OAK RIDGE NATIONAL LABORATORY

Review

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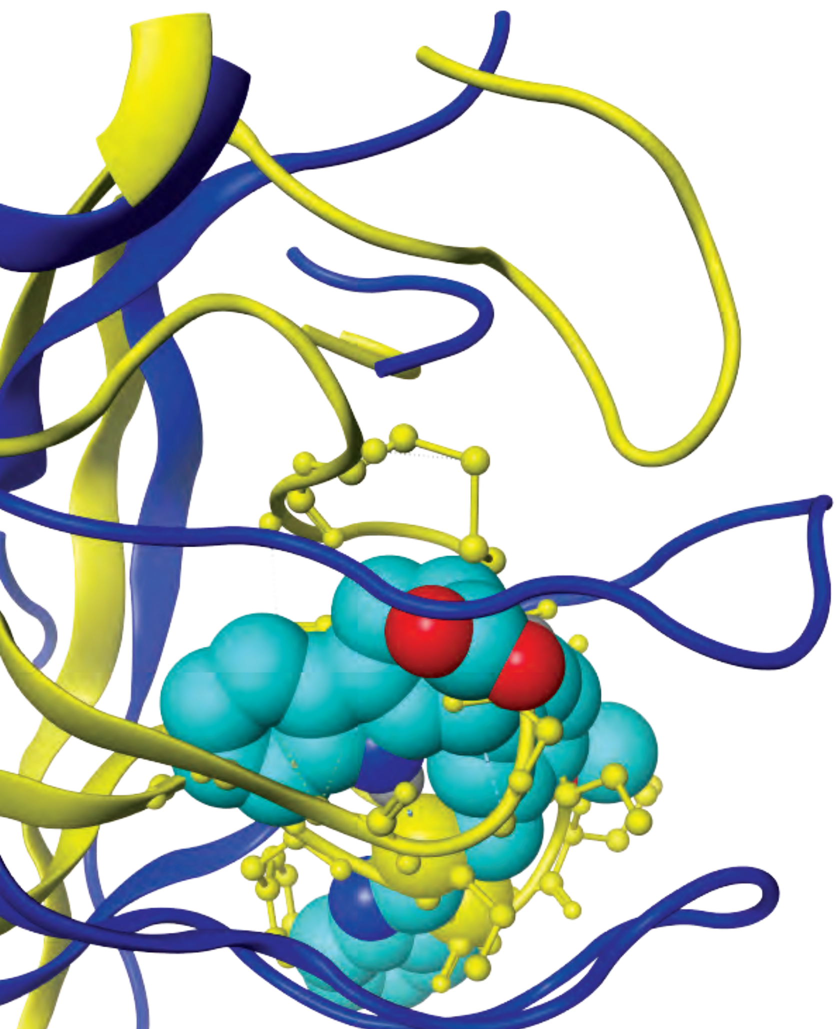


On the Cover

ORNL aquatic ecologist Terry Mathews leads studies on the concentration of mercury levels in water-based ecosystems.

ORNL science is helping the environment

Solutions to serious problems often demand new science and technology. This is especially true with environmental cleanup, where we must manage substances that are unpredictable or will be dangerous for millennia.

ORNL is in a unique position to contribute to these solutions. As the Department of Energy's largest science and energy laboratory, we are home to a collaborative and multidisciplinary community of highly skilled researchers and to some of the country's most powerful analytical tools.

We have reason to be confident in our abilities. Consider the ORNL-led Salt Waste Disposal Technologies Team, which developed a technology that removes radioactive cesium from waste at DOE's Savannah River Site, leaving only one part in 40,000. The team's approach, which includes both complex chemistry and engineered "cage" molecules, is turning millions of gallons of waste into a safer form.

In this issue, we highlight how ORNL's talented researchers and unique research environment are addressing some of the world's most perplexing environmental challenges.

The cesium-removal project won the research team a Secretary's Achievement Award from Energy Secretary Ernest Moniz. In another case, ORNL researchers are providing profound insight into the behavior of mercury in the environment, solving a puzzle that had perplexed scientists for decades. Lab scientists also used high-tech tools to develop a relatively low-tech—and inexpensive—approach to reducing the amount of uranium in groundwater.

Also in this issue, we explore a few of the many insights provided by ORNL's Titan supercomputer. A team led by the University of Illinois' Klaus Schulten has performed the largest biomolecular simulation ever—more than 100 million atoms. A team led by Jerome Baudry of ORNL and the University of Tennessee is pushing the boundaries of virtual drug testing, eliminating much of the time and expense of physical testing. In addition, a team led by Virginia Tech's James McClure is adding to our knowledge of the environment with an advanced simulation of the interaction of different types of material underground.

We also celebrate technical accomplishments from the present and the past. Recently, ORNL scientists announced development of an instrument that combines the capabilities of atomic force microscopes and mass spectrometers. Looking back, we examine the accomplishments of the Molten Salt Reactor Experiment, which operated for about five years in the 1960s, and the High Flux Isotope Reactor, which is 50 years old and still going strong.

Finally, we talk with talented young researchers about their science careers, and we hear from established scientists who joined us in recent months to participate in the Eugene P. Wigner Distinguished Lecture Series in Science, Technology, and Policy.

Thank you for your interest in *ORNL Review*. Enjoy the issue.

Thomas Mason

Thomas Mason
Laboratory Director

ORNL process could be white lightning to electronics industry

A new era of electronics and even quantum devices could be ushered in with the fabrication of a virtually perfect single layer of "white graphene," according to ORNL researchers.

The material, technically known as hexagonal boron nitride, features better transparency than its sister, graphene, and is chemically inert (non-reactive) and atomically smooth. It also features high mechanical strength and thermal conductivity.

Unlike graphene, however, it is an insulator instead of a conductor of electricity, making it useful as a substrate and the foundation for the electronics in cell phones, laptops, tablets and many other devices.

"Imagine batteries, capacitors, solar cells, video screens and fuel cells as thin as a piece of paper," said ORNL's Yijing Stehle, postdoctoral associate and lead author of a paper published in *Chemistry of Materials*. She and colleagues are also working on a graphene hexagonal boron 2-D capacitor and a fuel cell prototype that are not only "super thin" but also transparent.

With their recipe for white graphene, ORNL researchers hope to unleash the full potential of graphene, whose performance has not yet matched its theoretical value. With white graphene as a substrate, researchers believe they can help solve the problem while further reducing the thickness and increasing the flexibility of electronic devices.

While graphene, which is stronger and stiffer than carbon fiber, is a promising material for data transfer devices, graphene on a white graphene substrate features several thousand times higher electron mobility than graphene on other substrates. That feature could enable much faster data transfers.

"Imagine your message being sent thousands of times faster," Stehle said.

