OAK RIDGE NATIONAL LABORATORY

Review

Beyond Scotch tape

OAK RIDGE National Laboratory

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On the Cover
ORNL materials scientist Kai Xiao examines a gallium selenide crystal used to produce 2-D nanomaterials.

Big opportunities at the nanoscale

For many years, nanotechnology has been one of the most exciting areas of research and development. Scientists can now produce materials as little as one atom thick, making them essentially two-dimensional.

At this scale even materials that are unremarkable in their bulk form can show extraordinary properties, from super strength to super resistance to superconductivity. As we move forward, we're sure to find many uses for them.

ORNL is deeply involved in the hunt both for promising new nanomaterials and for technologies that allow us to produce them economically. Our Center for Nanophase Materials Sciences is home to some of the world's most powerful microscopes, operated by a staff of talented researchers. With these resources we are able to analyze and manipulate materials atom by atom, opening up new characteristics and capabilities.

In this issue of *ORNL Review* we take a look at some of the lab's nanotechnology efforts and talk to some of the researchers involved. We also explain how some of our cutting-edge microscopes allow us to do this work, and we talk to an MIT research team about ORNL's relationship with visiting scientists (pages 8–11).

These instruments provide invaluable data and lots of it. Elsewhere in this issue you can learn about a computing platform that gives researchers a better handle on their data by connecting ORNL's powerful scientific tools—including the lab's world-class neutron science facilities as well its advanced microscopes—with advanced web and data services (page 14). Computing itself is the tool for a project using ORNL's Titan supercomputer to provide a detailed explanation of just how nuclei split (page 15).

Two stories in this issue focus on nuclear power. One highlights modeling and simulation software that supports work with fuel assemblies (page 24). The other looks at the development of methods to analyze the meter-thick concrete walls of our aging nuclear power plants (page 18).

Also in this issue you will find an infographic reviewing ORNL-developed home technologies that promise to bring down your utility bills while helping the environment and making the United States more energy independent (pages 16–17). In addition, we look at efforts to advance our understanding of neutrinos: tiny, nearly undetectable elementary particles (page 20).

As always, we talk with grad students and postdocs early in their research careers to find out what they're up to and ask about their plans (pages 30–31). We sit down with a leading researcher and a prominent business leader, both of whom gave Eugene P. Wigner Distinguished Lectures in Science, Technology, and Policy (pages 26–28). And we close with a look back at ORNL history, this time focusing on the lab's first efforts in advanced computing.

Please enjoy this issue of *ORNL Review.*

Thomas Mason

Thomas Mason
Laboratory Director

It's official: Element 117 is 'tennessine'

The recently discovered element 117 has been officially named "tennessine" in recognition of Tennessee's contributions to its discovery, including the efforts of ORNL and its Tennessee collaborators at Vanderbilt University and the University of Tennessee.

"The presence of tennessine on the periodic table is an affirmation of our state's standing in the international scientific community, including the facilities ORNL provides to that community as well as the knowledge and expertise of the laboratory's scientists and technicians," ORNL Director Thom Mason said.

The International Union of Pure and Applied Chemistry—which validates the existence of newly discovered elements and approves their official names—gave its final approval to the name "tennessine" following a nearly yearlong process that began on December 30, 2015, when it and the International Union of Pure and Applied Physics announced verification of the existence of the superheavy element 117 more than five years after scientists first reported its discovery in April 2010.

ORNL had several roles in the discovery, the most prominent being production of the radioisotope berkelium-249 for the search. The berkelium-249 used in the initial discovery and subsequent confirmatory experiments for element 117 was produced by ORNL and DOE's Isotope Program and was provided as a U.S. contribution to those experiments.—*Bill Cabage*

For more information: http://go.usa.gov/x8nwc

Serendipitous discovery turns CO_2 into ethanol

In a new twist to waste-to-fuel technology, ORNL scientists have developed an electrochemical process that uses tiny spikes of carbon and copper to turn carbon dioxide, a greenhouse gas, into ethanol. Their finding, which involves nanofabrication and catalysis science, was serendipitous.

"We discovered somewhat by accident that this material worked," said ORNL's Adam Rondinone, lead author of the team's study published in *ChemistrySelect*. "We were trying to study the first step of a proposed reaction when we realized that the catalyst was doing the entire reaction on its own."

The team used a catalyst made of carbon, copper and nitrogen and applied voltage to trigger a complicated chemical reaction that essentially reverses the combustion process. With the help of the nanotechnology-based catalyst, which contains multiple reaction sites, the solution of carbon dioxide dissolved in water turned into ethanol with a yield of 63 percent. Typically this type of electrochemical reaction results in a mix of several different products in small amounts.

"We're taking carbon dioxide, a waste product of combustion, and we're pushing that combustion reaction backward with very high selectivity to a useful fuel," Rondinone said. "Ethanol was a surprise. It's extremely difficult to go straight from carbon dioxide to ethanol with a single catalyst."

Given the technique's reliance on low-cost materials and ability to operate at room temperature in water, the researchers believe the approach could be scaled up for industrially relevant applications. They plan to refine their approach to improve the overall production rate and further study the catalyst's properties and behavior.—*Morgan McCorkle*

For more information: http://go.usa.gov/x8Rr2

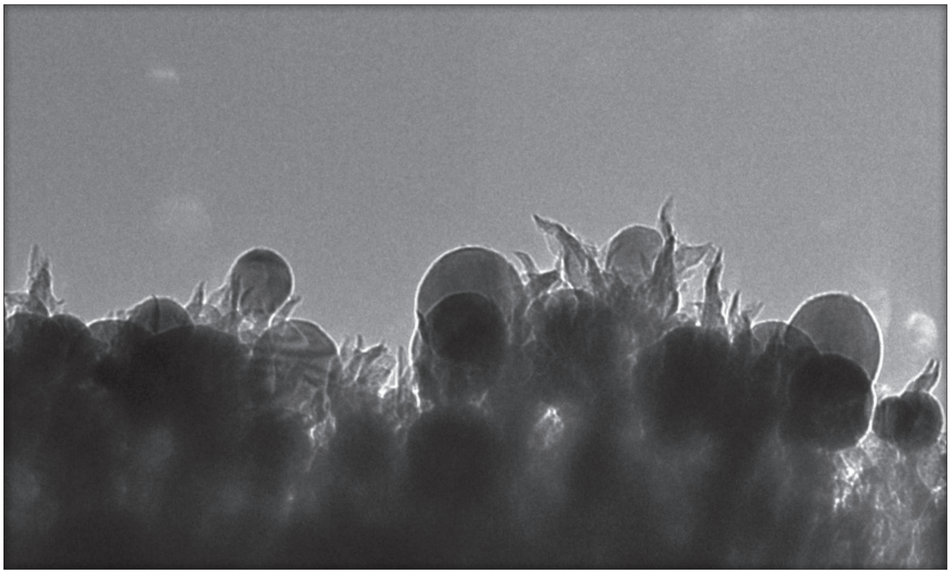
Embedding instruments at 700 degrees Celsius

When it comes to a challenging application for embedded instrumentation and control, none quite beats an environment of molten salt at 700 degrees Celsius.

That's the application chosen by ORNL scientists to demonstrate the advantage of embedding controls—or systems that drive moment-by-moment adjustments to a machine or process to improve efficiency and reliability.

"We wanted to do something that would be very difficult, if not impossible, to do using conventional machine-design techniques," said ORNL's Alexander Melin. "But we also wanted a testbed that could benefit a great deal from embedded instrumentation and control."

The scientists chose to investigate a pump that could tolerate placement in a fluoride salt reactor—circulating the molten salt used as a coolant. ORNL is



ORNL researchers developed a catalyst made of copper nanoparticles (seen as spheres) embedded in carbon nanospikes that can convert carbon dioxide into ethanol. Image credit: ORNL

ORNL's Titan supercomputer.
Image credit: Andy Sproles, ORNL

leading DOE's research and development effort on these advanced reactors amid renewed interest.

The solution being explored by the group is to use a canned rotor pump that eliminates the need for rotating seals and mechanical bearings. The sensorless design "uses the physics of the system and some clever mathematics to detect shaft position without having a physical sensor," Melin explained.

Future research could involve building a magnetic suspension to test the pump in a liquid salt environment.—*Stephanie Seay*

For more information: http://go.usa.gov/x8Rrt

Projects get time on supercomputers at ORNL, ANL

Fifty-five promising research projects will get access to the world-class supercomputers at Oak Ridge and Argonne national laboratories through the Innovative and Novel Computational Impact on Theory and Experiment program.

The projects will share 5.78 billion core hours and support a broad range of large-scale research campaigns to advance knowledge in critical areas ranging from sustainable energy technologies to next-generation aerospace designs to novel materials.

The INCITE program is the primary means of accessing DOE's Leadership Computing Facilities at the two national laboratories. ORNL's Titan system is currently the world's third most powerful supercomputer, capable of 27 million billion calculations each second (i.e., 27 petaflops). ANL's Mira system, ranked number nine in the world, is capable of 10 petaflops.

Researchers from academia, government research facilities, and industry compete for the awards, which average more than 105 million core hours. Domain and computational scientists at the leadership centers partner with each INCITE project, aiding in code and methods development, helping with optimization, streamlining workflow, troubleshooting unforeseen problems, and assisting with data analysis and visualization.

"Once again this year we're delighted to have this opportunity to play a key role in enabling breakthrough science through the 2017 INCITE program," said James Hack, director of the National Center for Computational Sciences, home to the Oak Ridge Leadership Computing Facility. "Our user community continues to propose ever more ambitious and computationally demanding campaigns. Helping that community fully exploit the unique capabilities of our facilities is always a welcome challenge."—*Eric Gedenk*

For more information: http://go.usa.gov/x8RrY

ORNL wins seven R&D 100 Awards

ORNL researchers have received seven R&D 100 Awards in recognition of their advancements in science and technology. The honorees were recognized on Nov. 3 at the 54th annual R&D 100 Conference, sponsored by *R&D Magazine*.

This year's seven honors bring ORNL's total of R&D 100 Awards to 200 since their inception in 1963. This year ORNL researchers and their collaborators were recognized for the following innovations:

Oak Ridge Graph Analytics for Medical Innovation, or ORIGAMI, is an artificial intelligence system designed to search, collect and connect medical literature resources to improve medical research discovery.

The Roof Savings Calculator Suite is a web-based tool for simulating energy flow and loss in businesses and homes and predicting the cost-effectiveness of cool roofing and attic technologies based on building type and location.

G-Mode: Full Information Acquisition in Scanning Probe Microscopy and Spectroscopy uses a custom controller to rapidly collect and thoroughly process information flow from a microscope detector in its entirety, yielding all accessible information about minute changes sensed by the probe as it interacts with nanoscopic volumes of a sample.

Virtual Environment for Reactor Applications, or VERA, is a physics simulation tool that visualizes the internal processes of commercial nuclear fission power plants and predicts reactor behavior in a number of potential scenarios.

U-Grabber is an adsorbent material designed to inexpensively and efficiently extract uranium and other metals from water. The material is made from polyethylene fibers, similar to PVC, woven into braids and grafted with chains of a uranium-attractive chemical called amidoxine.

Open Port Sampling Interfaces for Mass Spectrometry removes the most difficult barrier to mass spectrometry—producing and transferring viable samples into the device—and allows easier, universal input of samples via accessible intake ports.

Waste Tire Derived Carbon is a proprietary process for repurposing discarded car tires as a source of carbon powder, a sooty hydrocarbon byproduct that can be modified for incorporation into anodes of lithium-ion batteries.

ORNL also received a special recognition award from *R&D Magazine* for the **Wireless Power Transfer Based Electric and Plug-In Vehicle Charging System**, submitted by Toyota Motor Engineering & Manufacturing North America and codeveloped by a team of ORNL researchers with support from Cisco Systems and the International Transportation Innovation Center.—*Sean Simoneau*

For more information: http://go.usa.gov/x8RZP

Seven from ORNL elected AAAS fellows

Seven ORNL researchers have been elected fellows of the American Association for the Advancement of Science.

AAAS is the world's largest multidisciplinary scientific society and publisher of the *Science* family of journals.

Bryan Chakoumakos, lead of the Structure of Matter Group in the Quantum Condensed Matter Division, was nominated by the AAAS section on geology and geography for "outstanding contributions to the physical, chemical, earth and materials sciences through the application of the techniques of neutron and X-ray diffraction and materials synthesis."

David Dean, director of the Physics Division and ORNL Isotope Program, was nominated by the AAAS section on physics for "distinguished contributions to the field of nuclear theory, particularly for development and application of innovative computational techniques and for academic leadership and public service."

