first continuously operated nuclear reactor.

Building on the Graphite Reactor's success in producing isotopes following the war, the research community began looking at ways to study and produce elements beyond plutonium, or element 94. That led to construction of the High Flux Isotope Reactor at ORNL in 1965.

"The intense thermal neutron flux of HFIR enabled it to produce transplutonium isotopes such as californium and berkelium in quantities that allowed the development of the new field of heavy element chemistry," Roberto said. "The adjacent Radiochemical Engineering Development Center provided a unique capability to do very high-precision chemical separations and obtain very pure products of these isotopes."

A half century later, HFIR and REDC continue to be the world's principal source of transplutonium isotopes.



Shelley VanCleve and Nathan Sims of ORNL's Isotope and Fuel Cycle Technology Division work with berkelium-249. Image credit: Carlos Jones, ORNL

ORNL chemist Shelley VanCleve.
Image credit: Carlos Jones, ORNL

Isotopes produced at HFIR have been sent to accelerator facilities in California and Russia, where they have been used as target materials enabling discoveries of many new elements. In the 2000s, ORNL researchers also became more involved as scientific collaborators, developing and supplying state-of-the-art digital electronics critical to element discovery.

"This is big science that works best when large groups who represent the best capability in their particular area can work together," Roberto said.

A U.S.-Russian experiment in 2009 led to the lab's second official element discovery—element 117, which was announced in 2010 and named tennessine to recognize the contributions of ORNL and its Tennessee university partners, the University of Tennessee and Vanderbilt. ORNL's third new element, moscovium, was discovered in the same collaboration as a decay product of tennessine.

After seven decades of shaping the periodic table, ORNL researchers aren't resting on their laurels. They're already involved in experiments to look for elements 119 and 120, using targets produced at ORNL and irradiated in accelerators in Japan and Russia.

"The idea of playing a small part in discovering a new element is very exciting. With each campaign we have learned something new, expanding on our techniques to provide a quality product. The gratitude and excitement of those researchers receiving the material feeds our desire to do more."

— ORNL chemist **Shelley VanCleve**

"The idea of playing a small part in discovering a new element is very exciting," said Shelley VanCleve of ORNL's Isotope and Fuel Cycle Technology Division. "With each campaign we have learned something new, expanding on our techniques to provide a quality product. The gratitude and excitement of those researchers receiving the material feeds our desire to do more."

The effort is driven in part by the search for the "island of stability," where scientists anticipate that superheavy elements will have longer lifetimes, enabling detailed studies of the chemistry and physics of these extreme atoms and nuclei.

"We don't think the periodic table ends at 120," Roberto said. "However, discovery times are getting longer, and new approaches will be needed to go further."

ORNL and its international partners are betting that scientific progress and ingenuity will allow the discovery stories to continue.

"The researchers in superheavy element production make up a very small community worldwide, but the passion and excitement they possess for their work make me think the 'island of stability' is within reach," VanCleve said.

Expanding the periodic table

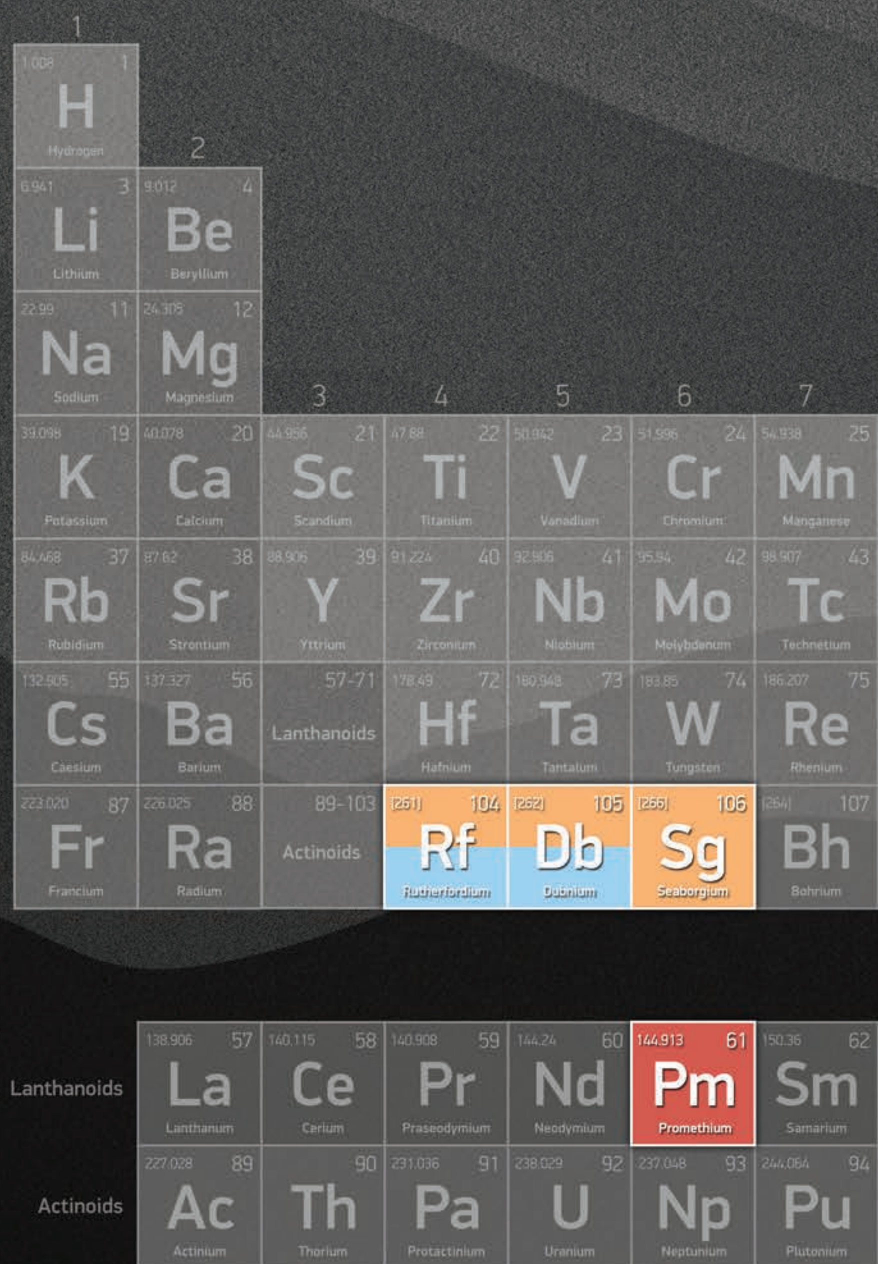
ORNL has been involved in the discovery or confirmation of 11 new elements since the lab was created by the Manhattan Project in 1943. During the International Year of the Periodic Table—2019—ORNL is celebrating the contributions of lab scientists, engineers, technicians and support staff who helped shape the periodic table as we know it today.