For more information: http://go.usa.gov/cKcG4

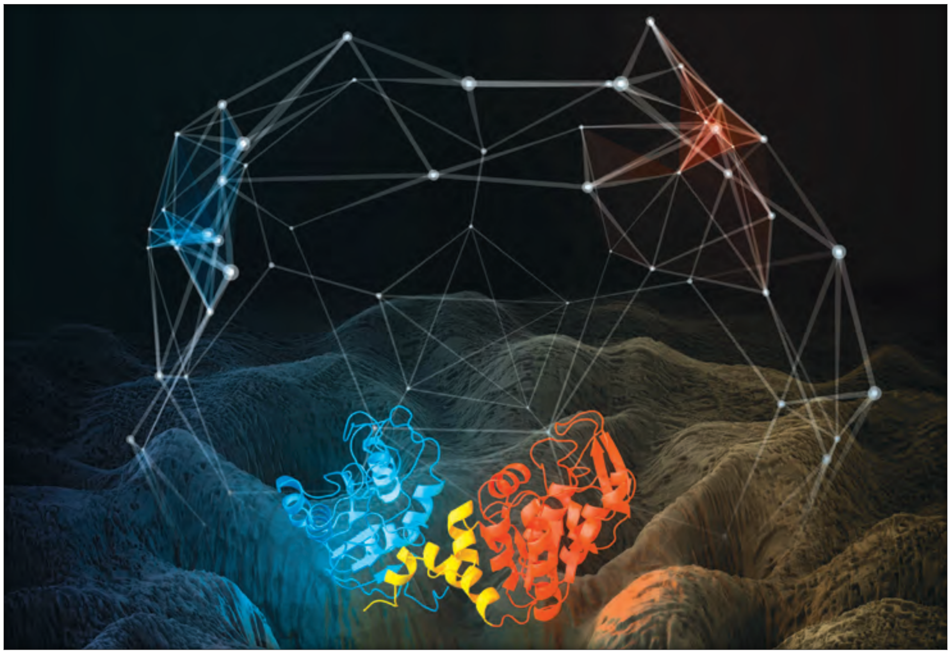


Illustration of the structure of a phosphoglycerate kinase protein that was subjected to molecular dynamics simulations. The relative motions of the red and blue domains of the proteins are highly complex and can be described in terms of motion of a configurational point on a rough energy landscape (illustrated). The transitions of the structure between energy minima on the landscape can be described in terms of a network (illustrated), which is found to be fractal (self-similar) on every timescale. Image credit: Thomas Splettstoesser, http://www.scistyle.com

Computing simulations look at protein dynamics

Supercomputing simulations at ORNL could change how researchers understand the internal motions of proteins that play functional, structural and regulatory roles in all living organisms. Research results are featured in *Nature Physics*.

"Proteins have never been seen this way before," said coauthor Jeremy Smith, director of ORNL's Center for Molecular Biophysics and a Governor's Chair at the University of Tennessee. "We used considerable computer power to provide a unified conceptual picture of the motions in proteins over a huge range of timescales, from the very shortest lengths of time at which atoms move (picoseconds) right up to the lifetimes of proteins in cells (roughly 1,000 seconds). It changes what we think a protein fundamentally is."

Studying proteins—their structure and function—is essential to advancing understanding of biological systems relevant to different energy and medical sciences, from bioenergy research and subsurface biogeochemistry to drug design.

Results obtained by Smith's University of Tennessee graduate student, Xiaohu Hu, revealed that the dynamics of single protein molecules are "self-similar" and out of equilibrium over an enormous range of timescales.

With the help of ORNL's Titan—the fastest supercomputer in the U.S., located at the Oak Ridge Leadership Computing Facility—Smith's team developed a complete picture of protein dynamics, revealing that the structural fluctuations within any two identical protein molecules, even if coded from the same gene, turn out to be different.

"A gene is a code for a protein, producing different copies of the protein that should be the same, but the internal fluctuations of these individual protein molecules may never reach equilibrium, or converge," Smith said. "This is because the fluctuations themselves are continually aging and don't have enough time to settle down before the protein molecules are eaten up in the cell and replaced."

For more information: http://go.usa.gov/cKct5

Oak Ridge dedicates National Historic Park

Oak Ridge recently dedicated the city's new Manhattan Project National Historical Park, memorializing the community's role in ending World War II.

"The Manhattan Project National Park has been a work in progress for the last decade," said Oak Ridge Mayor Warren Gooch. "It is going to honor tens of thousands of some of the most dedicated and hardest working people from all over the world who came here to work on the Manhattan Project, carried out their missions, and brought forth new things and new ways to help our country."

Niki Nicholas of the National Park Service, who will oversee the new Oak Ridge national park at the outset, said her agency looks forward to welcoming visitors to Oak Ridge.

"This is a very complex story to be told," Nicholas said. "It comes at the beginning of the National Park Service's centennial. The opportunities for the different issues to talk about and interpret are enormous."

Colin Colverson, attorney-advisor in the Department of Energy's Office of Chief Counsel, said the national park concept will build on the public tour opportunities that have been available in Oak Ridge during the past 20 years.

"The department is ready to take on its partnership with the park service in facility maintenance, safe access and the complex technical story that comes from the Manhattan Project," Colverson said.

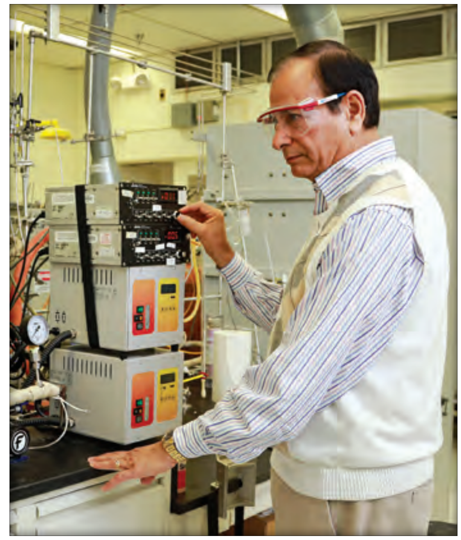
For more information: http://go.usa.gov/cQZ6G

ORNL study explains biofuel conversion

A new ORNL study explains the mechanism behind a technology that converts bio-based ethanol into hydrocarbon blendstocks for use as fossil fuel alternatives.

Scientists have experimented for decades with a class of catalysts known as zeolites, which transform alcohols such as ethanol into higher-grade hydrocarbons. As ORNL researchers were developing a new type of zeolite-based conversion technology, they found the underlying reaction unfolds in a different manner than previously thought.

"For 40 years, everyone thought that these reactions must go first from ethanol to ethylene, and then from there it forms longer chains. We were able to show that it's not how this occurs," said ORNL's Brian Davison, coauthor on the study published in *Nature Scientific Reports*.



Chaitanya Narula led analysis of an ORNL biofuel-to-hydrocarbon conversion technology to explain the underlying process. Image credit: Jason Richards, ORNL

The researchers' analysis found that this energy-consuming intermediary step is not necessary for the conversion to happen. Instead, an energy-producing "hydrocarbon pool" mechanism allows the zeolite catalysts to produce longer hydrocarbon chains directly from the original alcohols.

"It challenges a long-held but incorrect assumption," said ORNL coauthor Chaitanya Narula. "It has been assumed that you must go from ethanol to ethylene, which is endothermic and requires energy. We showed this step doesn't occur, and that the overall reaction is slightly exothermic."

ORNL researchers tracked the molecular transition in labeling experiments with deuterium, a hydrogen isotope, to confirm the hydrocarbon pool mechanism.

The research, supported by DOE's BioEnergy Technologies Office, has implications for the energy efficiency and cost of catalytic upgrading technologies proposed for use in biorefineries. Uncovering the mechanism behind the reaction helps support the potential economic viability of ORNL's direct biofuel-to-hydrocarbon conversion approach.

For more information: http://go.usa.gov/cKx2G

ORNL's historic Graphite Reactor is one of the Oak Ridge sites that are part of the Manhattan Project National Historical Park. Image credit: Lynn Freeny, DOE

Chemical complexity promises improved structural alloys

Designing alloys to withstand extreme environments is a fundamental challenge for materials scientists; energy from radiation can create imperfections in alloys.

In response, scientists in an ORNL-led research center are investigating ways to design structural materials that develop fewer, smaller flaws under irradiation.

The key, they report in the journal *Nature Communications*, is exploiting the complexity that is present when alloys are made with equal amounts of up to four different metallic elements.