Baohua Gu, team lead of Molecular-Scale Biogeochemical Processes in the Environmental Sciences Division, was nominated by the AAAS section on industrial science and technology for "distinguished contributions to molecular-scale mechanisms that control cycling of natural organic matter, contaminants and toxic metals and for technology innovations to remediate contaminants in the environments."

George Ostrouchov, senior research staff and analytics task lead in the Scientific Data Group of the Computer Science and Mathematics Division, was nominated by the AAAS section on statistics for "distinguished leadership in the field of statistical computing, particularly to enable parallel computation on big data with statistical software, and for service to profession."

Brian Sales, distinguished research scientist and lead of the Correlated Electron Materials Group in the Materials Science and Technology Division, was nominated by the AAAS section on physics for "pioneering research for clean energy technologies, including thermoelectric and superconducting materials, and materials for nuclear waste storage."

Tjerk P. Straatsma, lead of the Scientific Computing Group in the National Center for Computational Sciences, was nominated by the AAAS section on chemistry for "distinguished contributions in the field of computational science, particularly for the development, efficient implementation and application of advanced chemical physics modeling and simulation methods."

Brian Wirth, University of Tennessee-ORNL Governor's Chair for Computational Nuclear Engineering, was nominated by the AAAS section on physics for "advancing knowledge of radiation damage mechanisms and fuel performance in fission and fusion energy via multiscale modeling using high performance computing validated by experiments."

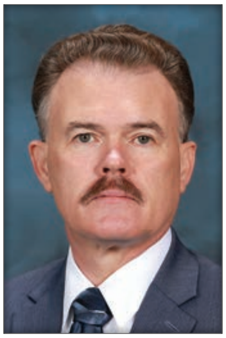

Bryan Chakoumakos


David Dean


Baohua Gu


George Ostrouchov


Brian Sales


Tjerk P. Straatsma


Brian Wirth

The new fellows will be inducted in February 2017 at the AAAS Annual Meeting in Boston.—*Sean Simoneau*

For more information: http://go.usa.gov/x8RCF

The Spallation Neutron Source. Image: Jason Richards, ORNL

Spallation Neutron Source celebrates 10 years

ORNL's Spallation Neutron Source recently marked a decade as a leading neutron science facility.

"The Spallation Neutron Source has opened neutron scattering science to a new generation of researchers at a time when advanced materials are critical to solving our challenges with energy and the environment," ORNL Director Thom Mason said in a September ceremony. Mason led the SNS project to its completion in 2006.

The SNS's combination of linear accelerator and accumulator ring sent its first protons to its one-of-a-kind mercury target in April 2006, beginning a process of commissioning instruments to take advantage of its unprecedented abundance of pulsed neutrons for research.

Over the intervening decade the facility has attracted researchers from around the globe to study materials with neutrons at peak intensities previously unavailable. Neutrons' properties make them ideal for studying the molecular and atomic structure of materials in ways not possible with other probes, such as phonons and electrons.

The tenth anniversary celebration took place in conjunction with a ceremony dedicating the renamed Shull Wollan Center—a Joint Institute for Neutron Sciences. Clifford Shull and Ernest O. Wollan, pioneered the field and created a key tool for scientific and technological advancement.—*Bill Cabage*

For more information: http://go.usa.gov/x8RCH

Neutron scattering pillar Herb Mook dies

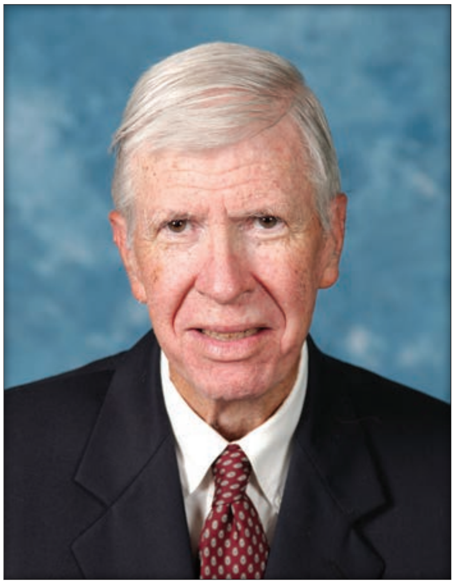
Herbert A. Mook Jr., solid-state physicist and one of ORNL's most venerable neutron scattering researchers, died Saturday, Oct. 1. He retired in 2014 following a career that included widely cited neutron scattering investigations into superconducting materials.

"Herb was, probably more than anyone else, responsible for me deciding to come to Oak Ridge in 1998," said ORNL Director Thom Mason. "He was one of our most highly cited and respected researchers and played a crucial role in building the science case for the Spallation Neutron Source, in part through the excellence of his own science."

Mook's ORNL career began in 1965 when he arrived from Harvard University to perform neutron diffraction studies at the Oak Ridge Research Reactor and the High Flux Isotope Reactor. His research focused on investigations of magnetism and on superconducting materials, which conduct electricity without resistance at extremely low temperatures.

His work has contributed to the scientific enterprise to develop materials that are superconducting at higher, more attainable temperatures. He was the first to demonstrate the coexistence of magnetism and superconductivity in rare-earth rhodium borides, which earned him DOE's Outstanding Scientific Accomplishment in Solid State Physics award in 1982, and was on a team that first observed the vortex lattice in high-temperature superconducting materials.

He is survived by his wife, Jane, two sons and several grandchildren.—*Bill Cabage*



Herb Mook

ORNL researchers advance drought-resistant crops

As part of an effort to develop drought-resistant food and bioenergy crops, ORNL scientists have uncovered the genetic and metabolic mechanisms that allow certain plants to conserve water and thrive in semi-arid climates.

Semi-arid plants such as agave have adapted to survive in areas with little rainfall by developing a specialized mode of photosynthesis called crassulacean acid metabolism, or CAM. Unlike plants in wetter environments, CAM plants absorb and store carbon dioxide through open pores in their leaves at night, when water is less likely to evaporate. During the day, the pores, also called stomata, stay closed while the plant uses sunlight to convert carbon dioxide into energy, minimizing water loss.

ORNL scientists are studying the unique metabolic mechanisms that allow CAM plants to conserve water, with the goal of introducing water-saving traits into bioenergy and food crops. The results of the team's latest study, which focuses on agave, are published in *Nature Plants* as the journal's cover story.

The CAM photosynthetic process, discovered in the 1950s, has largely remained a scientific curiosity, but researchers are now examining it as a potential solution to maintaining food and bioenergy crop yields during water shortages and drought.

"Today's demand on agricultural systems to provide food, feed, forage, fiber and fuel call for more comprehensive research into understanding the complexities of CAM plants," said ORNL coauthor Xiaohan Yang. "As we uncover each layer of the CAM process, our studies aim to speed up the evolution of crops to give them the ability to thrive in more arid environments as the availability of freshwater becomes limited."

To gain a comprehensive view of the complex CAM system, the team used ORNL's mass spectrometry capabilities to compare the molecular traits of agave with those of a control plant, Arabidopsis, which uses a more common photosynthetic process.—*Sara Shoemaker*

For more information: http://go.usa.gov/x9xp4

University of Tennessee grad student Kaitlin Palla studies agave plants in ORNL's greenhouse as part of the lab's research into water-efficient photosynthesis. Image credit: ORNL

Printed magnets outperform conventional versions

ORNL researchers have demonstrated that permanent magnets produced by additive manufacturing can outperform bonded magnets made using traditional techniques while conserving critical materials.

Scientists fabricated isotropic, near-net-shape, neodymium-iron-boron bonded magnets at DOE's Manufacturing Demonstration Facility at ORNL using the Big Area Additive Manufacturing machine. The result, published in *Scientific Reports*, was a product with comparable or better magnetic, mechanical, and microstructural properties than bonded magnets made using traditional injection molding with the same composition.

While conventional sintered magnet manufacturing may result in material waste of as much as 30 to 50 percent, additive manufacturing will simply capture and reuse those materials with nearly zero waste, said Parans Paranthaman, a group leader in ORNL's Chemical Sciences Division.

Using a process that conserves material is especially important in the manufacture of permanent magnets made with neodymium and dysprosium—rare-earth elements that are mined and separated outside the United States. Neodymium-iron-boron magnets are the most powerful on earth, used in everything from computer hard drives and headphones to clean-energy technologies such as electric vehicles and wind turbines.

The printing process not only conserves materials but also produces complex shapes, requires no tooling and is faster than traditional injection methods, potentially resulting in a much more economic manufacturing process, Paranthaman said.

"Manufacturing is changing rapidly, and a customer may need 50 different designs for the magnets they want to use," said ORNL researcher and co-author Ling Li. Traditional injection molding would require the expense of creating a new mold and tooling for each, but with additive manufacturing the forms can be crafted simply and quickly using computer-assisted design, she explained.—*Stephanie Seay*

For more information: http://go.usa.gov/x9xd4

Fighting antibiotic resistance with computer simulations

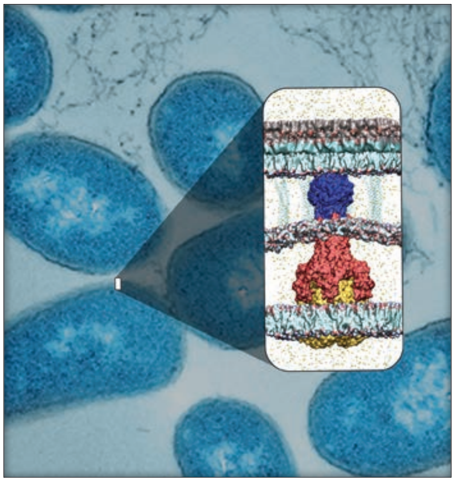
Supercomputer simulations at ORNL have played a key role in discovering a new class of drug candidates that hold promise for combating antibiotic resistance. In a study led by the University of Oklahoma with ORNL, the University of Tennessee and Saint Louis University, lab experiments were combined with supercomputer modeling to identify molecules that boost antibiotics' effect on disease-causing bacteria.

The researchers found four new chemicals that seek out and disrupt bacterial proteins called "efflux pumps," known to be a major cause of antibiotic resistance. Although some antibiotics can permeate the protective barriers surrounding bacterial cells, many bacteria have evolved efflux pumps that expel antibiotics back out of the cell and render the medications ineffective.

The team focused on one efflux pump protein, known as AcrA, which connects two other proteins in a tunnel shape through the bacterial cell envelope. Disrupting this centrally positioned protein could "throw a wrench" into the middle of the efflux pump and mechanically break it, unlike drug design strategies that try to inhibit overall biochemical processes.

"As a first in this field, we proposed the approach of essentially 'screwing up' the efflux pump's protein assembly, and this led to the discovery of molecules with a new type of antibacterial activity," said co-author Jeremy Smith, who serves as a UT–ORNL Governor's Chair and director of the UT–ORNL Center for Molecular Biophysics. "In contrast to previous approaches, our new mechanism uses mechanics to revive existing antibiotics' ability to fight infection." Details of the study were published in *ACS Infectious Diseases*.

Through laboratory experiments done in tandem with extensive protein simulations run on ORNL's Titan supercomputer, they scanned large numbers of chemicals to predict and select which would be the most effective in preventing AcrA proteins from assembling properly.—*Sara Shoemaker*



ORNL researchers used supercomputing to identify chemicals that seek out and disrupt the assembly of bacterial proteins called efflux pumps, known to be a major cause of antibiotic resistance. Image credit: ORNL/University of Oklahoma

For more information: http://go.usa.gov/x9xv8

Neutron diffraction probes CO_2 in extreme environments

Carbon dioxide is a key component in the carbon cycle of Earth, both in the atmosphere and in the mantle, or hot layer under Earth's crust. Studies of high-pressure, high-temperature phases of solid carbon dioxide are important to understanding the forms that carbon may adopt at the extreme pressures and temperatures of Earth's interior.

Through a Deep Carbon Observatory collaboration, Adam Makhluf of UCLA's Earth, Planetary and Space Sciences Department and Chris Tulk of ORNL's Chemical and Engineering Materials Division are using neutrons to study the fundamental role carbon dioxide plays in Earth's carbon cycle, especially in the composition of carbon reservoirs in the deep earth and the evolution of the carbon cycle over time.