Targeting the superheavies

Superheavy elements with an atomic number of **104** or higher were synthesized beginning in the 1960s by bombarding specialized targets with atomic beams. Unique actinide target materials produced at ORNL have enabled the discovery and confirmation of eight superheavy elements—**104, 105, 106, 114, 115, 116, 117** and **118**—in experiments that spanned the course of five decades.

Born of Fire

The radioactive element **61** was discovered in 1945 during the Manhattan Project by chemists working at ORNL's Graphite Reactor. They named it promethium after Prometheus, the mythical figure who stole fire from the gods to share with humans.



Categories

- Discovery credit: **61, 115** and **117**
- Target supply: **104, 105, 106, 114, 115, 116, 117** and **118**
- Alpha and X-ray detection: **102, 103, 104** and **105**

Tennessine

A U.S.-Russian experiment in 2009 that produced the first atoms of element **117** relied on a berkelium-249 target only available through ORNL, thanks to the lab's High Flux Isotope Reactor and radiochemical separation capabilities. ORNL also developed digital detector technology used in confirming element **117** and its decay products, including element **115**. In honor of ORNL and its Tennessee university partners, element **117** was officially named tennessine in 2016.

Early work in detection

In the 1970s, researchers at ORNL used alpha and X-ray detection to provide the first unequivocal identification of elements **102**, **103**, **104** and **105**, helping confirm the initial discoveries made at facilities in Dubna, Russia, and Berkeley, California.

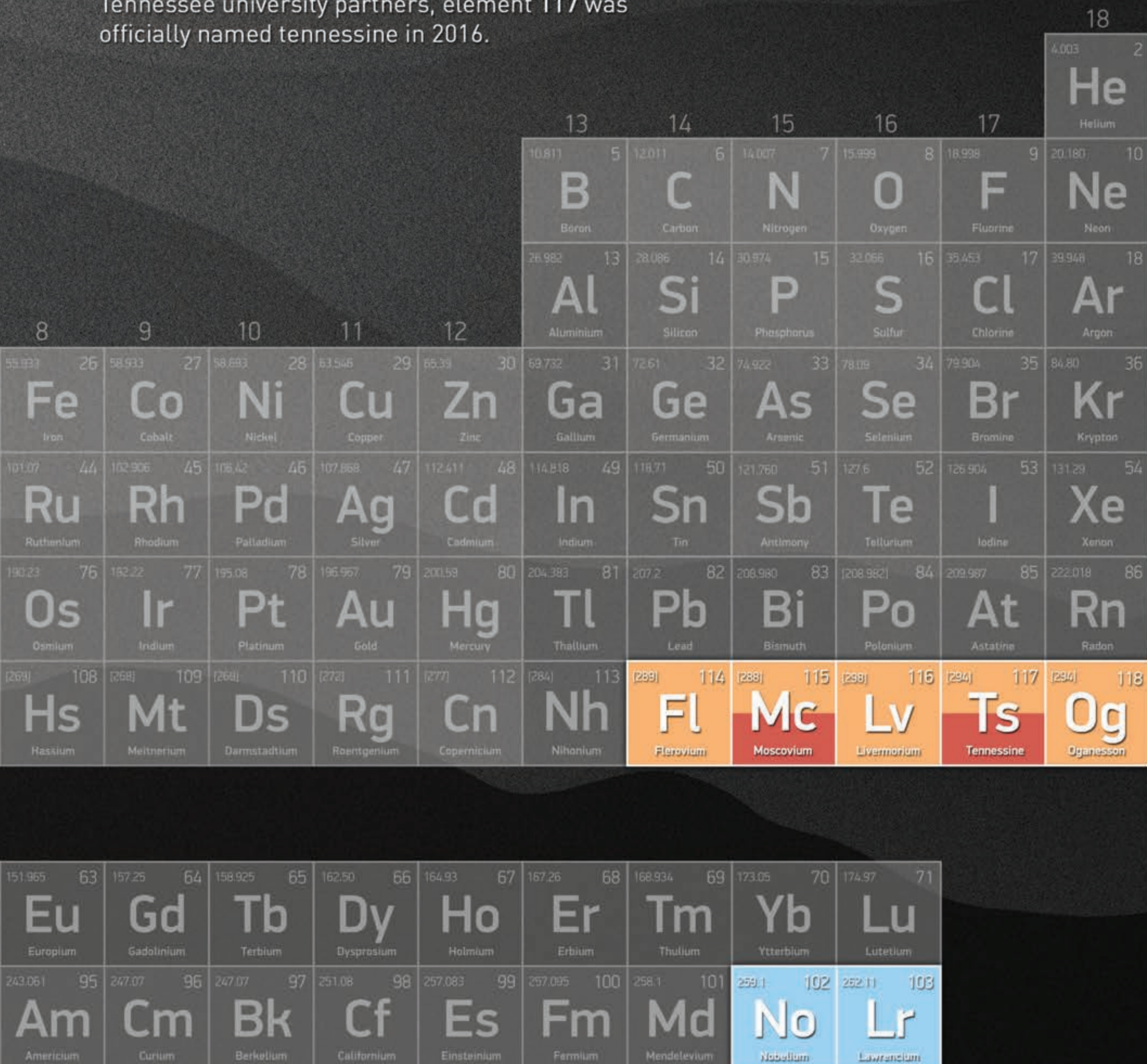


Image credit: Brett Hopwood, ORNL

Solving a beta decay puzzle

by Jonathan Hines
ornlreview@ornl.gov

Unstable nuclei don't remain unstable forever. Eventually they undergo a process called beta decay, converting a proton into a neutron, or vice versa, to form another element.