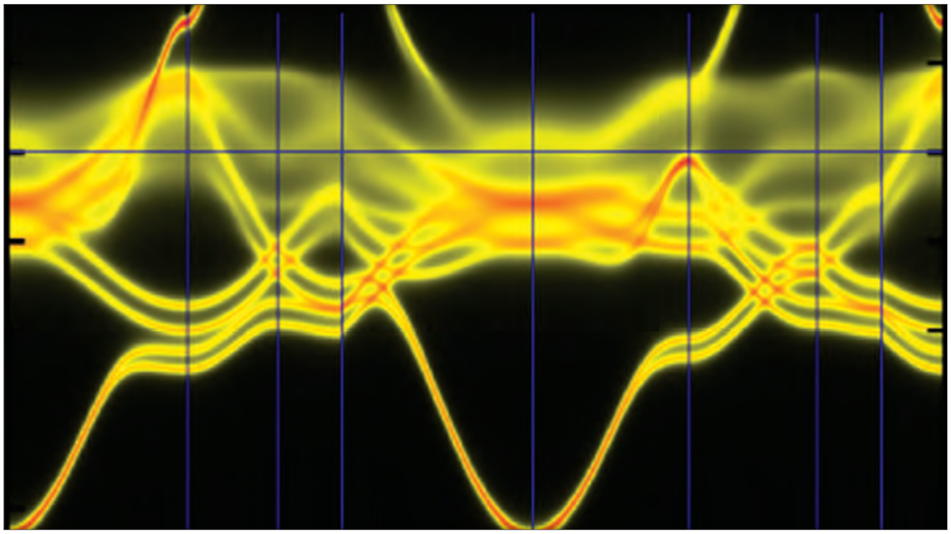
"Chemical complexity gives us a way to modify paths for energy dissipation and defect evolution," said first author Yanwen Zhang of ORNL and the University of Tennessee, Knoxville.

Zhang directs an Energy Frontier Research Center called "Energy Dissipation to Defect Evolution," funded by DOE's Office of Science. Partner institutions include Oak Ridge, Lawrence Livermore and Los Alamos national laboratories and the universities of Michigan, Wisconsin–Madison and Tennessee–Knoxville.

Radiation can harm spacecraft, nuclear power plants and high-energy accelerators. Nuclear reactions produce energetic particles—ions and neutrons—that can damage materials as their energy disperses, causing the formation of flaws that evolve over time.

The goal of the EDDE study was to find how compositional complexity can lead to differences in heat and electricity conduction and influence defect dynamics at early stages that affect the robustness of a structural material at later stages. The results revealed that advanced alloys achieve greatly enhanced irradiation performance through chemical diversity, optimizing electronic structure and atomic arrangements.

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

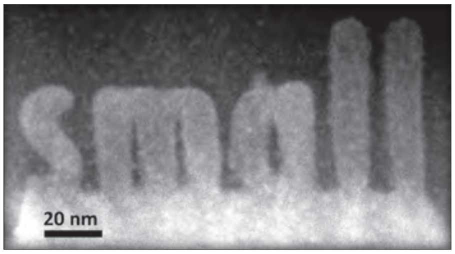


In complex alloys, chemical disorder results from a greater variety of elements than found in traditional alloys. Traces here indicate electronic states in a complex alloy; smeared traces indicate reduced electrical and thermal conductivity. Image credit: G. Malcolm Stocks, ORNL

Sculpting 3-D structures at the atomic level

Electron microscopy researchers at ORNL have developed a unique way to build 3-D structures with finely controlled shapes as small as one to two billionths of a meter.

The ORNL study, published in the journal *Small*, demonstrates how scanning transmission electron microscopes, normally used as imaging tools, are also capable of precision sculpting of nanometer-sized 3-D features in complex oxide materials.



ORNL researchers used a new scanning transmission electron microscopy technique to sculpt 3-D nanoscale features in a complex oxide material. Image credit: Stephen Jesse, ORNL

By offering single atomic plane precision, the technique could find uses in fabricating structures for functional nanoscale devices such as microchips. The structures grow epitaxially, or in perfect crystalline alignment, which ensures that the same electrical and mechanical properties extend throughout the whole material.

"We can make smaller things with more precise shapes," said ORNL's Albina Borisevich, who led the study. "The process is also epitaxial, which gives us much more pronounced control over properties than we could accomplish with other approaches."

ORNL scientists happened upon the method as they were imaging an imperfectly prepared strontium titanate thin film. The sample, consisting of a crystalline substrate covered by an amorphous layer of the same material, transformed as the electron beam passed through it. A team from ORNL's Institute for Functional Imaging of Materials, which unites scientists from different disciplines, worked together to understand and exploit the discovery.

"When we exposed the amorphous layer to an electron beam, we seemed to nudge it toward adopting its preferred crystalline state," Borisevich said. "It does that exactly where the electron beam is."

The use of a scanning transmission electron microscope, which passes an electron beam through a bulk material, sets the approach apart from lithography techniques that only pattern or manipulate a material's surface.

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

One instrument probes chemistry, topography and mechanics

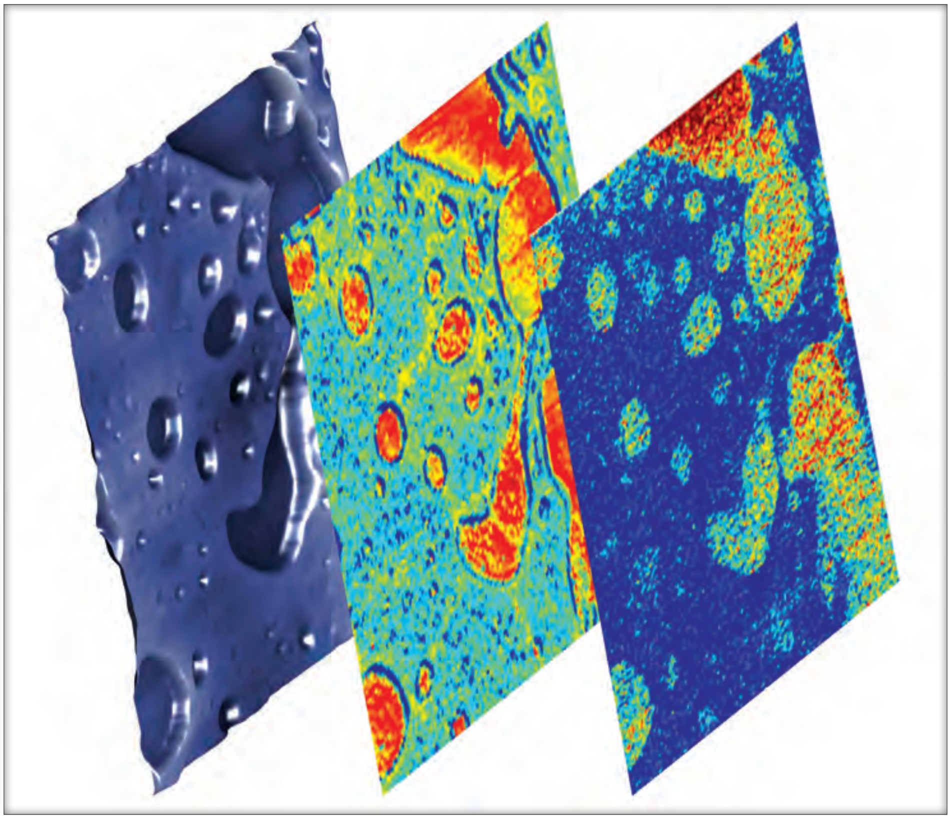
ORNL scientists have combined the cornerstone capabilities of atomic force microscopes and mass spectrometers into one instrument. Their all-in-one instrument can probe a sample in three dimensions and overlay information about surface topography, atomic-scale mechanical behavior near the surface, and chemistry at and under the surface. This multimodal imaging will allow scientists to explore thin films of phase-separated polymers important for energy conversion and storage.