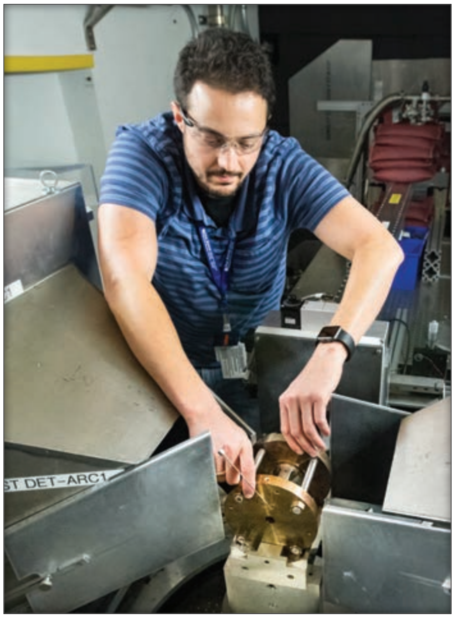
Makhluf and Tulk are using ORNL's Spallation Neutron Source to provide insight into carbon dioxide's behavior under intense conditions.

"At high pressures and temperatures, it is thought that carbon dioxide can take on unusual bonding arrangements that make it very similar chemically to silicon dioxide," Makhluf said. "There may be much more carbon than we think inside of the Earth because of substitution reactions with the most ubiquitous oxide on earth, silicon dioxide."

Studying such specific aspects requires very small samples that can be put under extreme high pressure, a process possible with an apparatus called a diamond anvil cell. This cell pressurizes the sample between two diamonds and allows researchers to place the sample in the neutron beam to produce crystallographic data. Although this high pressure is necessary to analyze the carbon dioxide, high temperatures are also essential to fully interpret the results.

"No one has ever laser heated such a large sample under high pressure," Makhluf said. "This study is meant to advance neutron science in diamond anvil cells so that other users can investigate samples at extreme temperatures."—*Katie Bethea*

For more information: http://go.usa.gov/x9xvF



UCLA's Adam Makhluf is using neutrons at ORNL's Spallation Neutron Source to study the fundamental role carbon dioxide plays in Earth's carbon cycle, especially in the composition of carbon reservoirs in the deep earth and the evolution of the carbon cycle over time. Image credit: Genevieve Martin, ORNL

Ultrathin Destiny:

Exploring the 2-D nanomaterials frontier

by Sara Shoemaker
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Materials are identified by their properties, desirable or otherwise. Iron is strong, but it rusts. Plastics are versatile and useful but end up polluting the environment because they don't easily decay.

Scientists and engineers improve materials by manipulating them to get just the right properties, a process that leads to improvements such as longer-lasting automobiles made with non-rusting steel and packaging and consumer products made with biodegradable materials.

The latest frontier in materials research is the nanoscale. Scientists now design materials atom by atom, determining the best arrangement of elements for the job at hand. At ORNL, researchers are focusing on ultrathin layered materials where each layer is no more than several atoms thick—in other words, materials so thin they are considered two-dimensional.

At such a small scale, the materials are transformed. Researchers can permeate their nanostructures with exotic properties: nearly unbelievable combinations of light weight and strength, or efficient, long-lasting energy storage, or resistance to extreme temperatures, or even superconductivity.

Imagine electronic devices that run for days on a single charge or transparent solar cells that can efficiently harvest energy from every window. High-powered ultrathin transistors could be woven

See ULTRATHIN DESTINY, page 10

ORNL materials scientists Kai Xiao and Akinola Oyedele explore the practical applications of 2–D nanomaterials.
Image credit: Jason Richards, ORNL

High-impact

MIT research comes to ORNL

by Sean Simoneau
ornlreview@ornl.gov

Shengxi Huang

Two-dimensional nanomaterials may be infinitesimally small, but they are a big deal for the chemists and materials scientists who trek to ORNL to study them. One such user is Shengxi Huang.

Huang is a doctoral candidate at the Massachusetts Institute of Technology working with Mildred Dresselhaus, a noted physicist, engineer, and long-time ORNL collaborator known as "The Queen of Carbon Science."

Dresselhaus pioneered research in carbon nanotubes, graphene and other carbon nanostructures. When Huang joined the research group shortly after arriving at MIT, Dresselhaus assigned her to work on 2-D materials at ORNL's Center for Nanophase Materials Sciences, which has the specialized facilities and active research interest necessary for their work, in this case allowing them to apply a technique known as low-frequency Raman spectroscopy.

Huang and Xi Ling, a former group member and current professor of chemistry at Boston University, came to ORNL to study a family of 2-D materials called transition metal dichalcogenides.

These materials are promising semiconductor candidates and exhibit excellent optical properties, such as strong photoluminescence and absorption, that can be applied to next-generation optoelectronic devices.

"I think these materials are potentially quite useful in making ultrathin and flexible devices," Huang said. "For example, our screens would be less rigid and could be rolled up or folded into a bag. They can be quite unique."

Working with CNMS researchers including Bobby Sumpter and David Geohegan, the MIT team used low-frequency Raman spectroscopy to characterize the properties of 2-D materials such as molybdenum disulfide and black phosphorus, also known as phosphorene.

Traditional Raman spectroscopy measures and identifies chemical composition and molecular structures using high frequencies. Low-frequency Raman is more advanced and costly, but it is also more powerful and can be used to measure the number of monolayers in a material and gauge the strength of the coupling between layers.

"Besides their unique facilities, ORNL is also staffed by experts in the field who can assist us with our research," Huang said. "There are people who are really good at maintaining and operating these machines and can make them do what you want and more. They can work unique functions into the spectrometers, which is also an important capability."

Huang is currently studying gallium telluride, which exhibits superior photoresponsitivity and may be the best known photodetecting 2-D material in existence. She plans on returning to ORNL to study the material's photoresponse capabilities with the lab's ultrafast optical spectrometers.

"We want to study the optic dynamics of these materials to help solve some mysteries as to why they have such high photoresponsivity and fast photoresponse times," she said.

The science of 2-D material physics is largely unexplored and constantly evolving. The continuing partnership between Dresselhaus's group and ORNL will push the boundaries of the field by combining state-of-the-art facilities, technological innovation, and the seasoned expertise of researchers from both parties.

"Oak Ridge probably has the best facilities in the U.S. for what we do. It is really good that they are open to users, especially in academia, to use their facilities and set up collaborations," she said. "People at MIT are very interested in exploring new fields, so the collaborations between the two institutions can be quite useful."

The laser-based ultrafast spectroscopy equipment at ORNL's Center for Nanophase Materials Sciences allows researchers to study phenomena in materials that happen on a timescale of a millionth billionth of a second. Image credit: Jason Richards, ORNL

ULTRATHIN DESTINY, from page 8

into clothing and perform smartphone-like communications or monitor personal biometrics.

"What's fascinating is that age-old layered materials like graphite and molybdenum disulfide are suddenly being rediscovered as atomically thin 2-D layers with radical new properties," ORNL group leader David Geohegan said. "A single layer behaves much differently from a bilayer, and so on, up to a few layers thick when the material begins to behave more or less like the bulk crystal, or starter material."

The study of 2-D materials has become a hot field. Geohegan and his group at the lab's Center for Nanophase Materials Sciences can synthesize and process a variety of ultrathin layered crystals and characterize where each atom is with sophisticated microscopes. Using the power of ORNL's Titan supercomputer, theorists can also model these materials like never before to understand the origins of their functionality.

By concentrating on growing and assembling 2-D layers that absorb and emit light, Geohegan's group not only develops ultrathin electronics but also reveals the quality of the crystals. "Right now a grand challenge is to grow atomically thin materials as well as they grow in nature," he said.

Kai Xiao, a materials scientist in Geohegan's group, leads the effort at the CNMS to understand the practical application of these atomically thin 2-D crystals by finding ways to wire up actual prototype devices with novel structures. Indeed, semiconducting 2-D materials may well be the future of electronics.

Semiconductors—materials that meticulously control the flow of electricity—are the key to microprocessors and modern technology. Labeled either n-type or p-type—depending on whether extra electrons are available to be conducted—they can be combined to create the p-n junction that is the building block of a transistor. The power of electronics depends on packing more and more transistors into devices like smartphones; as a result, we need smaller transistors.

Enter 2-D materials. While the features on today's silicon-based semiconductors continue to shrink, manufacturers could greatly benefit from new materials created from the thinnest layer up. Xiao's team is already there. "By stacking atomically thin 2-D layers like ultrathin Lego blocks, we can develop a prototype using new 2-D nanomaterials with custom properties ideal for semiconductors," Xiao said.

Moving beyond Scotch tape

Before you can experiment with a 2-D material, however, you must produce it. Two-dimensional materials burst onto the science scene in 2004 with the simple production of graphene, which is graphite in a single-atom sheet form. The silvery metal-

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Oak Ridge company to produce graphene in mass

by Leo Williams
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Perhaps no nanomaterial has gotten more attention than graphene, a one-atom-thick layer of carbon that is in many ways the Superman of materials: 300 times stronger than steel, unmatched at conducting heat, so dense that no gas can slip through.

Graphene may also illustrate our accelerating pace of technology. It was first produced as recently as 2004—a feat that helped bring the 2010 Nobel Prize in Physics to two researchers in the United Kingdom—yet an Oak Ridge company is gearing up to produce a million square meters annually before the end of this decade.

Vig Sherrill

That company, General Graphene, will be using a technique developed by ORNL physical chemist Ivan Vlassiouk. The chemical vapor deposition process takes a carbon-containing gas such as methane, strips out the non-carbon elements, and deposits the carbon to create graphene. What's more, it does so without requiring a vacuum.

Graphene vapor deposition technology was matured through ORNL's Technology Innovation Program and licensed to General Graphene partners Vig Sherrill and Greg Erickson in 2014. Since then they've been working with investors to identify funding and with ORNL to refine the technology.

The company is testing two prototypes before going into production. The first produces about 2 square feet of graphene a day, while the second will boost that by a factor of 50, to about 10 square meters a day. The company hopes to be in full production by early 2018.

The primary obstacle to widespread use of graphene is cost, largely because existing production technologies can deliver only low volumes of high-quality graphene. Sherrill noted that a square meter of graphene went for $100,000 as recently as two years ago. At less than a milligram, that made graphene among the most expensive materials in the world.

The cost has come down about an order of magnitude in the meantime, to $10,000 to $20,000, Sherrill said, with General Graphene working to bring it down to around $100 a square meter in the next few years.

At that point, the material would be available to everyone from manufacturers to research laboratories, a process that will open up possible uses, including flexible electronic touch screens and lightweight components for transportation, according to Sherrill.

"Graphene has 300 times the strength of steel," he said, "so 30 or 40 years from now you'll be able to make a car tire so light you could hold it on your pinkie. Or imagine a 747 wing you could hold in your hand."

The super-strong material could even be incorporated into textiles, he said.

"Imagine if your shirt were made of graphene. It wouldn't just be bulletproof; it could take a howitzer shell. You would be dead, but your shirt would be fine.

"Our goal is to sell it to everyone from do-it-yourselfers, to labs, to production facilities. Once it's at a level that can be afforded, I believe graphene is going to be like plastic. People are going to use it for things we can't dream of."

ULTRATHIN DESTINY, from page 10

like graphite commonly found in pencils flakes off easily into thin layers using the clear adhesive tape you can buy at a grocery store. By repeating this process, layers of graphite can be exfoliated, or peeled and separated from the bulk material, again and again until reaching a layer just one atom thick.

As arcane as that may sound, the adhesive technique is effective as a top-down method for studying 2-D materials. But that's just scratching the surface.

Xiao uses this approach to extract the ultrathin layers exfoliated from beautiful semiconductor crystals grown at ORNL such as molybdenum disulfide and gallium selenide. When the crystals are reduced to flakes, they are considered 2-D and can be stacked, rotated, doped (with another element inserted into its crystal structure), and otherwise manipulated to produce new materials with different properties.

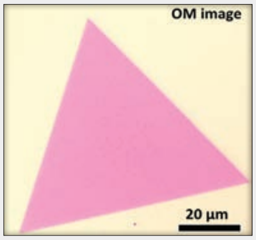
"Although using the top-down Scotch tape method is an easy way to make high-quality 2-D nanomaterials for fundamental research, it is hard to control the layer number and size," Xiao said. "Also, it is nearly impossible to align the atoms precisely, so we need to try and grow the layers epitaxially one on top of another."