For decades, scientists have worked to develop a theory that explains this behavior from first principles, that is, from fundamental calculations that avoid assumptions. Such a theory would be able to better predict how stars create heavier elements and why neutrons inside the nucleus decay more slowly than free neutrons.

New findings, made possible by ORNL's Titan supercomputer, show scientists have finally found an answer. By accounting for subtle effects that take place between nucleons (protons and neutrons), an international collaboration—including ORNL scientists—demonstrated that theory can now accurately describe some decay properties with enough precision to allow for direct comparison with experiment.

To solve the problem, the team simulated the isotope tin-100 decaying into indium-100. Tin and indium are neighbors on the periodic table, and the two isotopes share the same number of nucleons, with tin-100 possessing 50 protons to indium-100's 49.

The achievement gives nuclear physicists increased confidence as they search for answers to some of the most perplexing mysteries related to the formation of matter in the universe. Beyond regular beta decay, scientists are looking to compute neutrinoless double beta decay, a theorized form of nuclear decay that, if observed, would explore important new physics and help to determine the mass of the neutrino.

In the past, nuclear physicists worked around this problem by inserting a fundamental constant to reconcile observed beta-decay rates of neutrons inside and outside the nucleus, a practice known as "quenching." But with machines like Titan, the team demonstrated that this mathematical crutch is no longer necessary.

"We found that quenching could largely be explained away by including two nucleons in the decay—for example, two protons decaying into a proton and a neutron, or a proton and a neutron decaying into two neutrons," said ORNL computational scientist Gustav Jansen.

> *"We found that quenching could largely be explained away by including two nucleons in the decay—for example, two protons decaying into a proton and a neutron, or a proton and a neutron decaying into two neutrons."*
>
> — ORNL computational scientist **Gustav Jansen**

Calculating beta decay precisely required the team to not only accurately simulate the structure of the mother (original) and daughter (transformed) nuclei but also account for interactions between two nucleons during the transition. This additional treatment presented an extreme computational challenge due to the combination of strong nuclear correlations and interactions involving the decaying nucleon.

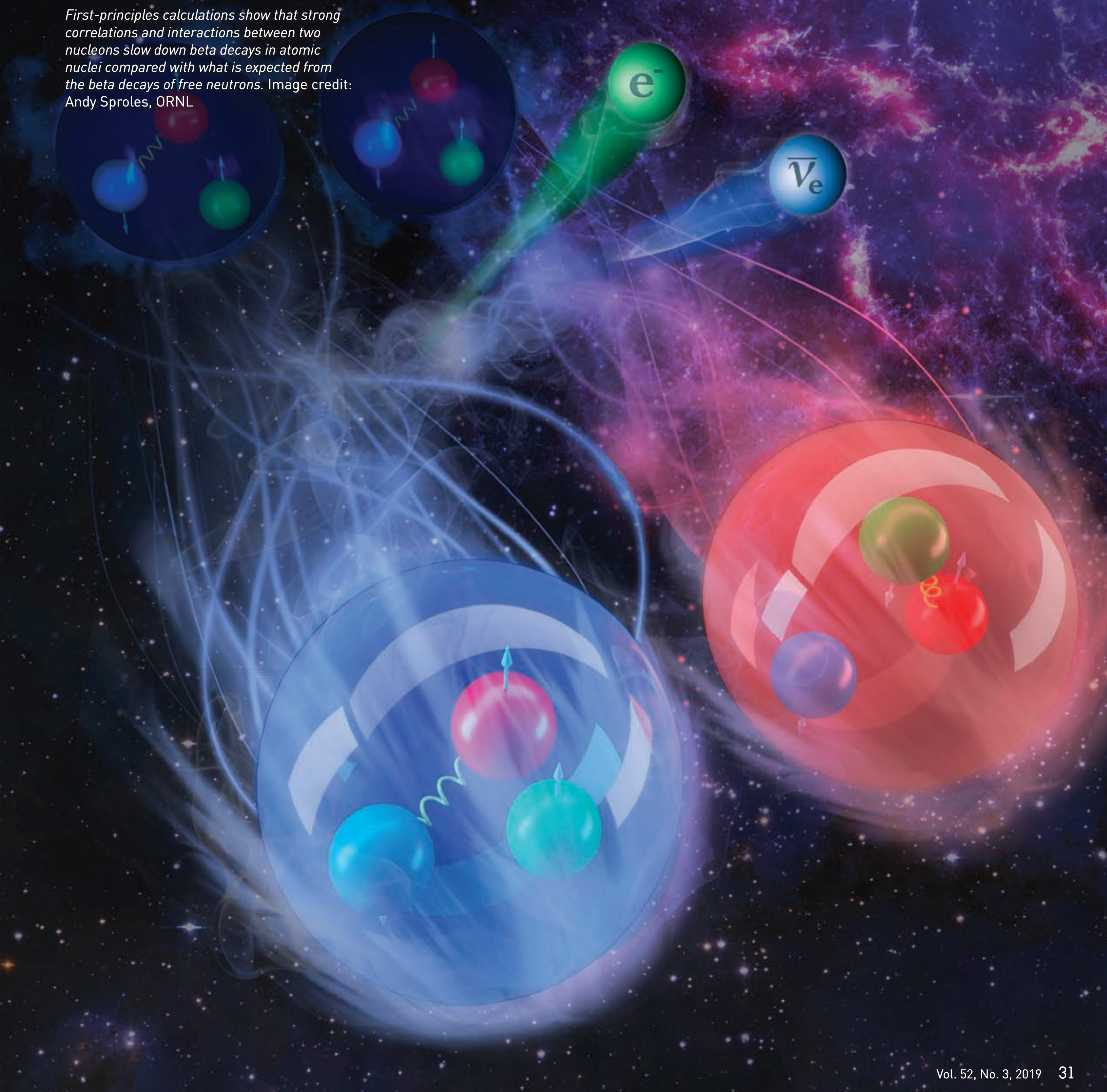
Many elements have isotopes that decay over long periods. For example, the half-life of carbon-14, the nucleus used in carbon dating, is 5,730 years. Other nuclei, however, exist only for fractions of a second before ejecting particles in an attempt to stabilize.

When tin-100 transforms into indium-100, the nucleus undergoes beta-plus decay, expelling a positron and a neutrino to convert a proton to a neutron.