"Combining the two capabilities marries the best of both worlds," said physicist Olga Ovchinnikova. "For the same location, you get not only precise location and physical characterization, but also precise chemical information." With mass spectrometrist Gary Van Berkel, Ovchinnikova co-led a study that tested the versatile instrument's ability to probe a thin polymer film that separated into islands of poly-2-vinylpyridine in a sea of polystyrene.

"This is the first time that we've shown that you can use multiple methods through the atomic force microscope," Van Berkel added. "We demonstrated for the first time that you could collect diverse data sets together without changing probes and without changing the sample."

In 2015, Anasys Instruments of Santa Barbara, Calif., received a phase-2 Small Business Innovation Research grant from the U.S. Department of Energy to couple atomic force microscopy and mass spectrometry in a commercial product. Such a device would bring multimodal imaging out of the rarified realm of national labs and into the larger scientific community.

Ovchinnikova envisions companies using the technology to answer fundamental questions about product performance. If a polymer blend—in a rubber tire or plastic bottle—is failing, why is it failing? In a stressed area, how are nanomechanical properties changing? What is the exact chemical composition at points of failure?



For a 500-nanometer-deep polymeric thin film made of polystyrene (lighter) and poly-2-vinylpyridine (darker), one multimodal instrument imaged, from left, surface topography, elasticity of the bulk material and buried chemical behavior. Image credit: ORNL

"This is something that atomic force microscopy by itself could *never* see. It could just see differences in mechanics, but it could never really tell you precise chemistry in a location," she said.

For more information: http://go.usa.gov/cQc5e

New web app makes science a little easier for ORNL researchers

ORNL researchers will soon get a tool that makes their jobs less complicated and allows them to focus more of their effort on science.

RESolution—short for "research" plus "solution"—is a portal application developed to simplify the interaction among research and other ORNL computing systems and to provide broad project management tools tailored for the research environment. The ultimate goal is to help staff do their jobs more efficiently, and with less frustration, so they can focus on science and technology.

The RESolution dashboard interface streamlines access to ORNL systems and provides a home base for keeping up with tasks. Users can see items awaiting action and receive alerts about approaching events, such as expiration dates, deadlines, and funding limits. RESolution allows users to make decisions, track progress, and take action from their desktop or mobile device.

This advanced web application was developed by ORNL Information Technology staff and Knoxville, Tenn.-based software engineering firm Cadre5. It was the overall winner of the 2015 Excellence.Gov Awards, given by the American Council for Technology-Industry Advisory Council to honor the best government information technology programs.

RESolution was developed with lab-wide input from researchers, support staff, and lab leadership and benefitted from months of testing by 200 research and administrative staff.

Finding scientific solutions to environmental problems

by Leo Williams
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Over four decades in operation, the Hanford Site in eastern Washington state had as many as nine nuclear reactors at a time working with five processing complexes to produce plutonium for America's nuclear arsenal.

On the other side of the country, the Savannah River Site in South Carolina had as many as five reactors working through the Cold War to produce tritium and plutonium for the weapons program.

This security and nuclear research effort has produced wastes that are now the focus of a massive cleanup effort by DOE across several research and production facilities. Just between these two particular sites, hundreds of tanks now hold 90 million gallons of radioactive waste, enough to fill more than 130 Olympic-size swimming pools. Add to that millions of cubic feet of solid waste and tens of square miles of contaminated groundwater, and you get a feel for the agency's greatest environmental challenge.

"The needs are just enormous," said Michelle Buchanan, ORNL's associate laboratory director for physical sciences. "The tanks alone represent some of the toughest chemistry on the face of the earth. These wastes are a true witch's brew of chemicals."

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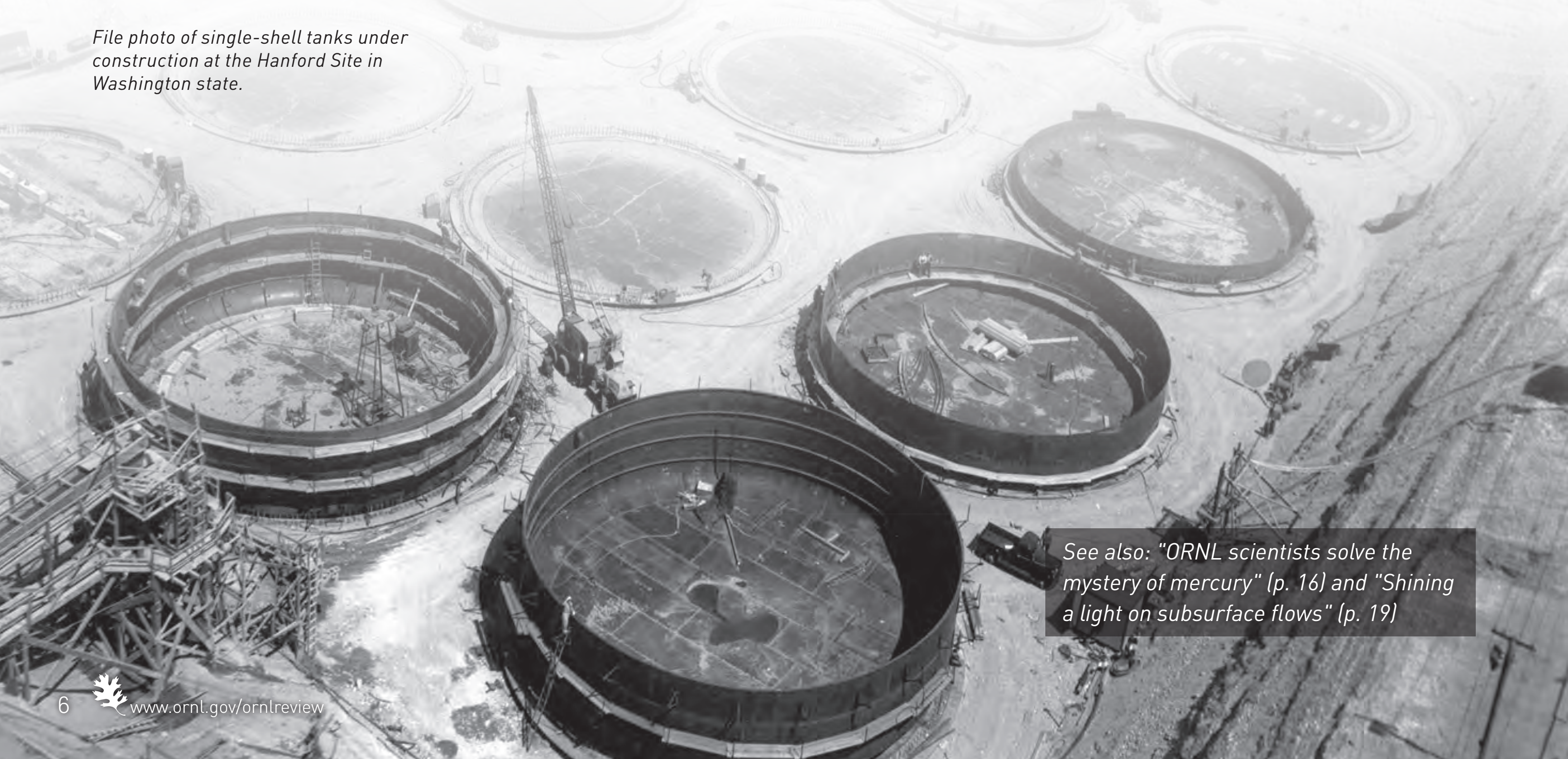

File photo of single-shell tanks under construction at the Hanford Site in Washington state.