As a result, Geohegan and Xiao's team explores a variety of high-tech methods such as chemical vapor deposition or pulsed laser deposition to directly grow the 2-D crystals in a controlled manner. This bottom-up approach ensures materials with consistent thickness, comparable to the way conventional semiconductors are grown. These scalable techniques promise to grow

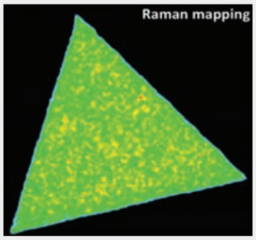
Skilled researchers using

ORNL's Center for Nanophase Materials Sciences and its talented microscopy specialists are uniquely positioned to analyze promising 2-D nanomaterials, from properties such as their electronic conductivity and ability to harvest light to the exact arrangement of their individual atoms. One promising material is gallium selenide, which is produced in flat, triangular crystals that are a hair's breadth wide and as thin as four atoms tall.

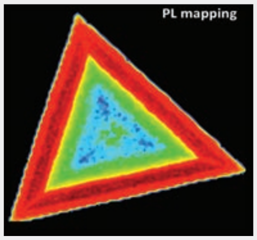
Here are a few of the cutting-edge microscopes ORNL uses to analyze and manipulate gallium selenide, along with specific tests they are able to perform.



Optical microscope image



Raman spectroscopy



Photoluminescence spectroscopy

Optical Microscopes

These microscopes show researchers regions of crystals down to a tenth of the width of a human hair.

- **Raman spectroscopy** is a technique that uses shifts in the color of a laser to measure the molecular vibrations of a material, allowing them to reveal the structure of atoms within a layer or how layered materials interact, depending on how they're stacked.
- **Photoluminescence spectroscopy** uses a laser to excite the electrons within a material and captures the light the material emits. This emitted light reveals the characteristic energy bands of the crystal that must be understood for optoelectronics, as well as the crystal's quality. The instrument can be chilled to 4°K (–452°F) to resolve these electronic bands and any defects by freezing the molecular vibrations.
- **Pump-probe ultrafast laser spectroscopy** splits an ultrafast laser pulse of light into two parts to measure very fast phenomena such as the creation and motion of electrons through the crystal. The first pulse of light creates the electrons, while the second bounces around a set of mirrors before arriving at the sample shortly thereafter—acting like a flashbulb to capture how the crystal responds to the excited electrons. The absorption of the second pulse is used to measure events as fast as 40 millionths of a billionth of a second long.

large-area 2-D crystals for future research and, eventually, in commercial applications.

Using a suite of powerful scanning tools, ultrathin layers are "read" and mapped as sensors scan the surface to reveal the individual atoms in the layers like stars in a honeycomb galaxy, the heavier atoms a bit brighter than the others. The resulting latticework of molecules takes on shapes and structures unique to the materials' particular properties.

ORNL microscopists on the CNMS team, including Juan-Carlos Idrobo Tapia and An-Ping Li, measure the electronic properties of the layers with atomic resolution, which provides CNMS team theorists including Bobby Sumpter, Liangbo Liang and Mina Yoon a roadmap of the electronic interactions between the atoms in the 2-D galaxy to guide their computations.

By bridging the gap from atoms to real devices, the team is able to explain why different 2-D material combinations would be successful or not for new technology and to predict the next step.

"How these layers react and change when subjected to various stimulations—like light or electrons—tells us about a material's characteristics and behavior," Xiao said. "It leads us to question what's there and what's missing and how can we use that information to our advantage when creating new materials."

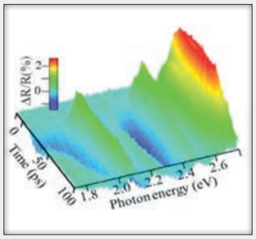
ORNL's work in 2-D nanomaterials has been described in many high-impact science journals, garnering recognition across the global physics community. Hopefully, as these materials find application, the pathway to commercialization will happen at the speed of nanotechnology.

advanced microscopes

Scanning Transmission Electron Microscopes

Aberration-corrected STEM instruments focus electrons into a beam that is smaller than the size of an atom and then scan the beam on the sample to show its atomic structure, including defects (holes in the lattice) and dopants (atoms of a different element).

- Electron energy loss spectroscopy can be used during STEM imaging to identify the element corresponding to each atom and the effects of bonding, dopants, or defects by the loss of transmitted electron energy as measured by an electron energy analyzer.



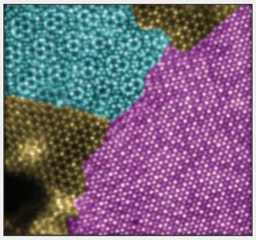
Pump probe laser spectroscopy

Helium Ion Microscope

This microscope uses helium ions instead of electrons to image materials and is much better at imaging surfaces. It can also be used to cut materials with extremely high resolution or create defects in a sample that can then be examined with a STEM.

Scanning Tunneling Microscopes

STMs bring a conducting probe tip very near the sample and inject electrons that tunnel through the vacuum between the instrument and through the sample to a conducting substrate. STMs can scan across the sample to also measure atomic positions and are especially good at mapping the electronic structure of a material and defect states in materials.



Scanning transmission electron microscopy

ORNL system unites

imaging and computing in the search for new materials

by Jonathan Hines
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A rapid increase in the volume of information captured by advanced microscopes presents a unique problem to materials scientists: How do you make effective use of all this data?

At ORNL, researchers are engineering a solution by uniting the lab's state-of-the art imaging technologies with advanced data analytics and high-performance computing. The combination of experimental power and computational might promises to accelerate research into better batteries, atom-scale semiconductors, and efficient photovoltaics, to name a few applications.

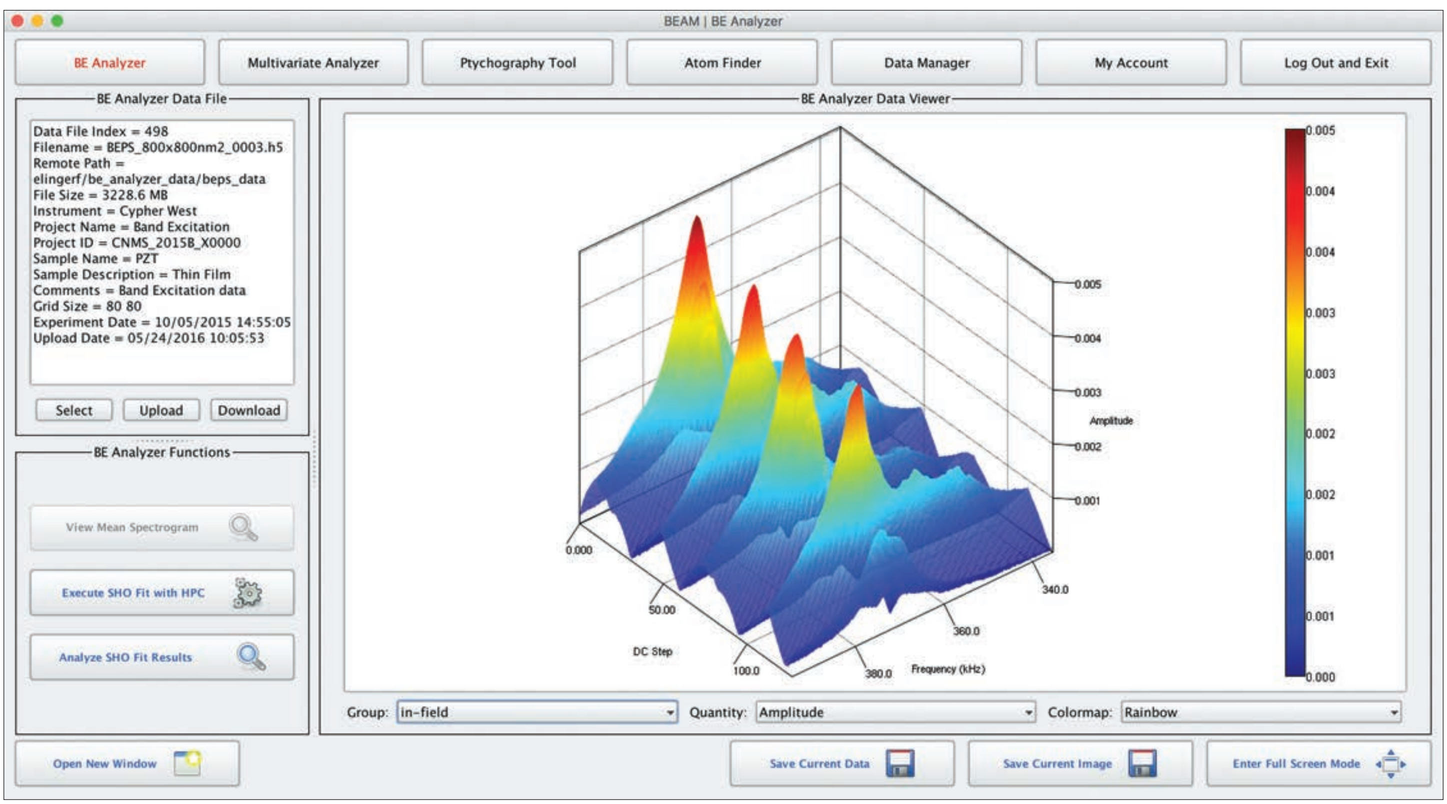
Developing a system that delivers these advanced capabilities in a seamless manner, however, demands an extra layer of software to pull it all together.

Enter the Bellerophon Environment for Analysis of Materials, an ORNL platform that combines scientific instruments with web and data services and computers, all through a user-friendly interface. Designed to streamline data analysis and workflow at ORNL user facilities such as the Center for Nanophase Materials Sciences and Spallation Neutron Source, BEAM gives materials scientists a direct pipeline to scalable computing, software support, and high-performance cloud storage services provided by ORNL's Compute and Data Environment for Science. Additionally, BEAM offers users a gateway to ORNL's world-class supercomputers.

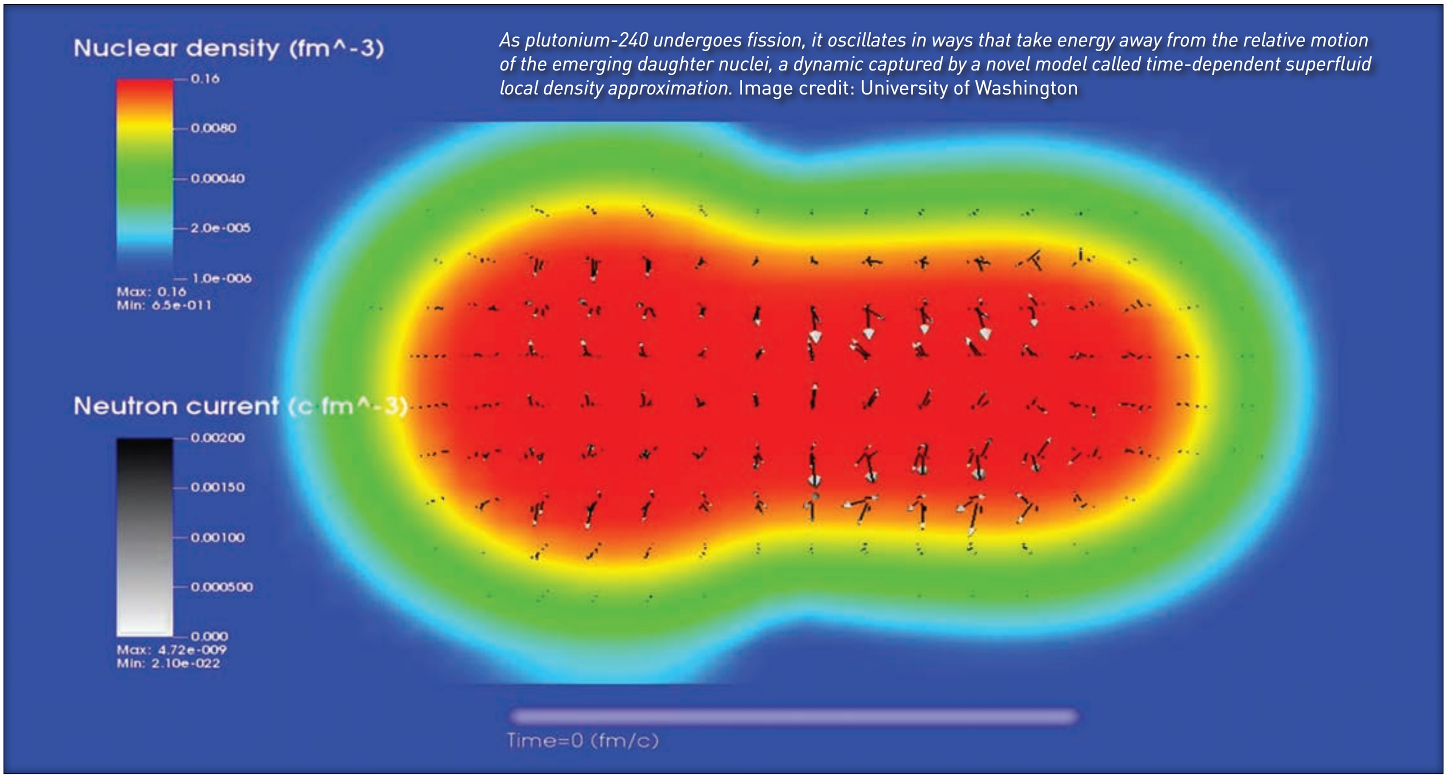
The system allows scientists to process, analyze and visualize large experimental datasets nearly as soon as they are created, a drastic improvement over traditional time-consuming data analysis.