With its equal number of protons and neutrons, tin-100 exhibits an unusually high rate of beta decay, giving the ORNL team a strong signal from which to verify its results. Furthermore, the tin-100 nucleus is "doubly magic," meaning the nucleons fill out defined shells inside the nucleus that make it strongly bound and relatively simple in structure.

"This means we can reliably compute it using our coupled cluster method, which calculates properties of large nuclei by accounting for forces between the individual nucleons," said Thomas Papenbrock, a researcher at ORNL and the University of Tennessee.

To model beta decay, however, the team also had to calculate the structure of indium-100, a more complex nucleus. By borrowing ideas from quantum chemistry, which treats electrons as waves, the ORNL team successfully developed a treatment of the strong correlations between nucleons.



First-principles calculations show that strong correlations and interactions between two nucleons slow down beta decays in atomic nuclei compared with what is expected from the beta decays of free neutrons. Image credit: Andy Sproles, ORNL

Summit expedites analysis of genetic disease origins

by Elizabeth Rosenthal
rosenthalec@ornl.gov

Genetics can be responsible for the onset and progression of diseases ranging from degenerative neurological disorders to some cancers.

To determine how genetic diseases form, a team led by Ivaylo Ivanov of Georgia State University used ORNL's Summit supercomputer to model the transcription preinitiation complex, or PIC—a complex of proteins vital to gene expression.

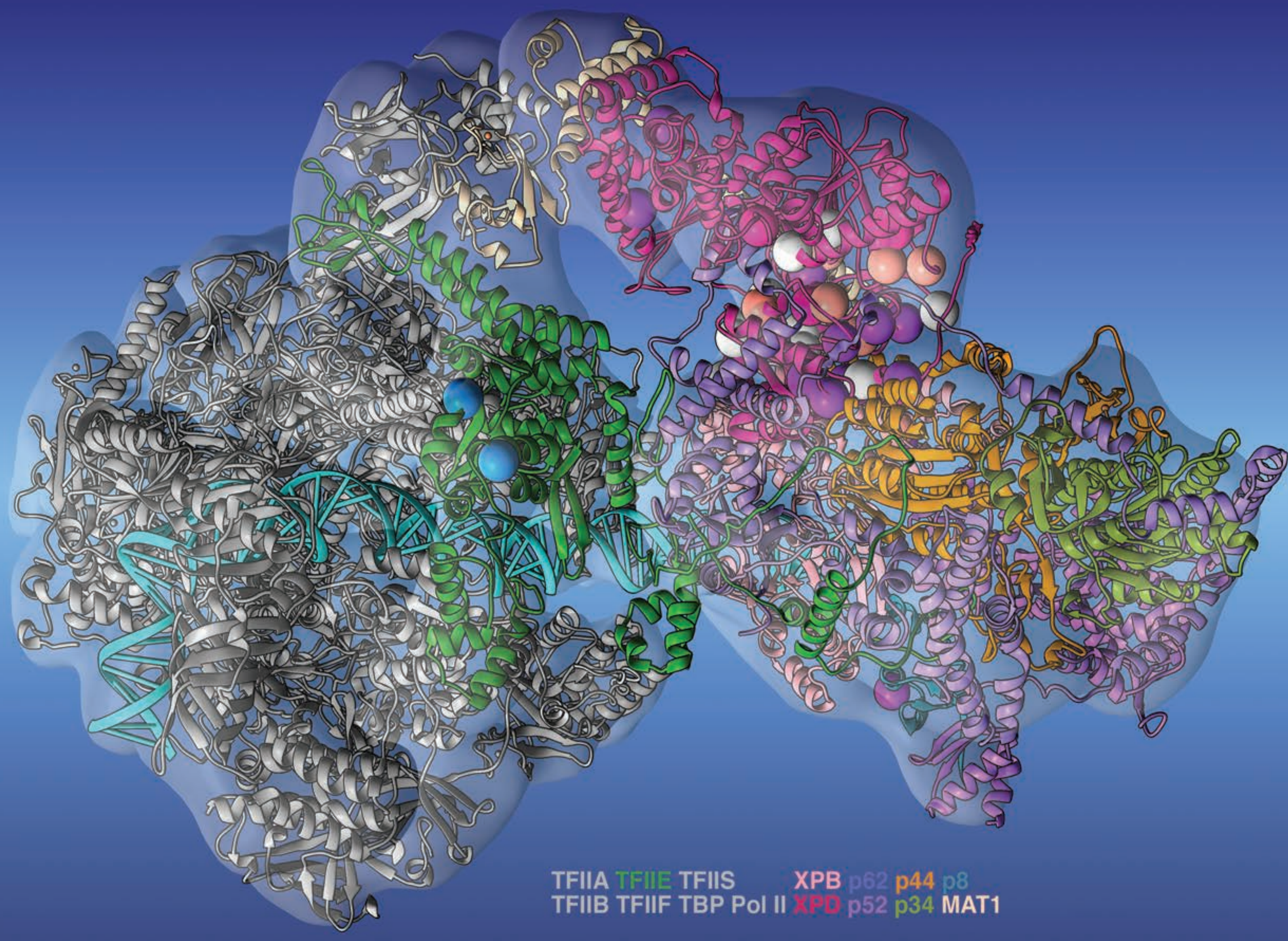
Gene expression involves the conversion of genetic information that originates in DNA to produce functional molecules such as proteins—the building blocks of all living organisms—through steps known as transcription and translation. Making sense of the relationship between a patient's genotype (unique genetic makeup) and phenotype (the external manifestation of a disease) could reveal how gene mutations interfere with gene expression and cause genetic disorders.

"Like a broken gear in a machine, mutational changes break down the function of the defective protein, a process that involves alterations in both structure and dynamics," Ivanov said. "This confluence of factors presents a challenge for conventional structural biology methods."

By using computational techniques to obtain a better understanding of how these inherited mutations affect protein function, the researchers aim to eventually inform the development of more effective treatments for genetic diseases.

During transcription, an enzyme called RNA polymerase II and a host of general transcription factors, or GTFs, assemble in a region of DNA called a promoter to produce the PIC. Opening the promoter depends on transcription factor II human, or TFIIH, a GTF consisting of multiple protein chains that unwinds the double helix strands of DNA to initiate transcription.