See also: "ORNL scientists solve the mystery of mercury" (p. 16) and "Shining a light on subsurface flows" (p. 19)

The Salt Waste Disposal Technologies Team receives a 2013 Secretary's Achievement Award from Energy Secretary Ernest Moniz.

ORNL process isolates troublesome cesium

by Leo Williams
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A scientific breakthrough by ORNL researchers is allowing millions of gallons of dangerous waste in South Carolina to be removed from the environment and processed for safe disposal.

The waste is a toxic, highly radioactive soup left over from the Savannah River Site's days creating and processing plutonium. Thirty-seven million gallons was created in a process (invented at ORNL) known as PUREX, for "plutonium and uranium redox extraction."

The straightforward part of the cleanup has long since been completed. By raising the pH level of the waste with sodium hydroxide, the site's overseers induced all but one of the most radioactive isotopes to drop to the bottom of the tanks as a sludge. The sludge has been sluiced out and is being turned into glass through a process called vitrification.

But that remaining isotope, cesium-137, was not so cooperative, remaining soluble in the salt portion of the waste. Its presence meant that the bulk of the waste was still highly radioactive, and regulators have demanded that it be separated and vitrified as well.

Science to the rescue

To remove the cesium, ORNL scientists developed a solvent-extraction process that uses both complex chemistry and engineered molecules to isolate, transfer, and ultimately concentrate the isotope. At that point, it is ready to be combined with other radionuclides and vitrified.

The scientists' chemical achievement, as scaled up, demonstrated, and implemented at SRS, earned the 76-member Salt Waste Disposal Technologies Team a 2013 Secretary's Achievement Award from Energy Secretary Ernest Moniz.

Team leader Bruce Moyer of ORNL's Chemical Sciences Division said the accomplishment is noteworthy at least in part because ORNL's impact had grown

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Researchers use soybean oil

to reduce uranium in groundwater

by Leo Williams
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Soybean oil is especially versatile. It fries chicken. It makes a tasty salad dressing. Believe it or not, it can remove uranium from groundwater, too.

ORNL investigators have developed a method for reducing both nitrate and uranium in groundwater by using the energy found in soybean oil. Their approach is simpler, cheaper and less disruptive than traditional alternatives such as excavation and pump-and-treat technologies.

"It's one of those things that is really elegant; there's a lot of beauty in it," explained ORNL geochemist Scott Brooks.

Brooks, hydrogeologist David Watson and microbiologist Chris Schadt developed their approach while working with a disposal site at the nearby Y-12 nuclear weapons plant. The site, known as the S-3 ponds, was used from the early 1950s to the early '80s to hold liquid waste from uranium operations. Although the ponds have since been cleaned up and capped—the site is now a parking lot—a plume of contaminated groundwater extends several miles from the ponds.

That plume was the focus of a field research center sponsored by DOE's Biological and Environmental Research program, with researchers looking for ways to understand and manipulate the interaction of chemistry, microbes and contaminants in groundwater. The center hosted investigators from around the country and sent samples of contaminated soil and groundwater to facilities around the world.

The soybean oil approach—Brooks and his colleagues refer to it as emulsified vegetable oil, or EVO—grew from a focused exploration among ORNL researchers. While the technique itself appears low-tech, the process to develop it was not. Along the way they took advantage of cutting-edge analysis tools, especially the Advanced Photon Source at Chicago's Argonne National Laboratory.

"It went from very basic fundamental laboratory studies to applying it in the field and taking a look at the coevolution of the chemistry and the biology," Brooks said.

"We would write our concept on a blackboard and say, 'We think if we do this, that should happen, and if that happens, this should happen.' Then we worked to solidify all that into a robust mathematical model, so we could say, 'If we add exactly this much, we ought to see exactly that amount of change.'"

> *"It went from very basic fundamental laboratory studies to applying it in the field and taking a look at the coevolution of the chemistry and the biology."*
>
> —Scott Brooks, ORNL geochemist

The soybean oil is emulsified—converted to small droplets to penetrate more deeply into the groundwater. It doesn't reduce either the nitrate or the

ORNL technician Tonia Mehlhorn with buckets of soybean oil used to treat uranium in groundwater. Image credit: David Watson and Kenneth Lowe, ORNL

uranium directly. Rather, it feeds useful microbes that are already in the soil. First, the team needed to tackle the nitrate, relying on bacteria known as nitrate reducers. The bacteria are anaerobic, meaning they don't need oxygen. Rather, they rely on nitrogen in the acid, transferring energy to and from it in the same way other organisms do with oxygen.

"We normally think of living things as requiring oxygen to live," Brooks said. "Your body uses oxygen as a place to dump electrons, and its cells harness energy from that. Bacteria have much broader capabilities. They still generate energy by moving electrons through their cell machinery, but in the absence of oxygen they have to put those electrons someplace else. And nitrate reducers put those electrons into nitrate and reduce it into nitrite or nitrous oxide."

Not only do the nitrate reducers act on the nitrate, they also break down fats within the oil and make them available for the next stage in the cleanup: reducing uranium.

"Many metal-reducing bacteria can reduce uranium, either directly or indirectly," Brooks said. "In some cases, they produce reduced iron that can chemically reduce the uranium."

The microbes don't change uranium into something else. Rather, they cause it to stick to particles in the ground or to simply precipitate out of the water, much as the salt in a glass of saltwater eventually drops to the bottom of the glass.

So far, it looks like the oil does just that. Researchers found that a single injection of the oil reduced the nitrogen and uranium for a year and can keep uranium levels in the water low enough that it's not a hazard to people who consume that water.

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Nuclear legacy

DOE has worked for decades to clean up its nuclear legacy, and the effort has been largely successful. Starting with more than 100 contaminated sites in 1989, the agency has completed cleanup at all but the 16 most challenging.

The remaining sites—which include some at DOE's Oak Ridge facilities—are the toughest. In some cases they are prohibitively expensive to address using existing technology; in others, the technology just doesn't exist. Consider, too, that radioactive waste will need to be isolated for thousands of years, and you can see the need both for new research and for strategies that make use of recent discoveries.

It's a challenge in need of new solutions, some of which will certainly come from the agency's largest science lab, ORNL. ORNL hosts unique and powerful research tools, including the world's second most powerful supercomputer, the world's most intense reactor-based and pulsed neutron beams, and a variety of world-class scanning probe and scanning transmission electron microscopes. It also provides a collaborative environment for talented chemists, environmental scientists, engineers, geologists, biologists, materials scientists, physicists and computational scientists to put their heads together to solve common problems.

State of flux

Of all of DOE's environmental challenges, the most vexing are the waste tanks, which hold a mishmash of highly radioactive, chemically hazardous and often corrosive substances. Some are liquid, some sludge, and even if you could analyze them completely, they are in a state of constant flux.

"A big need is to characterize those tanks, and to do it on a continuous basis," Buchanan said. "The tanks are not in equilibrium. Things are always changing. So being able to come up with new sensors and analytical techniques where you can remotely and in situ [in place] monitor concentrations and speciation [chemical form] is very important."

Ultimately, the tank contents must be treated—meaning the most radioactive materials must be pulled out and put into the most stable form possible—and disposed of in such a way that they're unlikely to harm us or our descendants.