"Processes that once took days now take a matter of minutes," said ORNL software engineer Eric Lingerfelt, BEAM's lead developer. "Once researchers upload their data into BEAM's online data management system, they can easily and intuitively execute advanced analysis algorithms on resources like CADES's compute clusters or ORNL's Titan supercomputer and quickly visualize the results. The speedup is incredible, but most importantly the work can be done remotely from anywhere, anytime."

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



ORNL's Bellerophon Environment for Analysis of Materials combines scientific instruments with web and data services and computers, all through a user-friendly interface. Image credit: ORNL



As plutonium-240 undergoes fission, it oscillates in ways that take energy away from the relative motion of the emerging daughter nuclei, a dynamic captured by a novel model called time-dependent superfluid local density approximation. Image credit: University of Washington

Team uses Titan

to improve fission modeling

by Jonathan Hines
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In 1938, while trying to fatten the atom, German chemist Otto Hahn accidentally split it instead. Since then scientists have been trying to pinpoint exactly how nuclear fission unfolds at the microscopic level.

The most successful modern techniques for analyzing nuclei rely on supercomputers to calculate changes in the nucleus's density. Extending these methods to explain the splitting of heavy, fissile elements like uranium and plutonium, however, requires something extra.

A new approach pioneered by the University of Washington's Aurel Bulgac and colleagues expands commonly used density functional theory to include superfluid pairing between identical particles in nuclei (e.g., protons and protons or neutrons and neutrons). Being superfluids, these pairs move without resistance, affecting the energy needed to split the nucleus during fission. The team's method, called time-dependent superfluid local density approximation, has shown promise for capturing the dynamics of nuclear evolution without having to rely on simplifications.

In a first study of its kind, Bulgac's team applied the technique to a fissioning plutonium-240 nucleus using ORNL's Titan supercomputer. The simulation achieved notable fidelity, with the predicted kinetic energy agreeing with experimental results. Additionally, the simulation suggested that the final stages of fission last about 10 times longer than previously calculated, a finding with wide ramifications for nuclear science and astrophysics.

"Our simulation shows the nucleus takes a longer route to scission, or split. It doesn't simply break into two parts but oscillates in ways that take energy away from the relative motion of the emerging daughter nuclei," Bulgac said. "It's like hiking down a mountain. You can go straight down, or you can zigzag to the bottom. The second option takes much longer, but you end up at the same place."

The results from Bulgac's team are encouraging for researchers who need an improved understanding of fission fragments' excitation energies—the energy needed to boost a nucleus to a higher energy above its ground state. Currently these properties are virtually impossible to glean from experiment. Improved methods would benefit researchers who study nuclear fuel composition, nuclear forensics, and astrophysics, in which fission plays a role in producing the remnants of exploding stars.

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

New technologies to make your home more efficient

Buildings use an enormous amount of energy. By developing technologies that do more with less, ORNL's Building Technologies Program is helping to minimize both energy consumption and the carbon emissions that come with it. Here are a few of the promising technologies that are already available for your home or may be coming soon.

Heat pump water heater

This water heater is more than 300% efficient because it draws heat into the tank from the surrounding environment as well as from the electricity that drives it. As an added benefit, it cools and dehumidifies the surrounding environment. Versions driven by natural gas are under development. See http://go.usa.gov/xKefT, https://goo.gl/PFQ6hL. **Potential savings (tons of coal): 19 million***

Magnetocaloric refrigerator/freezer

Put some metals in a magnetic field and they heat up; remove the field and they cool back down. Refrigerator/freezers based on this principle (known as the "magnetocaloric effect") eschew harmful refrigerants and can cut up to 30% of energy use. ORNL and GE are using the lab's innovation and manufacturing expertise to overcome substantial technical challenges and bring a commercial version to market. See http://goo.gl/ZMwlHf, http://go.usa.gov/xZZdH. **Potential savings (tons of coal): 7 million***

Air/water flashing and sealant

Air leakage accounts for about 4% of U.S. energy use. LiquidArmor, a spray-on product from Dow Chemical, is faster and easier to use than readily available sealants such as tape, coatings with a reinforcing mesh, and flashings applied with a caulk gun. Developers used data from the heat, air and moisture penetration chamber at ORNL's MaxLab. See http://goo.gl/R4lbqF. **Potential savings (tons of coal): 43 million***

Energy-harvesting printed wireless sensors

Wireless sensors—powered by energy harvested from indoor light—report one or more of temperature, humidity and light level, allowing for better control, reduced energy consumption, greater comfort, and reduced electricity draw during peak load periods. The sensors are printed and can go for years at a time without maintenance. See https://goo.gl/UDouBv. **Potential savings (tons of coal): 12 million***

Composite insulation

Using vacuum technology like that of a coffee thermos, this insulation offers up to three times the efficiency of foam insulation boards. The savings estimate assumes walls of existing residential buildings retrofitted with 2" of insulation. See http://goo.gl/MGlg9j, http://goo.gl/xyOETN. **Potential savings (tons of coal): 32 million***

Integrated heat pump

Integrated heat pumps go beyond cooling and heating, tackling tasks such as water heating, dehumidification, and conditioning of fresh ventilation air. Diverted waste heat means cheaper hot water, and variable-speed compressors, fans and pumps increase efficiency during milder weather. Systems developed by ORNL in connection with Lennox Industries, Nortek Global HVAC, and ClimateMaster have cut energy usage by more than half over traditional heat pumps. See http://goo.gl/p6nHHX, http://goo.gl/ZT4t4P. **Potential savings (tons of coal): 42 million***

Ultrasonic clothes dryer

The ORNL-developed ultrasonic dryer uses high-frequency mechanical vibrations to dry your laundry, extracting moisture into a cold mist that can be removed with room-temperature air. The dryer is a triple win, saving energy (by being 3–5 times more energy efficient than conventional dryers), time (taking half the time to dry the same load), and your wardrobe (by being gentler on fabrics). **Potential savings (tons of coal): 13 million***

Cold climate heat pump

Traditional heat pumps work great in mild climates but fall short when the mercury plunges. The Cold Climate Heat Pump, developed with Emerson Climate Technologies, combines two compressors with a compressor discharge pressure control. A prototype system kept an Ohio home comfortable down to -13°F and saved 40% on energy usage in a peak heating load month. See http://go.usa.gov/xZgkC. **Potential savings (tons of coal): 7 million***

Thermoelectric clothes dryer

Thermoelectric elements look something like saltine crackers, with one side hot and the other cool. Air heated by the hot side evaporates moisture in your laundry (like a conventional dryer), but it is then directed to the cool side, where the water condenses and some energy is recovered. This process adds no moving parts to the dryer and leads to energy savings of 37%. See http://go.usa.gov/xKefR, http://go.usa.gov/x-KefU. **Potential savings (tons of coal): 5 million***

Infrared reflecting cool-colored coatings/shingles

White roofs reflect light better than dark roofs, lowering both roof temperature and cooling bills. Dark roofs, on the other hand, look nicer. ORNL has demonstrated unique pigments that deliver the best of both worlds, reflecting light in the invisible infrared spectrum. Dark-colored coatings/shingles with these pigments are commercially available and reflect light energy 500% better than conventional dark roofs. See https://-goo.gl/dWqHH6. **Potential savings (tons of coal): 7 million***

Magnetocaloric window air conditioner

Some metals heat up when placed in a magnetic field and cool down when the field is removed. ORNL is working to develop window air conditioners using this principle, which will be up to 30% more efficient than traditional air conditioners while avoiding the use of environmentally harmful gases. See http://goo.gl/eu2aUJ, http://goo.gl/vA253G. **Potential savings (tons of coal): 12 million***

* Number represents potential energy savings each year in the United States, expressed as the amount of coal needed to generate that amount of energy.

Seeing through concrete

by Jim Pearce
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When nuclear power plants in the United States were built, they were licensed for 40 years of operation. Today, most are either approaching that age or have already exceeded it.

"Several years ago, the Nuclear Regulatory Commission began to look at the safety implications of extending these licenses to 60 years," said Dwight Clayton, an engineer in ORNL's Electrical and Electronics Systems Research Division. "They determined that, based on the science, extending the licenses from 40 to 60 years wouldn't be a problem. Then the question came up: Can we go from 60 years to 80 or even 100 years?"

This is where the science becomes less clear. In fact, the Light Water Reactor Sustainability Program in DOE's Office of Nuclear Energy was created to help answer these questions.

At about the 80-year mark, signs of degradation can begin to appear in a nuclear plant's concrete containment structures. To determine whether they are present in a specific structure, however, researchers need an instrument that can peer through as much as a meter of concrete.

"That's where our group comes in," Clayton said. "Our area of expertise is signal processing and instruments, so we looked at various technologies for evaluating concrete structures and settled on ultrasonic linear arrays. These devices use sound waves to examine the internal condition of concrete structures."

One challenge for Clayton's team was adapting commercially available arrays—designed to probe the foot-thick concrete common in buildings and bridge decking—to examine the meter-thick, heavily reinforced concrete common in nuclear power plants.

"The depth of the concrete and the amount of reinforcement make it hard to see through with any type of technology," Clayton said. "The sound waves produced by the arrays go into the concrete, are reflected off whatever is in the wall, and return. So they have to travel through as much as 2 meters of concrete."

That means Clayton's team had to boost the performance of its off-the-shelf arrays by a factor of three or more. They did this by developing heavy-duty signal-processing software to pull data signals out of the noise created by these obstacles. The additional processing

> *"Our area of expertise is signal processing and instruments, so we looked at various technologies for evaluating concrete structures and settled on ultrasonic linear arrays. These devices use sound waves to examine the internal condition of concrete structures."*
>
> — ORNL engineer **Dwight Clayton**

allows them to see defects in the concrete much more clearly.

The team is testing the system on a wall section that simulates a nuclear power plant wall. The mock-up contains various defects, so researchers can see how the system responds to each type of problem area. Delaminations, for instance, are places where the concrete separates. In addition, organic material such as construction debris (leather gloves or pieces of wood) may be inadvertently left in the concrete, where it can lead to corrosion in steel liners.

"We are going to be able to take into account these kinds of construction defects that may not be an issue for 40 years, but as you go beyond 40 or 60 years they start to become an issue," Clayton said.

Another important way that concrete can deteriorate over time is called alkali silica reaction. ASR is a slow chemical reaction that creates pockets of gel within concrete structures. As these pockets expand, they cause small cracks.

"When you see fine cracks on the side of a concrete bridge, most likely that's ASR at work," Clayton said. "It can also be freezing and thawing, but a lot of times it's ASR."

ORNL is working with the University of Tennessee to build a test wall that develops ASR within months, rather than years, to better understand the mechanisms of ASR and fine tune the ultrasonic linear arrays to detect it.

University of Minnesota researcher Kyle Hoegh positions an ultrasonic linear array on a test wall section. The device uses sound waves to examine the internal condition of concrete structures. Image credit: Dwight Clayton, ORNL

"By applying elevated temperature and 100 percent humidity to the test wall, we'll be able to accelerate the process," Clayton said. "We have a two-year project with UT, but these two years of testing will simulate a much longer time in the life of a normal concrete wall."

This work can be applied to all sorts of concrete structures, including bridges, stadiums and dams.

The team's goal is to provide the NRC and DOE with a concrete structure evaluation system that can be deployed by 2020.

"We will provide a sound, scientific method to see through concrete," Clayton said. "Whether or not this eventually results in new requirements for nuclear power plants is up to the NRC."

Neutrino experiments

explore the unknown with ORNL expertise, equipment

by Dawn Levy
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Approximately 100 trillion neutrinos bombard your body every second, but you do not notice these ghostly subatomic particles. Because they are electrically neutral and interact with other matter via the weak force, their detection is difficult—and the subject of challenging experiments.

In 2015 the Nobel Prize in physics went to researchers who demonstrated that neutrinos can change identities. The discovery meant that neutrinos have mass, albeit small. It also hinted at new physics beyond the Standard Model, which captures our current understanding of matter and energy but is incomplete.