Because TFIIH contributes to both transcription and DNA repair, mutations in three subunits of the GTF directly lead to genetic diseases, including autoimmune and neurological disorders. Although studying the molecular mechanism behind transcription is crucial to advancing biomedical applications, previous attempts to characterize the PIC have been limited by incomplete models.



The spheres in this model correspond to the positions of patient-derived mutations color-coded by disease phenotype. Image credit: Ivaylo Ivanov, Georgia State University

To create the most complete model of the human PIC to date, the researchers combined data from cryoelectron microscopy—a structural biology method that uses an electron beam to study cryogenically frozen protein samples—and large-scale simulations on Summit using the molecular dynamics code NAMD.

"Our new model gives us the most complete view of the structure of TFIIH, which helps us understand the dynamics of these proteins and lets us map the origins of patient-derived mutations, potentially enabling future biochemical experiments focused on understanding the structural mechanisms of TFIIH," Ivanov said.

The simulations revealed that mutations tend to cluster at crucial areas of TFIIH, which prevents the GTF from working properly and leads to disease. From these findings, the team gained valuable insights into three distinct genetic disorders associated with cancer, aging and developmental defects. Access to Summit significantly sped up the team's time to solution.

"Running on Summit accelerates our research," Ivanov said. "Instead of spending several months running on another system, we were able to complete our calculations in a matter of days, which saved us a lot of time and effort."

Future efforts that build on this accomplishment could more precisely pinpoint the mutations that cause genetic diseases, expound on the role TFIIH plays in transcription and DNA repair, and delve deeper into the stages of gene expression.

"We look forward to moving beyond merely describing the mechanisms of transcription to elucidating their connection to genetic diseases," Ivanov said.

Supercomputing for long-lasting batteries

by Rachel Harken
harkenrm@ornl.gov

In today's technology landscape, companies are continually improving electronic devices. Bigger screens, better cameras and smarter systems are just some of the advances these companies promise with each product upgrade.

But one question remains: Where are the long-lasting batteries?

A research collaboration recently made a discovery that might hold the answer to that question: a new liquid electrolyte material that conducts fluoride in fluoride-based rechargeable batteries, which pack a major energy punch.

As part of the project, a team led by Caltech's Thomas Miller used ORNL's Titan supercomputer to understand and refine the electrolyte's properties. The team confirmed the electrolyte's unprecedented ability to conduct fluoride ions and retain chemical stability at room temperature, making the breakthrough material the first of its kind in the battery world.

The study, published in *Science*, included chemists from Caltech, NASA's Jet Propulsion Laboratory, the Honda Research Institute and Lawrence Berkeley National Laboratory.

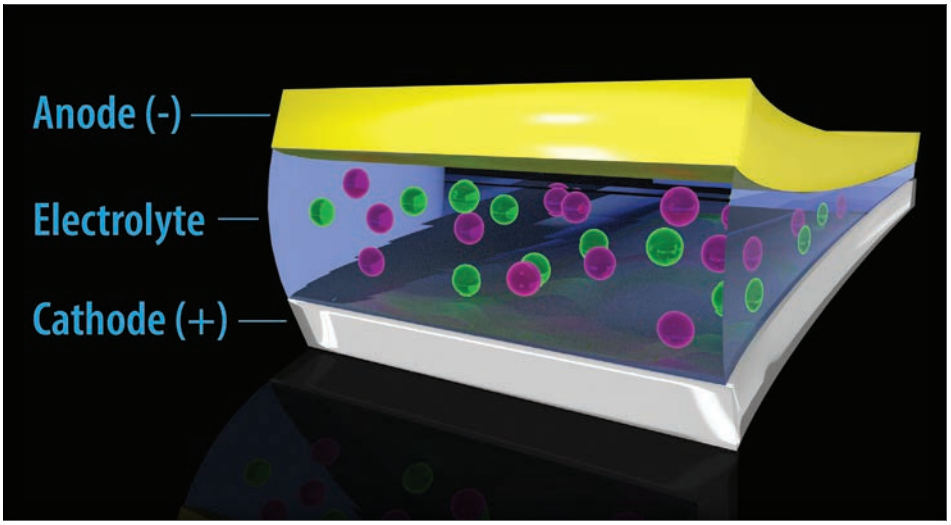
"We've taken an exciting step in the right direction," Miller said. "We have helped develop electrolytes that are sufficiently stable to make practical fluoride ion batteries a more achievable goal."

Fluoride batteries—which employ the same element added to toothpaste and tap water to prevent tooth decay—have long been studied for their potential to hold more charge than lithium batteries. The problem has been finding a suitable room-temperature electrolyte—the conductor material that plays a crucial role moving ions around inside a battery.