There are other problems, too. DOE must grapple with groundwater contamination at a number of sites, as contaminant plumes move toward public water supplies (See "Researchers use soybean oil to reduce uranium in groundwater," page 8). Groundwater is also a key concern for long-term storage, as investigators face the likelihood that even the best-engineered waste storage is bound to fail over the course of

"The tanks alone represent some of the toughest chemistry on the face of the earth. These wastes are a true witch's brew of chemicals."

—ORNL Associate Laboratory Director for Physical Sciences Michelle Buchanan

Computers and tanks

The waste tanks at Hanford and Savannah River may not be DOE's only environmental challenge, but they're at the top of the list.

Hundreds of tanks hold 90 million gallons of highly radioactive, extremely toxic liquids and sludges. The tanks are in constant flux, although they are nowhere near evenly mixed. Not only do we not know what to do with many of them; we're also still working to figure out exactly what's in there.

Supercomputing may help us better understand the problem and eventually solve it.

ORNL is home both to the world's second most powerful supercomputer, Titan, and to deep expertise in data analysis. Indeed, supercomputing is the only tool that can take data at wildly different scales—from quintillionths of a second to hundreds of years, say, or from individual atoms to areas the size of a refrigerator—and tie them together.

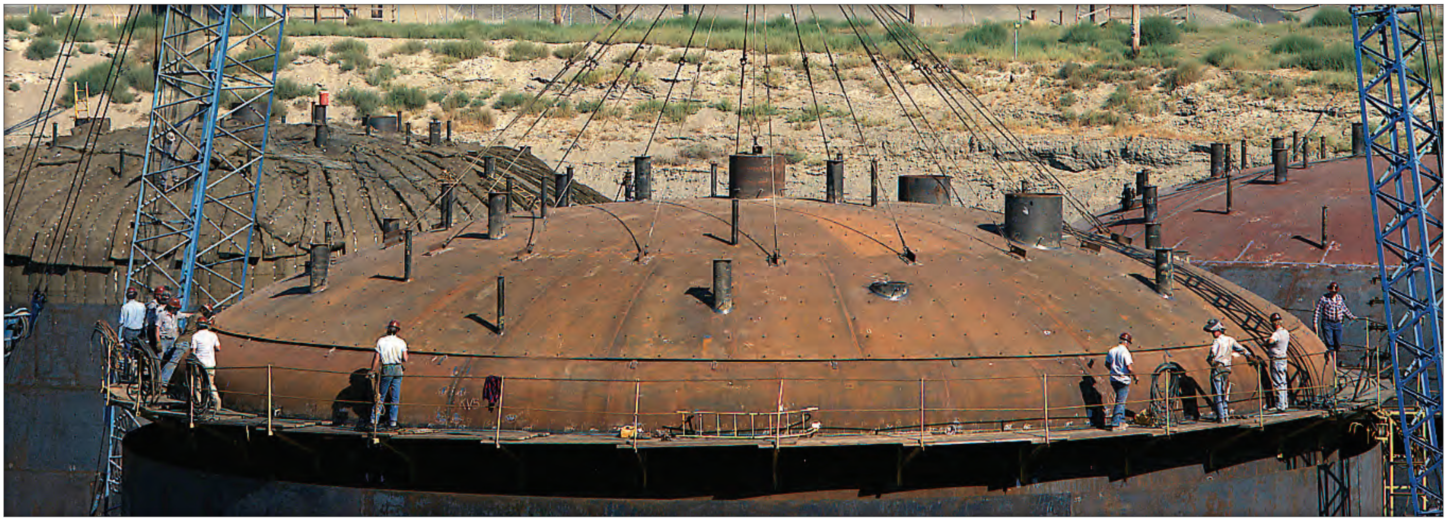
"Can we model all of those complexities to the level of accuracy where it would be useful for cleanup and risk assessment? Maybe not," said Bobby Sumpter, a computational chemical physicist at ORNL. "It is an area ripe for forefront-pushing. We're beginning to realize that we do have a lot of data and we do have models. We should be able to make each of them better."

It's an approach made possible by the phenomenal growth in computing power, he said. Today's most powerful computers are more than 100 times faster than those of a decade ago and more than 100,000 times faster than those of a decade before. Even so, Sumpter said, the problem will ultimately require machines dozens of times more powerful than today's top systems: exascale machines capable of more than a billion billion calculations each second.

"This is an exascale computing problem," he said. "It's not that you have an exascale computer and solve the problem. It's that you have an exascale computer, and you get the pieces of the models, and you incorporate the data you have to collect. It's a major effort."

Still, he said, such an effort would have been unthinkable not so long ago.

"They're trying to get this from where it is now to where it needs to be, realizing that we do have computer power to support it. Ten years ago, there was no chance that we could do that; the computer power wasn't there."



File photo of Hanford tank.

centuries. Converting the wastes to more stable forms and packaging them in highly corrosion-resistant containers represent major challenges for materials and corrosion scientists, but no material will be stable forever.

"The radionuclides eventually will get released—the repositories will collapse, the canisters will be breached, the cladding on spent fuel rods will decompose, and these things will get released into the local environment," explained ORNL geochemist David Wesolowski.

"Then the next question is, how long is it going to take?" Wesolowski said. "Once you get to the ultimate point to where the radioactive waste is exposed to the groundwater, how long is it going to take for it to migrate to places we care about?"

These and other challenges prompted the Secretary of Energy's Advisory Board earlier this year to gather scientists from national laboratories and universities around the country. Their task was to consider how scientific progress over the last decade or so can address these long-term problems. The Environmental Management Basic Research Needs Workshop Report will identify the risks and the science and technology needs that will help chart the roadmap for future federal funding to address these needs.

"The nice thing about the workshop is it brought together people with experience working with environmental management issues and people who are just good scientists who love to solve problems," Buchanan said.

"It's some of the most challenging science you can think of. Not only is it a great need; it's also fascinating science."

Rocks and neutrons

The world below our feet can be as important as the one we see around us. It provides much that we need, including drinking water, but it also carries contaminants that poison that water.

Much of what we know about underground contamination comes from scientists such as geochemist David Wesolowski and his group at ORNL. Using unique tools such as the neutron scattering capabilities at ORNL's Spallation Neutron Source and High Flux Isotope Reactor, Wesolowski and his colleagues see rocks very differently from the way most of us do.

"You can think of rocks as like a sponge," he said, "with pores ranging from very small, nanometer [billionth of a meter] size, to large cracks and pores you can see with your eyes."

When you look at how water flows through rock, it's important to know what gets trapped and what flows through: these are concepts known as porosity and permeability. As it turns out, neutrons are great at answering those questions. Neutrons penetrate deeply into matter, giving scientists a detailed, three-dimensional picture of rock sections, even ones that are contained within a pressure vessel to simulate conditions deep below ground.

One especially revealing technique involves deuterium, also known as heavy water. The hydrogen atoms in deuterium have a proton and a neutron in their nuclei, unlike those in common water, which have a proton but no neutron. While the two forms of water behave the same, they are easily distinguished in a neutron-scattering experiment.

If you flood a rock with regular water, let it drain and then flood it with deuterium, neutron scattering shows you which pores are connected and which are not.

"The neutrons give you a picture of the pore structure," Wesolowski said. "If those pores are filled with water, and that water can be replaced by heavy water, then you get a different scattering."

CESIUM from page 7

out of its science spinning off into environmental management.

"ORNL has really a lot to crow about," Moyer said. "This isn't our waste, and we don't really have a very big EM program at the lab.

"What we are strong at is science. We'd been studying this kind of chemistry for 10 years before we even started on the waste cleanup problem. And so when the real problem came along, we were ready to jump in and make this chemistry work, which no one else really had done."