Now three experiments are gearing up to advance our understanding of neutrinos, and all three benefit from expertise and facilities at ORNL.

"We're enthusiastic because these experiments will provide the means to answer basic questions about the universe," said ORNL physicist Alfredo Galindo-Uribarri. Physicists will use novel detectors to explore unknowns of the cosmos, from the properties of neutrinos to the possibility that neutrinos are a component of dark matter, which makes up one-quarter of the universe.

One experiment, with ORNL physicists in leadership roles, is the Majorana Demonstrator, which was built by international partners. It is located inside a former gold mine in South Dakota, where the Homestake experiment detected cosmic neutrinos from 1970 to 1994. A Nobel Prize recognized this work in 2002.

> *"We're enthusiastic because these experiments will provide the means to answer basic questions about the universe."*
>
> — ORNL physicist **Alfredo Galindo-Uribarri**

The Majorana Demonstrator uses germanium-76 as both source and detector in a search for neutrinoless double-beta decay. It is an initial experiment that will demonstrate the feasibility of a much larger one. If the decay process is observed, it will prove that the neutrino is its own antiparticle, provide a measure of neutrino mass, and possibly answer why the universe is made of matter and not antimatter.

Two other large, collaborative experiments, both sited at ORNL, will for the first time detect neutrinos generated at ORNL's Spallation Neutron Source and High Flux Isotope Reactor. The main purpose of both facilities is to produce neutrons, but during normal operations these world-class neutron "factories" also produce plentiful neutrinos. Why not use the neutrinos for experiments too?

From left, ORNL's David Dean, Alfredo Galindo-Uribarri and Chris Bryan check on a prototype detector at the High Flux Isotope Reactor. The prototype will mine neutrinos produced in the reactor's core from the decay of fission products to prepare for the PROSPECT experiment's detection instrument, now under construction at Yale. Image credit: Genevieve Martin, ORNL

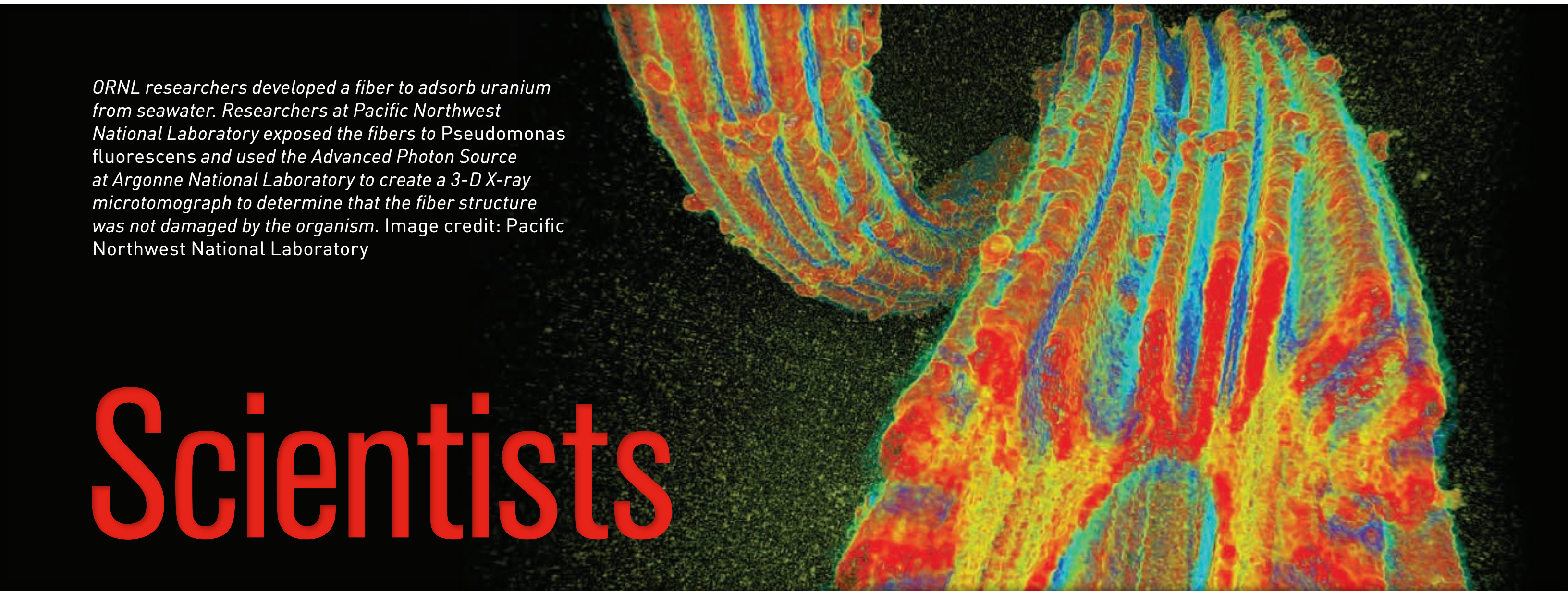
PROSPECT, an experiment at HFIR that is led by Yale University, will detect neutrinos produced in the reactor's core from the decay of fission products. It will mine information about neutrino oscillations—transmutations of electron neutrino, muon neutrino and tau neutrino "flavors" from one to another. Specifically, researchers want to find out if neutrinos oscillate over less than 20 meters. Short-baseline neutrino oscillations have not been definitively observed. Their observation would allow precision measurements of neutrino flux and energy spectrum and possibly reveal the existence of a fourth flavor, the "sterile neutrino." A prototype detector has been built at ORNL for tests preparing for the arrival of PROSPECT's detection instrument, now under construction at Yale.

At SNS collaborators on another experiment, called COHERENT and led by Duke University, will use the proton beam parasitically to generate neutrinos. COHERENT's partners aim to make first-of-a-kind measurements of a phenomenon predicted by the Standard Model but never observed—the scattering of low-energy neutrinos off various nuclei.

A beam of protons will hit a target of mercury, an element whose atoms have a big nucleus capable of releasing a slew of particles, including some that stop in the target, decay and release neutrinos. Because these particles decay at rest, the neutrinos they generate will be of low energy and suitable for the scattering experiments.

Owing in large part to ORNL facilities and expertise, these big physics collaborations may soon force neutrinos out of the dark shadows of the unknown universe and reveal their hidden natures.

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



ORNL researchers developed a fiber to adsorb uranium from seawater. Researchers at Pacific Northwest National Laboratory exposed the fibers to Pseudomonas fluorescens *and used the Advanced Photon Source at Argonne National Laboratory to create a 3-D X-ray microtomograph to determine that the fiber structure was not damaged by the organism.* Image credit: Pacific Northwest National Laboratory

Scientists find a cheaper way to extract uranium from seawater

by Dawn Levy
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Oceans hold more than four billion tons of uranium—enough to meet global energy demands for 10,000 years if only we could capture it from seawater to fuel nuclear power plants.

Researchers have been working on the problem for more than half a century. Scientists of the Japan Atomic Energy Agency pioneered uranium-capturing materials in the 1990s, while more recently partners of a DOE-led initiative have developed new adsorbents that reduce the cost nearly fourfold.

"For nuclear power to remain a sustainable energy source, an economically viable and secure source of nuclear fuel must be available," said ORNL chemist Phillip Britt, who provides technical and outreach leadership for the DOE program.

Scientists from two DOE labs lead key collaborations. ORNL researchers concentrate on designing, synthesizing and characterizing uranium adsorbents with higher capacity and selectivity, whereas Pacific Northwest National Laboratory scientists focus on marine testing of adsorbents. Major advances in the effort have been published in a special issue of the journal *Industrial & Engineering Chemistry Research*.

"Synthesizing a material that's superior at adsorbing uranium from seawater required a multidisciplinary, multi-institutional team including chemists, computational scientists, chemical engineers, marine scientists and economists," said Sheng Dai, technical overseer of the ORNL program.

That teamwork culminated in the creation of braids of polyethylene fibers containing chemical groups that bind uranium. To date the braids have only been tested in the laboratory with seawater, but they are also deployable in oceans, where nature can do the mixing to avoid the expense of pumping seawater through them.

> *"For nuclear power to remain a sustainable energy source, an economically viable and secure source of nuclear fuel must be available."*
>
> — ORNL chemist **Phillip Britt**

After several weeks underwater, the uranium-oxide-laden braids are collected. They are subjected to an acidic treatment that releases uranyl ions—a source of more than 6 grams of uranium per kilogram of fiber—and regenerates the adsorbent for reuse. Further processing and enrichment of the uranium produces fuel for nuclear power plants.

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

Speedy ion conduction

in solid electrolytes clears road for advanced energy devices

by Dawn Levy
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In a rechargeable battery the electrolyte transports lithium ions from the negative to the positive electrode during discharging. The path of ionic flow reverses during recharging.

Current commercial lithium-ion batteries that use organic liquid electrolytes are flammable and subject to leakage. Solid electrolytes, in contrast, overcome these challenges, but their ionic conductivity is typically low.

An ORNL-led team has discovered a previously undetected feature in a solid electrolyte that could efficiently facilitate ion transport. State-of-the-art microscopy revealed this feature, which is about 5 billionths of a meter—or 5 nanometers—wide.

"The solid electrolyte is one of the most important factors in enabling safe, high-power, high-energy, solid-state batteries," said Cheng Ma, the first author on this work, "but currently the low conductivity has limited its applications."

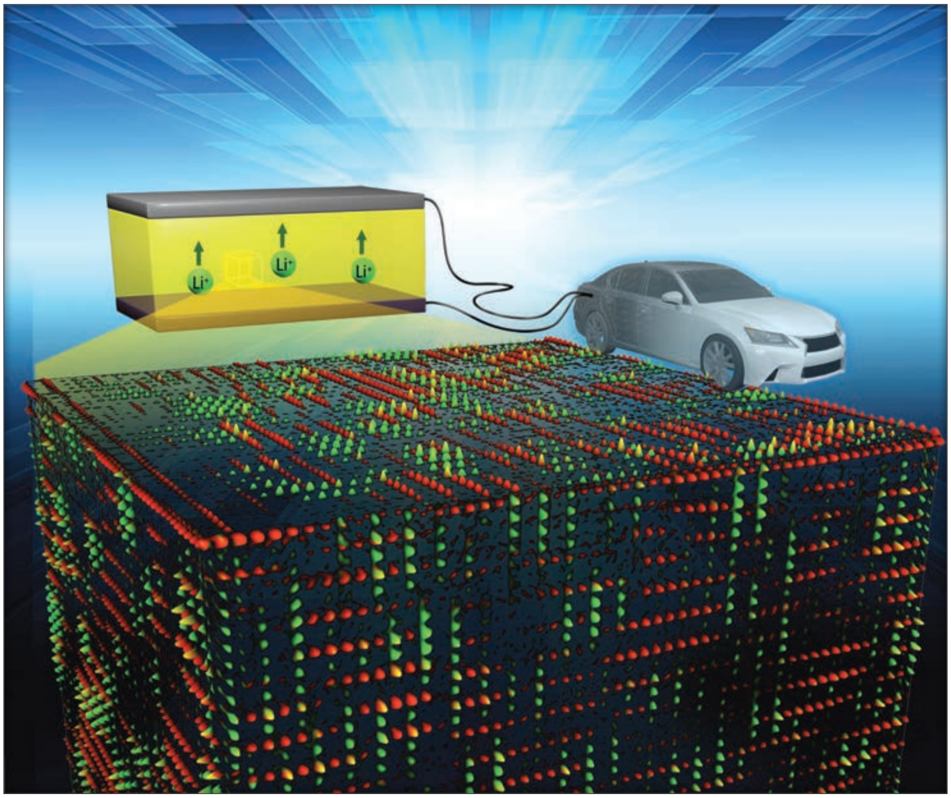
Miaofang Chi, the senior author of the study, said, "Our work is basic science focused on how we can facilitate ion transport in solids by tuning ion arrangement over length scales from subnanometer to microns. It is important to the design of fast ion conductors not only for batteries but also for other energy devices." These include supercapacitors and fuel cells.

To directly observe atomic features in the solid electrolyte, the researchers relied on the expertise of ORNL's Center for Nanophase Materials Sciences.

In the solid electrolyte lithium ions move fastest in planar pathways resulting from alternating stacks of atomic layers rich in either lanthanum or lithium. The ORNL-led team was the first to see that, without hurting this superior 2-D transport, tiny domains, or fine features approximately 5 to 10 nanometers wide, provided more directions in which lithium ions could move throughout the bulk material.