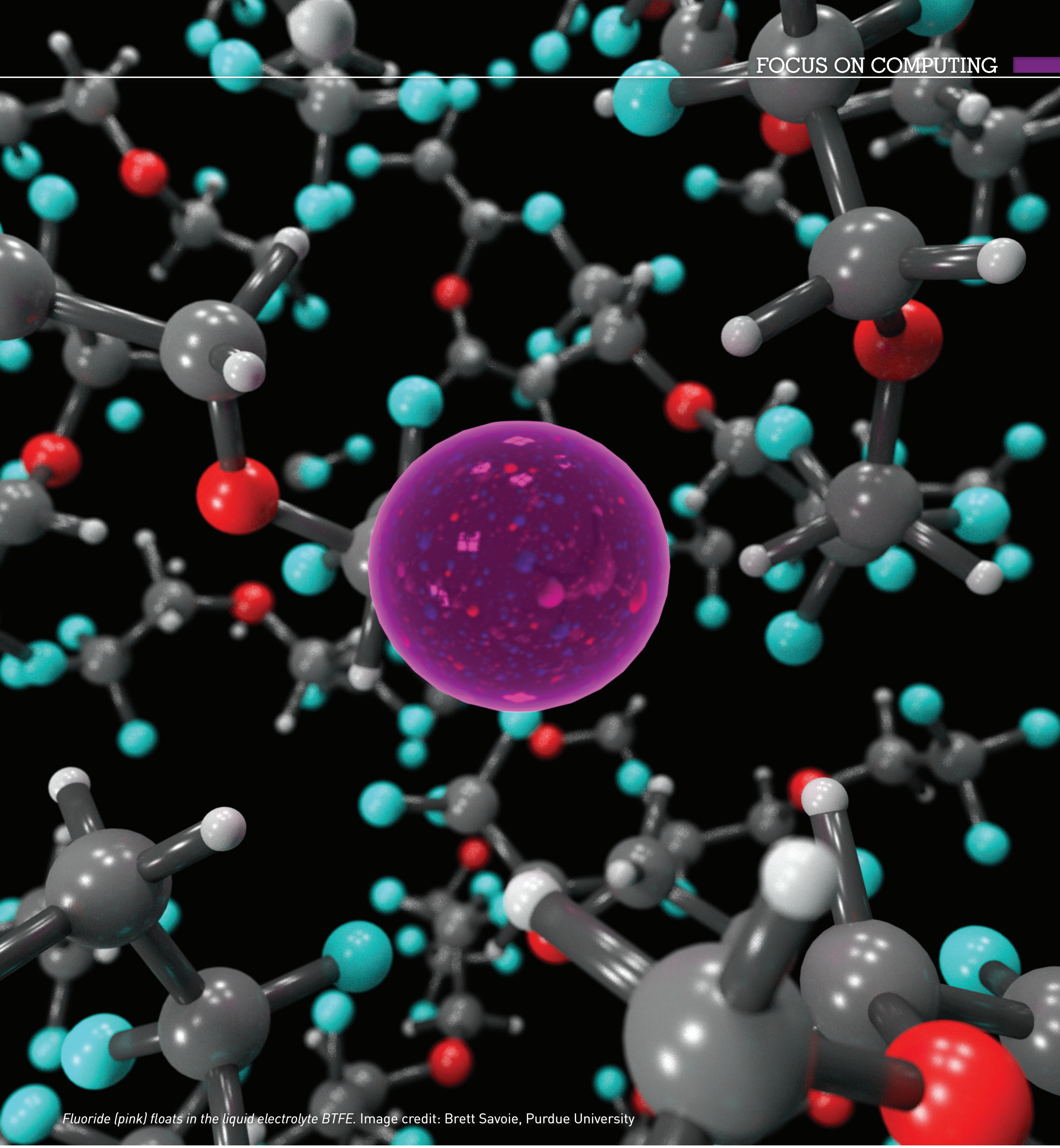
Lithium batteries shuttle lithium ions between the positive and negative terminals of a battery like grains of sand in an hourglass. In fluoride batteries, chemical reactions occur at the electrodes, where negatively charged fluorine anions form and break bonds to convert chemical energy to electrical energy. Fluorine anions can store a great deal of energy per ion, making them an attractive candidate for rechargeable batteries. In fact, higher energy-density fluoride batteries could hold up to eight times more charge than lithium batteries.

For fluoride to become a viable option for rechargeable battery technology, it would require a stable liquid electrolyte. The collaborative team decided to try a solvent material called bis(2,2,2-trifluoroethyl)ether, or BTFE, first proposed by intern Victoria Davis at JPL. Remarkably, the new solvent worked, making the fluoride ions stable enough to move from the anode to the cathode—which enabled the battery to drive electrical current. But the team didn't quite know why.

Miller's team used Titan and the Large-Scale Atomic/Molecular Massively Parallel Simulator at Sandia National Laboratories to look at BTFE's reactions with fluoride. The team discovered that positively charged regions in BTFE inter-



For fluoride batteries to generate electricity, charged atoms—called ions (pink and green)—travel between a negative node (anode) and a positive node (cathode) with the help of a liquid electrolyte solution. Image credit: Brett Savoie, Purdue University



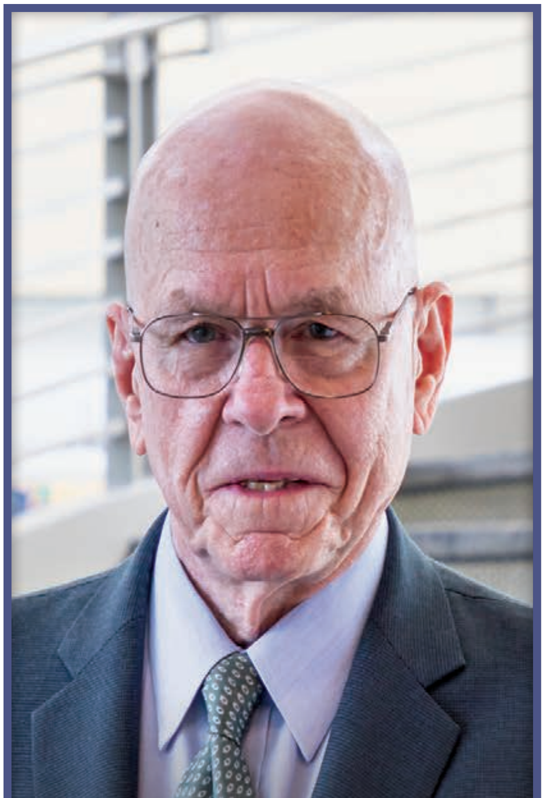
Fluoride (pink) floats in the liquid electrolyte BTFE. Image credit: Brett Savoie, Purdue University

acted strongly with the negatively charged fluoride to dissolve it.

"This liquid electrolyte allows for much more facile motion of the fluoride ions, even at room temperature, and its interactions help stabilize the fluoride," Miller said.

The discovery gives researchers a map for the mechanisms involved in stabilizing fluoride batteries and could aid in the development of new kinds of batteries with applications in cars, cell phones and other electronic devices.

"We will need to do more work before this can become a viable technology for widespread deployment," Miller said. "But we know that fluoride ion batteries certainly hold promise as a future battery technology."



K. Barry Sharpless shared the Nobel Prize for Chemistry in 2001 for his work on chirally catalyzed oxidation reactions. More recently, he received the 2019 Priestley Medal from the American Chemical Society for "the invention of catalytic, asymmetric oxidation methods, the concept of click chemistry and development of the copper-catalyzed version of the azide-acetylene cycloaddition reaction."

Sharpless pioneered the concept of click chemistry—rapid, irreversible reactions that "click" two molecules together—after sharing the Nobel Prize. It has since had countless applications in organic synthesis, medicinal chemistry, chemical biology, and materials science.