The key to the process is a molecule known as a calixarene–crown ether, which takes a ring-like calixarene molecule and adds a separate crown ether molecule to cap one end, thereby creating a cage. After much work, the team came up with a cage molecule so effective that it captures nearly all of the cesium while leaving other elements almost entirely alone.

As good as the cages are, however, they need help. Over the course of a decade and a half, the team had to clear some very complex hurdles.

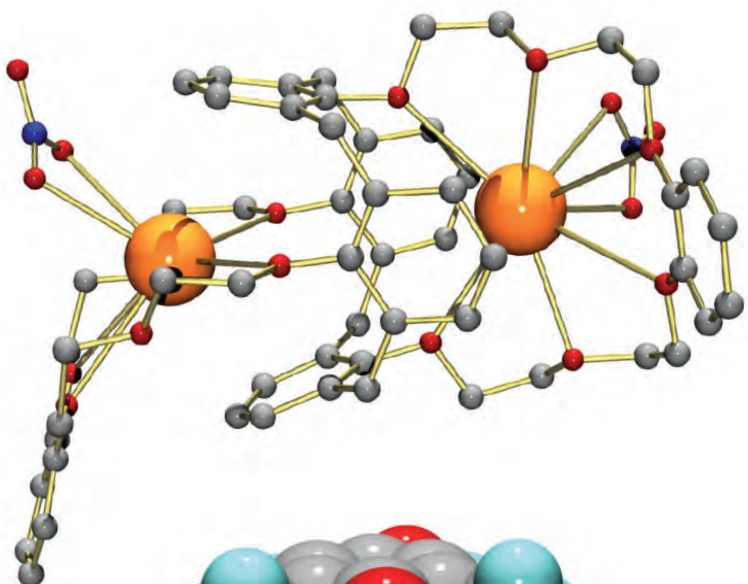
"There are no royalties involved, even though its impact is billions and billions of dollars. It, therefore, doesn't show up in the lab's commercialization metrics, but it's one of ORNL's biggest commercial successes."

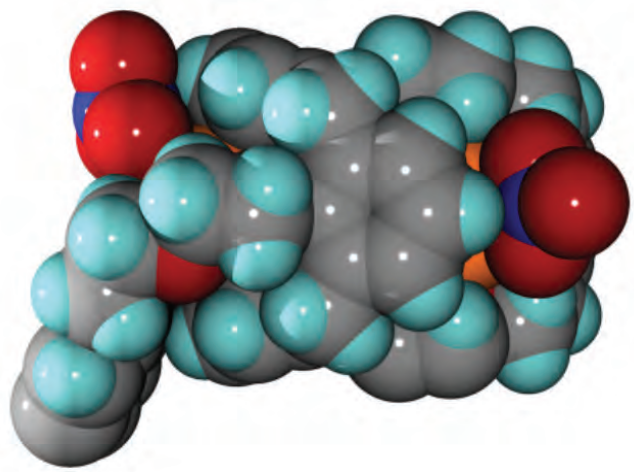
—ORNL chemist Bruce Moyer

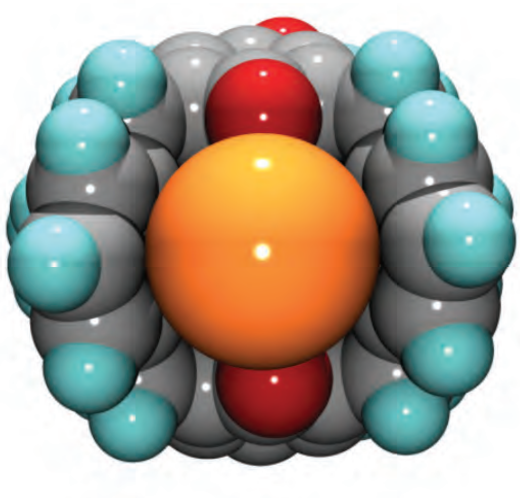
Challenges to overcome

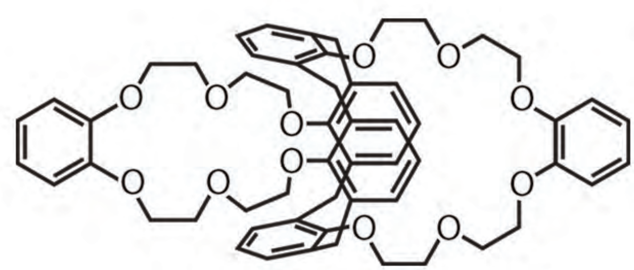
For instance, the cage molecules are contained in a solvent called Isopar L, but cesium ions won't go into the solvent unless they are paired with negatively charged ions. So the team added a modifier to the solvent that brings in nitrate anions found within the waste salt solution. Moyer credits Peter Bonnesen, a chemist now with ORNL's Center for Nanophase Materials Sciences, with engineering the clever structure of this modifier, for which ORNL holds a patent.

In addition, the cesium had to be coaxed out of the cage molecules and









Researchers took a ringlike calixarene molecule and capped it at one end with a crown ether molecule to create the perfect cesium trap. After they trap the cesium contained in tank waste, the calixarene–crown ethers are removed from the waste, cesium ions are separated from the traps, and the traps are reused.

Separating and treating cesium: the process

STEP 1: Getting to the cesium

1. Start with a kerosene solvent called Isopar L.

   The kerosene acts as the oil in an oil-and-water approach.

2. Add calixarene–crown ether cage molecules.

   Calixarenes are ring-like molecules. When they are capped at one end with a crown ether molecule, the resulting cage captures cesium so well that it ignores other elements in the waste such as potassium and sodium.

3. Add a solvent modifier called Cs-7SB

   The cesium ions must be paired with negatively charged ions—especially the abundant nitrate anions in the waste—before they can be coaxed into the solvent. The solvent modifier brings in the nitrates.

4. Effectiveness: 99.9975%

   In other words, the combination of solvent, solvent modifier and cage molecules pulls out nearly all of the cesium, leaving only one part in 40,000.

STEP 2: Separating the cesium from the cage molecules and solvent solution

1. Add a substance called guanidine to the solvent and then strip it with boric acid that has been mixed with water.
   The solvent solution costs about $10,000 a gallon. That means you have to reuse it, and that in turn means you have to remove the cesium. Guanidine causes the cesium ions to pop out of the cage molecules, and boric acid strips them out of the solvent.

STEP 3: Dispose and reuse

1. Send the boric acid and cesium off for vitrification.

   The cesium is now in the boric acid and ready to be turned into a glass through a process called vitrification.

2. Send the treated solvent back for reuse.

removed from the solvent. That took two approaches: first, a molecule that makes In addition, the cesium had to be coaxed out of the cage molecules and removed from the solvent. That took two approaches: first, a molecule that makes the cesium ions pop out of the cage molecules, and second, a boric acid stripping solution that pulls the released cesium out of the solvent.

The process has gone through two iterations, with the first removing 99 percent of the cesium. This was better than the original requirement of about 92 percent, but Moyer and others wanted to do much better. The revised solvent, known as NGS, or "Next Generation Solvent," includes a more soluble calixarene molecule for capturing the cesium as well as guanidine for stripping cesium out of the solvent.

This improved efficiency better than a hundredfold, to 99.9975 percent, so that the process leaves behind only one part in 40,000 of cesium in the original waste.

Using the tools of science

To get to this achievement, the team used a variety of scientific tools, including organic synthesis, X-ray crystallography, nuclear magnetic resonance spectroscopy, radiometric tracer methods, and computational modeling.

Engineers collaborating on the project—including Joe Birdwell at ORNL, Mark Geeting at SRS, Terry Todd at Idaho National Laboratory, and Monica Regalbuto and the late Ralph Leonard at Argonne National Laboratory—scaled up the process using centrifugal contactors, and Sam Fink's group at Savannah River National Laboratory was instrumental in testing and demonstration.