ORNL's Yongqiang Cheng and Bobby Sumpter performed molecular dynamics simulations that corroborated the experimental findings.

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



An ORNL-led research team found the key to fast ion conduction in a solid electrolyte. Tiny features maximize ion transport pathways, represented in red and green. Image credit: ORNL

Indispensable

nuclear modeling software gets a makeover

by Jason Ellis
ellisjk@ornl.gov

Nuclear plants worldwide operate safely with the help of a unique suite of modeling and simulation software that has enabled engineers to design the best processes for removing spent nuclear fuel and installing new fuel assemblies.

Launched in 1980, the SCALE code system can also analyze criticality safety and nuclear reactor physics, predict the distribution of nuclides in an irradiated material, and evaluate radiation shielding.

A team of developers led by ORNL recently gave SCALE a major upgrade, leaving much of its older Fortran programming and using the more modern C++ language to rewrite the software from the ground up. The resulting product is both more efficient and more accurate.

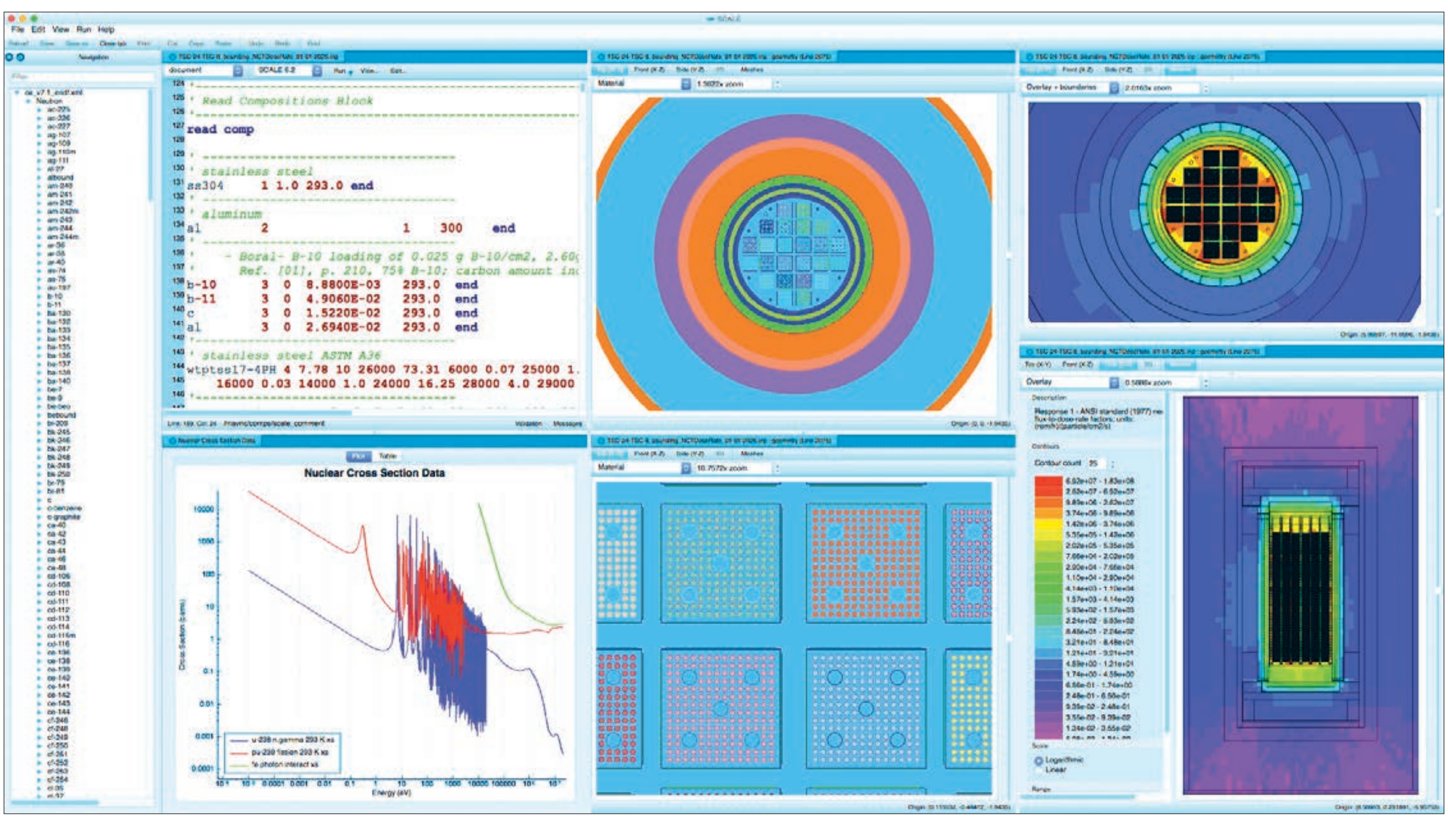
"The foundation was based on Fortran programming code that had many limitations built into the 40-year-old design," said Brad Rearden, manager of the SCALE code system in ORNL's Reactor and Nuclear Systems Division. "It was not going to sustain us moving forward. We took a pause and said we're not going to work like that anymore; we're going to re-do the foundation, which was a bold step."

The effort ensures the future of SCALE as a software that's as common to many in the nuclear industry as email is to the average office worker.

Looking at the transportation of spent nuclear fuel, SCALE simulates nuclear physics processes and allows engineers to design safety barriers needed for both regular operations and adverse conditions such as an accident. If a simulation shows that operating limits could be exceeded, additional safety measures can be built in.

The software is also useful during the production of nuclear fuel.

"For manufacturing processes, how much uranium can you safely process in



Among its many strengths, the SCALE code system supports the safe removal and transportation of spent nuclear fuel. Image credit: ORNL

Container with spent fuel rods. Image credit: Carlos Jones, ORNL

a single batch as you're making nuclear fuel? If you can include a little more thanks to our safety computations, it enables a more efficient process," Rearden said.

The development team has improved and expanded SCALE every year, but the "guts" of the system remained the same until this most recent version.

A 65-member team based at ORNL developed the newest iteration—SCALE 6.2—to enable efficient modern software maintenance and quality assurance while essentially eliminating bias that led to incorrect answers.

"We communicated with our sponsors that we needed to work on speed, efficiency, and accuracy, and at the same time, we needed a more structured approach to help modernize our software programming and verification techniques," Rearden said. "At this stage in the process, we have grown from 1 million lines of code to more than 2 million."

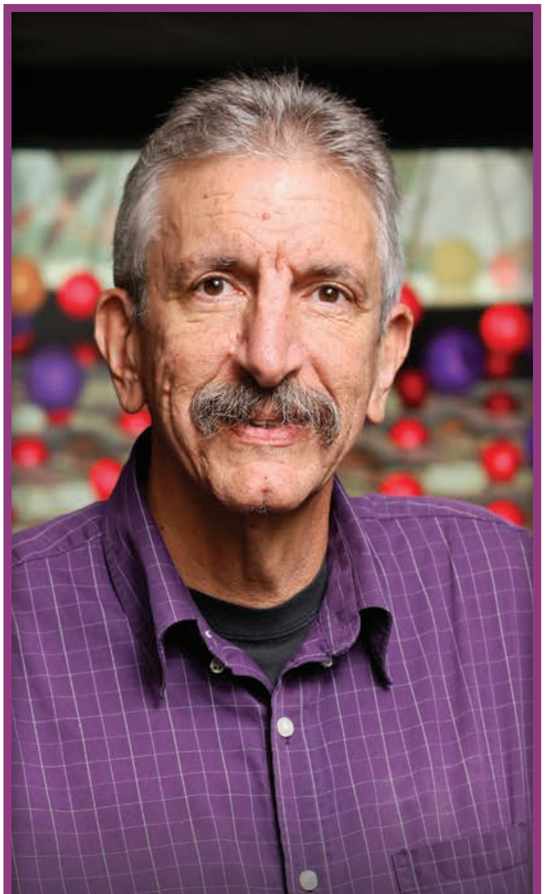
The 7,000 users in 56 countries worldwide have applauded the new SCALE 6.2 during numerous presentations and training sessions provided by Rearden's staff. And even though the latest update is the most drastic in SCALE's history, more is planned for this software. The goal is to complete the reconstruction project and launch version 7.0 in the next five years.

The second half of the plan also includes taking steps to enable SCALE's more advanced simulations to run with the world's leading supercomputers, including ORNL's.

"SCALE 6.2 is the halfway point of the modernization plan. For 7.0, we are looking at a fully integrated, parallel framework. We want to enable advanced simulations, especially looking at the next generation of reactors and optimized performance of existing systems," Rearden said.

> *"At this stage in the process, we have grown from 1 million lines of code to more than 2 million."*
>
> — SCALE manager **Brad Rearden**

For more information:
http://scale.ornl.gov



Caltech physicist Brad Filippone is a fellow of the American Physical Society and associate editor of the journal *Physical Review C*. He is also a spokesman for the neutron electric dipole moment experiment at ORNL's Spallation Neutron Source.

The experiment is committed to measuring the neutron's EDM, a nearly infinitesimal separation between its positive and negative charges. The answers provided by the experiment may help us understand shortcomings in the Standard Model of particle physics, a proposed adjustment to the model known as supersymmetry, and the reason why matter and antimatter didn't completely cancel each other out at the beginning of the universe.

Filippone delivered the Eugene P. Wigner Distinguished Lecture September 12, 2016, on the topic "Discovery Opportunities at Very Low and Very High Energies." This is an edited transcript of our conversation following his lecture.

Distinguished

Brad Filippone

1. Why does the Standard Model fail to explain why there is more matter in the universe than antimatter?

The problem is that at the beginning, just after the Big Bang, you had lots of energy, and that energy could turn into matter and antimatter in equal amounts. The Standard Model has no natural way to make one of those—matter or antimatter—go away. There are not enough new interactions in the Standard Model to make it happen. There are some interactions—very small—but they would not give us the amount of matter that we see today. There would hardly be any matter if we just used the Standard Model. It would all have annihilated, so there's a serious problem in trying to understand our present view. The Standard Model is our present view of fundamental forces and interactions, and it is not sufficient to account—as far as we can tell—for the amount of matter that we see in the universe today.

2. How would supersymmetry correct this shortcoming?

Supersymmetry is a theoretical model. More than a theory, it's a model that allows particles that we know about to have mirror images. According to it there is another set of particles that, when they interact, can produce potentially 118 new parameters that could allow me to get the matter–antimatter symmetry to work to get the right amount of matter. And so I have lots of free parameters. There is likely to be a whole range of values, and we anticipate that some of them will be sufficiently large to account for the matter that we see in the universe.

So supersymmetry just gives us a lot more knobs, a lot more potential ways to solve the problem. Whereas the Standard Model presently has no knobs to turn that you can adjust, supersymmetry would have many, many knobs that could be fixed so that the matter problem was solved.

3. Will the neutron EDM experiment help clear up this conflict? How?

The neutron EDM experiment is looking for one of these new kinds of interactions which would force the matter to survive. So we're looking for that new kind of interaction—if we observe the electric dipole moment. We don't

Lecturers

need supersymmetry to get an electric dipole moment, but if supersymmetry exists, it includes in it interactions that would automatically lead to electric dipole moments. Especially if the energy scale of supersymmetry is close to the Large Hadron Collider, that's almost ideal for giving us observable electric dipole moments in the next round of experiments. We could be able to see something in the next round of experiments. However, if we don't observe electric dipole moments, we start to close the door. Already the lack of particles observed at the Large Hadron Collider suggests that if there's supersymmetry, it's at a higher mass, and with electric dipole moments you can even push that mass to a higher level, or potentially see evidence for it. That might then motivate building a bigger accelerator to then go and look for those particles.

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

I enjoy telling the story of science that I do to more than just physicists. I had a great time doing that. I've also since my graduate days when I worked at Argonne National Lab, I've worked at national labs. I've worked at Los Alamos for many years; I'm working at Oak Ridge as well. So I'm quite familiar with the collaborations of universities and national labs. In many cases the universities are not capable of creating enough infrastructure to solve some of these big experimental problems. We're building these big projects. We don't have the expertise or the technology to do that in the universities, and so we are partnering with the national labs. I've done this for the last 30 years—different national labs with different projects, using their expertise and our students and knowledge to build projects that are complicated and large scale. And it's been very effective. I enjoy it.

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.

Charles Holliday is the chairman of Royal Dutch Shell, a position he took in May 2015. He spent 10 years as chairman and CEO of DuPont and has been a director at both Deere & Company and Bank of America.