Sharpless received a Ph.D. from Stanford University in 1968. After postdoctoral work at Stanford and Harvard University, he joined the Massachusetts Institute of Technology and in 1990 became W.M. Keck Professor of Chemistry at the Scripps Research Institute. He now leads the Sharpless Lab at Scripps.

He delivered the Eugene P. Wigner Distinguished Lecture May 16, 2019, on the topic "New Developments in Click Chemistry." This is an edited transcript of our conversation following his lecture.

Distinguished

K. Barry Sharpless

1. What is click chemistry?

It's a version of chemistry that is more efficient at making bonds. It's designed to put pieces together the way life does.

We try to make a very complicated molecule to interact with life. And so, I think the inspiration is to use life's trick—a few good modules going together—and that gives a drug or function that the biological system needs to survive.

Click chemistry is inspired by life, but we use reactions that life would never touch. We use almost perfect reactions. They have nothing that will stop them. Life likes to use fancy pieces and take them apart and put them back together. If we can make a bond with a human intention that is irreversible and perfect, we can, in effect, have control over something we've never had control over—that is, getting messages back from life that are quick. If it doesn't work, we don't care. We've only spent a few minutes making that compound.

That's what click chemistry aims to do: make drugs affordable and better, but also cheap. And that would be helpful. Water and air and food are taken as an ideal for humans to give each other, and medicines, up to a good level, should be the same way—not so expensive. It's an ideal for breaking the pharmaceutical industry's lock on these things.

2. What applications use this chemistry?

In biology, there must be thousands of reactions run every day with kits that are enabled by the best click reaction. Those kits can go into a newborn cell, one that's just been made, and it can make that cell light up. So the people who study life and death in animals and embryology or cancer, they can see whether the organism has made a new cell that day. The whole nucleus of the cell will light up, if they use this kit called Click-iT.

People will use that who don't have the slightest idea what it is, but that's great. I like the idea that it just works, and everybody uses it. If you're a biochemist, what could be more important than knowing whether life is still there?

Every field in science that has any chemistry in it—which is every field—it's just everywhere, because it's a reaction that you cannot stop on this earth. It's unstoppable.

We take known drugs and click things on them, and they get better and usually less toxic. Of course, not every one does, but on average so far, for every thousand new analogs made and tested, 20 are better. It's a pretty simple way to improve medicine. We are not starting from scratch, which

Lecturer

we could do, too. But we say here is a drug that's good. It's already working. If we put this widget here or here, does it make it better? And it's a more dramatic way to get on the board than to start from scratch.

3. Chemistry has recently been able to get living systems to speak to us. How does this work?

One of the things that we always like to know when we're doing science is why something happened. In medicinal chemistry and biology, the "why" gets really hard to answer. We want to know what part of the organism was affected by the outside agent that was added.

The organism gives an answer to this question, as it were, and the answer is a function. Your cancer gets better, or your blood sugar goes down. But you never really know why that happened, because most drugs just bind reversibly, and they affect different systems.

People say it's one target, but it's usually many things. And so what we can do is, we have this very quiet, very demure group called a fluorosulfate. It doesn't react with any part of biology if it's dead. It only reacts with and captures live proteins, and beyond that it only reacts with one or a few specific proteins from the thousands specified and made in an animal genome.

So it waits, as it were, for its prince. It's like a sleeping beauty; it's very quiet. But then when the prince gets close, something happens with the enzyme, and next thing you know, snap, it makes a permanent and specific link to the enzyme. The link may be inconsequential but will usually have consequences for the life functions of the organism. Not only can these specific annotations of proteins translate into useful medical functions for the organism at hand, but I can easily go back and find the exact spot on that singular protein where it is appended. In other words, I know what kiss caused the permanent bond.

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

We have a lot in common. I've always wanted to do useful things, and the national labs are doing useful things. I have the feeling that people are reaching out as much as they can to teach what they know and see if it will be useful.

Click chemistry took off because it was useful, but there are many things that won't take off in the world, just because they didn't get disseminated. You have all these fancy, expensive instruments, and you can offer help to people on the outside.

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 staff members, and put them to work at the lab's one-of-a-kind facilities. The result is research that makes us proud and prepares them for distinguished careers.

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

Jessica M. Vélez

Graduate student, Environmental Sciences Division
Ph.D. student, Energy Science and Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Various cities in North Carolina, Puerto Rico and Texas

What are you working on at ORNL?

I am characterizing a population of the ectomycorrhizal fungus *Cenococcum geophilum* isolated from soils taken from underneath *Populus trichocarpa* trees in the Pacific Northwest. I am also testing the growth of this population with a panel of heavy metals, including cadmium and copper, and hope to use fungi which are resistant to these in a greenhouse experiment with poplar.

What would you like to do in your career?

I aim to pursue a career in science communication and outreach on behalf of a nonprofit or research institution. I currently participate in several science communication initiatives and am leading a student project to develop a proposal to establish a science communication and outreach track for the Bredesen Center.

Why did you choose a career in science?

I began my secondary education in microbiology at the University of Texas in Austin in 2001 but ultimately completed a Bachelor of Arts in English in 2004. I returned to school to complete a more specialized scientific education and found my calling in outreach, service and the communication of science.

Peter A. Mouche

Postdoc, Materials Science and Technology Division
Ph.D., Nuclear, Plasma and Radiological Engineering, University of Illinois, Urbana-Champaign
Hometown: Naperville, Illinois

What are you working on at ORNL?

My research considers the design of safer materials for use within existing nuclear power plants. My project focuses on coating new fuel cladding material to help it withstand the harsh environments inside a reactor core. I deposit the coatings and then characterize them, particularly for mechanical stability.

What would you like to do in your career?

I want to advance existing material performance, as well as understand how new materials can be used in current or next-generation nuclear reactors. New fabrication methods have expanded the field of available materials, and ORNL is the best place to try new ideas and approaches.

Why did you choose a career in science?

I was fortunate to have amazing science and math teachers who piqued my interest in exploring the world. My parents encouraged me to run mini-experiments growing up; research was always a part of my life. Discovering why something unknown happens is a most amazing process.

Kendra Allen

Graduate student, Biosciences Division
Ph.D. student, Energy Science and Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Chicago, Illinois

What are you working on at ORNL?