Holliday has also been active in nonprofits, having served as chairman of Catalyst, an organization dedicated to expanding business opportunities for women, and of the Council on Competitiveness, an organization working to ensure U.S. prosperity. He holds a bachelor of science in industrial engineering from the University of Tennessee and honorary doctorates from Polytechnic University in Brooklyn, New York, and Washington College in Chestertown, Maryland.

In 2002 Holliday coauthored *Walking the Talk: The Business Case for Sustainable Development*, about corporate responsibility. On October 17, 2016, he delivered the Eugene P. Wigner Distinguished Lecture on "Sustainable Energy Transitions." This is an edited transcript of our conversation following his lecture.

Distinguished

Charles Holliday

1. Your book argues for sustainable development, while your Wigner lecture focused on sustainable energy transition. What do we mean when we use these terms?

"Sustainable" was originally defined by the Brundtland Commission some time ago, when the former prime minister of Norway, Ms. [Gro Harlem] Brundtland, defined it as meeting the needs of the current generation while allowing the next generation to have the capability to meet their own needs. It's really sustainable development.

So what the book argued, what we're talking about today with energy transitions, is finding a way of meet our current needs while leaving this planet in a form that the next generations can do it for themselves. We don't have to give them all the answers. We don't have to give them all the resources. We have to give them a fighting chance to make it.

And that's what we're about in energy transition. How can we transition from the current energy system, which is polluting the planet, and how can we go to the next system, which will allow future generations a chance to succeed. But if we can't meet our current needs—our housing, our food, our clothing today—for this generation, it just won't work.

2. How have your thoughts on sustainability evolved since the book came out in 2002?

This book, *Walking the Talk*, was about 62 examples of what companies were doing to actually make sustainability a reality today. So there were many case studies, if you will, for what was going on.

About 12 years after the book came out, we took on a little project where we went back and said, "How are these companies doing now? They talked a really good story 12 years ago." So we tried to find which companies were still in existence, which ones were still producing the products that they described in their short vignette, and which ones were really succeeding. And we looked for commonalities.

What we found was the common link between the very successful companies was a vision. They had something they were aiming for beyond just one short-term project. They knew where they wanted to take the company overall, and those that had a statable vision for their company that they could articulate, that they described in their first case study, tended to be doing a lot better today. So I think that might be a lesson you can take from it.

Lecturers

3. Where has business succeeded in pursuing sustainability, and where should it focus in the coming years?

Business had to earn credibility first with the public and the governments that police it. So you had to have the right ethical standards, you had to treat the environment the right way by the current rules, you had to think about those needs of your employees and the communities where you do business.

That is a first step that you must have before you can really think about going farther. And I can't stress enough the importance of ethical standards. We've seen examples in just the last year of major companies that didn't demonstrate the kind of ethical standards around their engineering that we needed.

With that in place, it's being sure you're listening to the people who are being impacted. I think the successful companies are the listeners. And they're finding ways to make sure they're hearing when they're listening. We do a lot of that in Shell, but I think DuPont also did a lot of that, so I think it's very critical as we move forward.

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

Oak Ridge is something I've been near most of my life, being originally from Tennessee and going to school at the University of Tennessee. But I've never visited here before. And when your director, Thom Mason, reached out, it didn't take me one minute to say yes, because it's something I've always wanted to see. So that's number one.

Number two, the reputation Oak Ridge has for working with business and with universities to create tangible results. I did a major study with the national academies a few years back around research universities and how the successful ones will partner with organizations like Oak Ridge. And one of our best examples in the entire country was Oak Ridge in doing that work. So I was really anxious to see exactly what was here, and the leading-edge stuff you're doing. I think you're a role model for the country. I think you're a role model for other national laboratories to follow. And that's also the feeling I get when I meet with my friends at the Department of Energy in Washington.

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

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

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

Katherine Royston

Postdoc, Reactor and Nuclear Systems Division
Ph.D., Nuclear Engineering, Virginia Tech
Hometown: Wellington, Florida

What are you working on at ORNL?

As a member of the Radiation Transport Group, the majority of my work involves radiation transport analysis using advanced computational tools. I am currently conducting radiation transport analyses and shield design for the US ITER Instrumentation and Control Group to ensure the safe operation of the ITER fusion device.

What would you like to do in your career?

In the near term I would like to expand my work to include more methods and software development. Ultimately I want a career where I am always learning and know that I am making a meaningful contribution to society.

Why did you choose a career in science?

I've always loved solving problems, and a career in science gives me new challenges every day.

Jason Dugger

Postdoc, Center for Nanophase Materials Sciences
Ph.D., Chemistry, The University of Texas at Austin
Hometown: Carlsbad, New Mexico

What are you working on at ORNL?

I am working under a Laboratory Directed Research and Development project where I'm designing a sample environment chamber that can apply electric fields to samples during neutron reflectometry experiments. We'll use this sample cell to study the electromechanical response of ionic block copolymers to electric fields.

What would you like to do in your career?

I'm very interested in molecular self-assembly and how intermolecular interactions give rise to specific functional properties on the macroscale. I hope to lead a research program that focuses on understanding these areas and how they can be exploited to solve global engineering problems in environmental and energy sciences.

Why did you choose a career in science?

I've always been curious about the way that the world works. Doing research not only puts me at the forefront of our understanding of nature but also exposes me to others that share that mindset. This is a path in life where you learn something new every day, and that's incredibly exciting for me.

Kemper Talley

Graduate student, Reactor and Nuclear Systems Division
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Easley, South Carolina

What are you working on at ORNL?

My research currently focuses on cumulative fission-product yields and multiple beta-delayed neutron emission modeling for various nuclear engineering applications. I work at the intersection of nuclear physics and nuclear engineering, bringing new nuclear theories and data to nuclear engineering applications.

What would you like to do in your career?

Accurate and reliable nuclear data is a key asset in creating new nuclear technologies and improving existing technologies. I want to continue to update engineering models with new experimental data and theories as well as motivate new experiments that are of key importance to nuclear data needs.

Why did you choose a career in science?

I chose a career in science because I have this deep desire to know more about the universe.

Stephen Signore

Graduate student, Environmental Sciences Division
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Clearwater, Florida

What are you working on at ORNL?

I analyze operations and maintenance data to better inform risk-based reliability assessments of hydroelectric powertrain components to maximize the reliability, availability and value of the system. This research is necessary due to the changing demands of the grid for hydroelectric units resulting in increased start/stop cycling of hydroelectric units.

What would you like to do in your career?

I am interested in staying in the hydroelectric-power-asset-management-community. Work done in collaboration by ORNL and hydroelectric utilities provides a complex real-world problem of significant value to both private and public stakeholders.

Why did you choose a career in science?

I chose a career in science because it enabled me to become a part of something bigger than myself. I love the challenge of solving real-world problems and sharing the results with those that will benefit from my work.

Callie Goetz

Graduate student, Low Energy Nuclear Physics Experimental Program
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Nashville, Tennessee

What are you working on at ORNL?

The goal of my work is to make nuclear reactors safer. I'm working in the Physics Division studying three isotopes of bromine that are strongly produced by fission. When fission products decay, they dissipate heat in the nuclear reactor even after the reactor is shut down. This heat can cause meltdown in emergency situations, so understanding it is the first step toward a cleaner, greener future.

What would you like to do in your career?

I would like to continue to combine my two passions for science and service. My career to date has been double-pronged. I am currently working as a scientist as well as serving as chief operating officer of a nonprofit called "Ask a Scientist."

Why did you choose a career in science?

Science allows me to apply my passion for problem-solving to real-world problems that affect us all.

Jason Whitham

Postdoc, Biosciences Division
Ph.D., Microbiology/Forest Biomaterials, North Carolina State University
Hometown: East Granby, Connecticut

What are you working on at ORNL?

As part of the Bioenergy Science Center, I work in close collaboration with teams using genetic manipulation, physiological characterization, systems biology, and analytical chemistry to understand and improve microbial fuel and chemical production from lignocellulosic feedstocks. My contributions include identification of multiple genetic targets for improved performance of microbial catalysts.

What would you like to do in your career?

Make an impact. Do cool things that will inspire my future children and others. Make discoveries and inventions used to produce green fuels and chemicals at an industrial scale for sustaining and improving the lives of U.S. citizens and people around the world.

Why did you choose a career in science?

Money was never a major factor. Neither was acclaim. A natural aptitude toward science and technical application, the timing of NC State energy initiatives in 2008, supportive family and friends, and prayerful seeking of God's will in my life have led me further and further into this area of science.

Weinberg takes a flier on computing at ORNL

by Tim Gawne
gawnetj@ornl.gov

Scientific computing found a home at ORNL in 1947, less than five years after the lab was created by the Manhattan Project.

Alvin Weinberg, newly minted head of the Physics Division, shared his decision with Eugene Wigner, the lab's first research director, who by this time had returned to Princeton.

Weinberg's confidence in this computing experiment was underwhelming. "I have set up the mathematicians and computers in business for themselves with (mathematical biologist Alton) Householder in charge," Weinberg wrote to Wigner. "This is an experiment whose success is not necessarily assured."

Nevertheless, the Mathematics and Computing Section of the Physics Division was born. By the next year it morphed into the Mathematics and Computing Panel, with the mission of providing "a consulting service on mathematical, statistical and computational problems" for researchers at the lab.

This was not the computing organization we now know at ORNL, with supercomputers regularly among the world's most powerful. In fact, ORNL didn't have its own computer at all. Instead, the panel borrowed time on machines at other institutions: the IBM Model 604 calculators at Oak Ridge's two other federal installations and the Mark 1 at Harvard.

ORNL was eventually saved from having to beg for computer time when it acquired a hand-me-down machine from the canceled Nuclear Energy for the Propulsion of Aircraft project. It was only in the early '50s that the lab got into the high-performance computing game with ORACLE, the Oak Ridge Automatic Computer and Logical Engine.

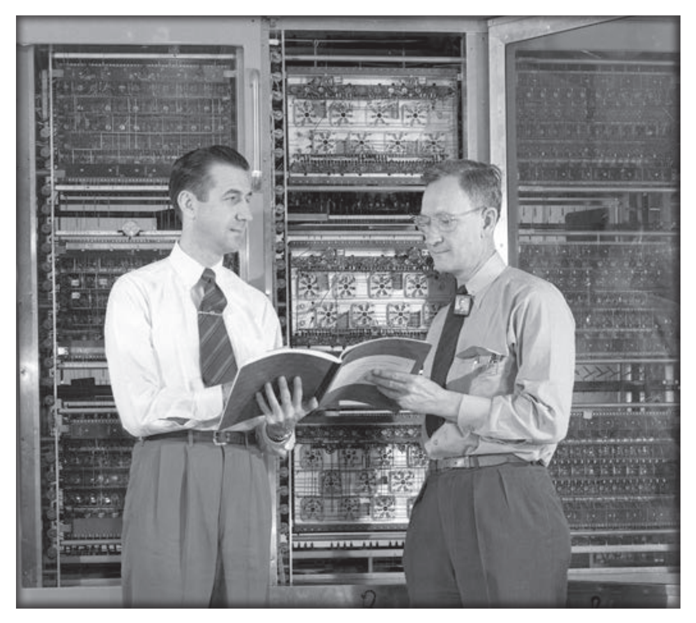
ORACLE, which became the world's fastest computer in 1954, owed its design to the godfather of modern computing, John von Neumann. In 1945, von Neumann and colleagues described an architecture that would be able to store and overwrite executable programs, thereby differentiating it from machines that were simply large calculators. Seven years later, a dozen members of ORNL's Instrumentation and Controls Division were holed up at Argonne National Laboratory to create ORACLE, with von Neumann serving as consultant.

We shouldn't read too much into the word "modern" here. This was not commodity computing; it was vacuum tube home brew at its finest.

After ORACLE was installed at ORNL, Householder did some globe-trotting—including visits to several European institutions—to see where the lab's new machine stood. "Whatever may be the reason for it," he concluded, "the machines now operating, and those under development, are generally relatively slow. Only three of those under development promise anything like ORACLE speeds."

Looking back, those days seem like ancient history, and, indeed, six decades is forever when you're talking about the world of computing. Householder is remembered with a named fellowship offered by the lab's Computer Science and Mathematics Group, and the vacuum tube–powered ORACLE seems almost quaint when compared to ORNL's Titan system, which can go through up to 27 million billion calculations each second.

Nevertheless, the two systems had identical purposes: to accelerate scientific discovery across disciplines utilizing world-class tools. Under the circumstances, one can reasonably conclude that Weinberg's experiment was a resounding success.



Earl Burnette of the I&C Division and A. S. Householder, chair of the Math Panel.

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