The goal of my work is to understand the effects of biomaterials on the physical and chemical environment of microbial communities. By examining the processes of bacteria as they are encapsulated, we hope to understand their functionality and use in complex materials.

What would you like to do in your career?

I would love a career that focuses on my passions of interdisciplinary research in the sciences and engineering, collaboration of community partners and government entities, and research-based teaching within science classrooms. I am unsure what role that is, but I am excited to see where the journey takes me!

Why did you choose a career in science?

I chose a career in science because it gave me foundational critical and systematic thinking skills, allowing me to accomplish goals that I previously thought were impossible and to be the example I always wanted to see growing up.

Lu Han

Postdoc, Chemical Sciences Division
Ph.D., Macromolecular Science and Engineering, Case Western Reserve University
Hometown: Baoding, China

What are you working on at ORNL?

My research in ORNL focuses on polymer chemistry and polymer engineering for various applications, including binder development for binder jet additive manufacturing toward high-mechanical-property, low-carbon-content 3D printed parts; polymer nanocomposites; self-healing materials; and complex architecture polymer synthesis.

What would you like to do in your career?

I would love to continue research into polymer chemistry, where my passion is and where I can make a contribution to society.

Why did you choose a career in science?

Science helped me understand the world as a kid. I love to explore the unknown, to help people understand the world and make it a better place. I am always fascinated by the beauty of chemistry. The colors, crystals and symmetry are the most beautiful things in the world!

Matthew Mulvehill

ASTRO Intern, Center for Nanophase Materials Sciences
M.S., Chemical Engineering
Hometown: Arcadia, California

What are you working on at ORNL?

The project I am working on focuses on the electrolysis of carbon dioxide to ethanol as an alternative fuel. I am designing a pressurized recirculating electrolysis cell system to study the effects of various conditions on the reaction to further mature the technology for a possible full-scale plant deployment.

What would you like to do in your career?

After I pursue and obtain a Ph.D. with research involving alternative or renewable energy technology, I want to find a career that allows me to learn and innovate in the energy industry. I will be a part of the solution to any energy problem the world faces in the future.

Why did you choose a career in science?

I find fulfillment through three senses that science allows me to chase: a sense of discovery when learning something new about an interesting subject, a sense of accomplishment from creatively solving a problem, and a sense of inspiration that stems from knowing your work will have the chance to benefit somebody's life.

Swapneeta Date

Postdoc, Environmental Sciences Division
Ph.D., Biomedical Sciences, Texas Tech University Health Sciences Center
Hometown: Pune, India

What are you working on at ORNL?

Seafood is an important food source for millions of people around the world, but several types of fish contain high levels of a potent neurotoxin, methylmercury. I am trying to decipher the molecular details of how certain anaerobic bacteria form methylmercury, which eventually ends up in fish.

What would you like to do in your career?

I am passionate about both doing high-impact research and facilitating good research. Therefore, I am interested in a career in scientific leadership and management. I would like to follow the footsteps of great scientific leaders such as Dr. Marcia McNutt, an exceptional scientist and president of the U.S. National Academy of Sciences.

Why did you choose a career in science?

Everything that we take for granted today—wireless internet, healthy life for 90 years, plentiful food—has resulted because thousands of scientists have dedicated their lives to answering whats, whys and hows. A career in science is my way of contributing to the greater good while standing on the shoulders of giants.

Fifty years after Apollo 11, ORNL 'moon scoop' remains a source of family pride

by Abby Bower
ornlreview@ornl.gov

Glen and Alice Ellis, 1940s. Image credit: Mike Ellis

Late in the evening of July 20, 1969, the Ellis family's eyes were glued to their black-and-white television. Michael, 11, Jeanne, 14, and Lee, 18, waited alongside their parents, Glen and Alice Ellis, in their Lenoir City, Tenn., basement to watch humanity's first walk on the moon.

Like more than 600 million others worldwide, the Ellis kids wanted to witness the spectacle of the lunar landing. But they had a more personal interest as well: They wanted to see if the astronauts would use a device that—just months earlier—had been a blueprint sprawled across their father's drawing board at ORNL.

The device that fascinated them was a collapsible "moon scoop," known to NASA as the lunar contingency soil sampler.

The aluminum-and-Teflon scoop had an important job. Minutes after Neil Armstrong descended from the lunar module, he used it to quickly take a sample of rock and soil that would ensure scientists back home could study at least a piece of the moon if the mission had to be abandoned early.

Glen Ellis, a draftsman at ORNL, drew the plans for the moon scoop. A man who rarely brought his work life home, Glen shared little about his job with his five children, but he told his family about this project.

"It was a big deal because we did know that he was involved in it," says Michael Ellis, Glen's youngest son. "He did talk about making this scoop."

The details, however, were always a bit of a mystery. The Ellis family was never certain if Glen had both developed the concept for the scoop and drawn the plans or if he had drafted someone else's idea.

A few weeks ahead of the 50th anniversary of Apollo 11, a new origin story surfaced. Gene Shaver Jr., a nephew of Glen Ellis, says that the idea for the moon scoop came from a day Glen spent at the golf course with the rest of his design team. The way Glen used to tell it, the "bingo" moment came after an unfortunate golfer hit a ball in the water and had to fish it out with the kind of ball retriever golfers use. A similar design, Glen thought, might help an astronaut scoop rocks on the moon. He returned to the lab with his team, and the plans took life.

If that story is true, it's fitting that during the Apollo 14 mission Alan Shepard used the shaft of the contingency sampler—with a smuggled golf club head attached—to famously play golf on the surface of the moon.

Today, one of the contingency samplers is on display at the Smithsonian's National Air and Space Museum in Washington, D.C., and two of Glen's grandsons work at ORNL. Kevin Gaddis is a radiochemist in the Isotope and Fuel Cycle Technology Division, while Ryan Gaddis manages the computer systems used for employee training.

Their grandfather's professional legacy inspires them "to do work that matters," Kevin says. He keeps Glen Ellis's original blueprints for the moon scoop hanging on his living room wall.

The aging documents act as a reminder of the time a man walked on the moon 50 years ago, but more importantly, as a reminder of his grandfather.

Astronaut Neil Armstrong participates in lunar surface simulation training on April 18, 1969 using a "moon scoop" produced at ORNL. Image credit: NASA

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