"You name it, and our team did it," Moyer said. "We studied the structure of the complexes of cesium nitrate and other metals with a couple dozen calixarene–crown ethers. We had a couple of really good organic chemists, and we got to be experts at the synthesis. Then we studied the structure using X-ray crystallography and NMR spectroscopy.

"Then we did the thermodynamics—basically figuring out how strong is the extraction and what is the chemical way you can describe and model the extraction."

The project is using a pilot facility at SRS while the $2 billion-plus Salt Waste Processing Facility is being constructed. Moyer said the project is an enormous achievement in technology transfer for ORNL, even though it is a government-use application rather than a commercial one and brings in no licensing fees.

"There are no royalties involved, even though its impact is billions and billions of dollars. It, therefore, doesn't show up in the lab's commercialization metrics, but it's one of ORNL's biggest commercial successes."

Vehicle analysis without the vehicle

ORNL's **Vehicle Systems Integration Laboratory** evaluates new vehicles before they exist. Simulated real-world conditions combine with advanced data collection to give engineers the information they need, both on individual components and on entire systems. As a result, they can create high-performance, energy-efficient designs quickly and at minimal cost.

How can we make vehicles cleaner and more efficient?

Rising fuel consumption and clean air regulations necessitate more aggressive research into advanced vehicle components and integration.

Annual consumption of petroleum by vehicles in US (2014): 200 billion gallons

- 200 billion gallons of petroleum consumed = 1.5 times the volume of Sydney Harbor

Annual CO_2 emissions by vehicles in US (2014): 4 million pounds

- 4 million pounds = 267 African elephants

Potential savings from 2025 fuel standards: $1.7 trillion

- $1.7 trillion = $5,000 for every U.S. citizen

Components

Improving efficiency, durability and cost while making components lighter and smaller.

Engine/generator
Produces power by burning gasoline or other fuel

Electric motor
Produces power from electricity

Transmission
Transfers power from the engine/motor to the drive wheels

Battery/fuel cell
Powers the electric motor

Powertrain
Group of components that generates power and deliver it to the drive wheels

After-treatment systems
Reduce harmful emissions (e.g., catalytic converter)

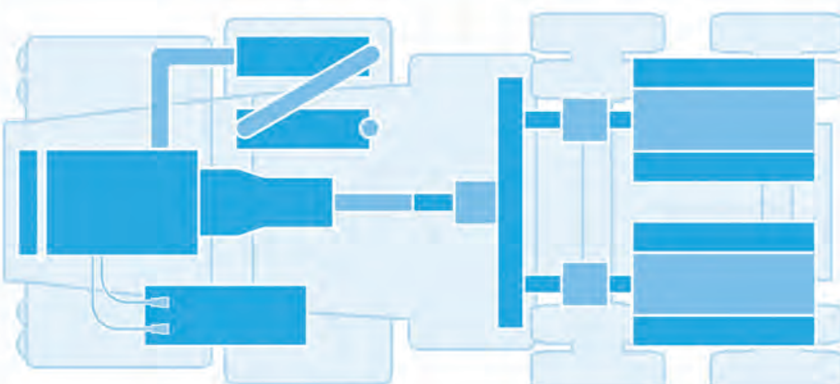
Simulating vehicles of all types and sizes.

Driving style

Whether you're a lead foot or a defensive driver, going up the side of a mountain or tooling along the plains, we can simulate it.

Test laboratory

Components believe they're in an operating vehicle. Sophisticated instruments monitor emissions and efficiency.



Benefits of the VSI Lab approach

- Cost-effective
- Repeatable
- Safer
- Realistic

Future transportation

Not only does the lab evaluate vehicles that have yet to be built, it also works with advanced combustion modes and other technologies that may not yet be market-ready. As a result, your dream car of the future may already be taking a virtual spin at ORNL.

Scientists Scott Brooks and Carrie Miller collect water quality data in East Fork Poplar Creek, sampling the site for mercury. Image credit: Jason Richards, ORNL

ORNL scientists

solve the mystery of mercury

by Ashanti B. Washington
ORNLReview@ornl.gov

Oak Ridge has a unique relationship to the science of mercury contamination. In the 1950s and '60s, the city's Y-12 nuclear weapons plant released around 350,000 pounds of mercury into local waterways, making the region a de facto laboratory for mercury in the environment.

Today, four Oak Ridge National Laboratory scientists are collaborating on landmark mercury research that gives policymakers and people across the world a better understanding of mercury's insidious behavior in the environment—and how to clean up contaminated water, soil and infrastructure.

As it encounters streams, soil and organisms, inorganic mercury transforms to a more toxic, organic form called methylmercury, which is linked to birth defects and other health concerns. Organisms can readily absorb this methylated form of the contaminant, causing it to linger in the environment.

ORNL geochemist Eric Pierce, an expert in the migratory patterns of mercury and other metal pollutants, hopes to limit this lingering effect by preventing methylmercury from moving or seeping deeper into the earth. The trickiest issue, he says, is that the contaminant's change between forms can affect its movement—making a blanket solution nearly impossible.

Instead, Pierce looks at promising combinations of on-site technologies to restrain mercury.

One method, for instance, encapsulates mercury by mixing a stabilizing compound with tainted soil. The technique could be used alongside tools such as reactive caps, or fabric layers interspersed with a material that chemically traps mercury.

"Ultimately, we're figuring out the right combination of on-site treatment technologies that keep local ecosystems thriving," Pierce says.

Helping to understand the role of methylmercury in ecosystems is Terry Mathews, an aquatic ecologist in ORNL's Environmental Sciences Division. She's part of the Biological Monitoring and Abatement Program, leading studies on the concentration levels of mercury in water-based ecosystems.

"For over 30 years, we've been gathering data, testing more than 40 sites along the watersheds and aquatic bodies in East Tennessee," she says. "My team and I monitor the diversity and abundance of regional aquatic species to understand when and how mercury is transferred from contaminated water to aquatic microorganisms to the top rung of the food chain."

Using the state's impressive diversity of freshwater organisms, Mathews and her team made a puzzling discovery.

"It's actually counterintuitive," she said. "Even though we have drastic reductions in aqueous mercury concentrations, methylmercury levels in fish have remained elevated."

The key to understanding how species amplify mercury levels is smaller than you'd think, according to Dwayne Elias, a microbiologist in ORNL's Biosciences Division.

Zooming in on microbes and tiny creatures like periphyton and algae at the base of the food chain, Elias is part of a team that uncovered the gene "switch" underlying mercury's transformation into its neurotoxin form. He has since found the switch in nearly 1,500 global environments, from the ocean floor to the Arctic permafrost.

"For the last 40 years, people have been trying to identify the genes and proteins that control the methylation process to create this very toxic compound," says Elias. "ORNL accomplished this in five years."

"For the last 40 years, people have been trying to identify the genes and proteins that control the methylation process to create this very toxic compound. ORNL accomplished this in five years."

—ORNL microbiologist Dwayne Elias

ORNL geochemist Scott Brooks isn't worried about microbes in frosty locales. He's focusing on the contaminant and organisms in ORNL's own backyard along East Fork Poplar Creek.

"I identify where in the ecosystem methylmercury is generated, its characteristics, and how to use that information to change how it's formed, or how we remediate it," Brooks says.

Brooks leads a team that studies the activity of mercury at specific sites, identifying chemical compounds that interact with mercury in the ground. Underground are subsurfaces, or zones where mercury density varies wildly, requiring a nuanced treatment approach. It's a huge problem.

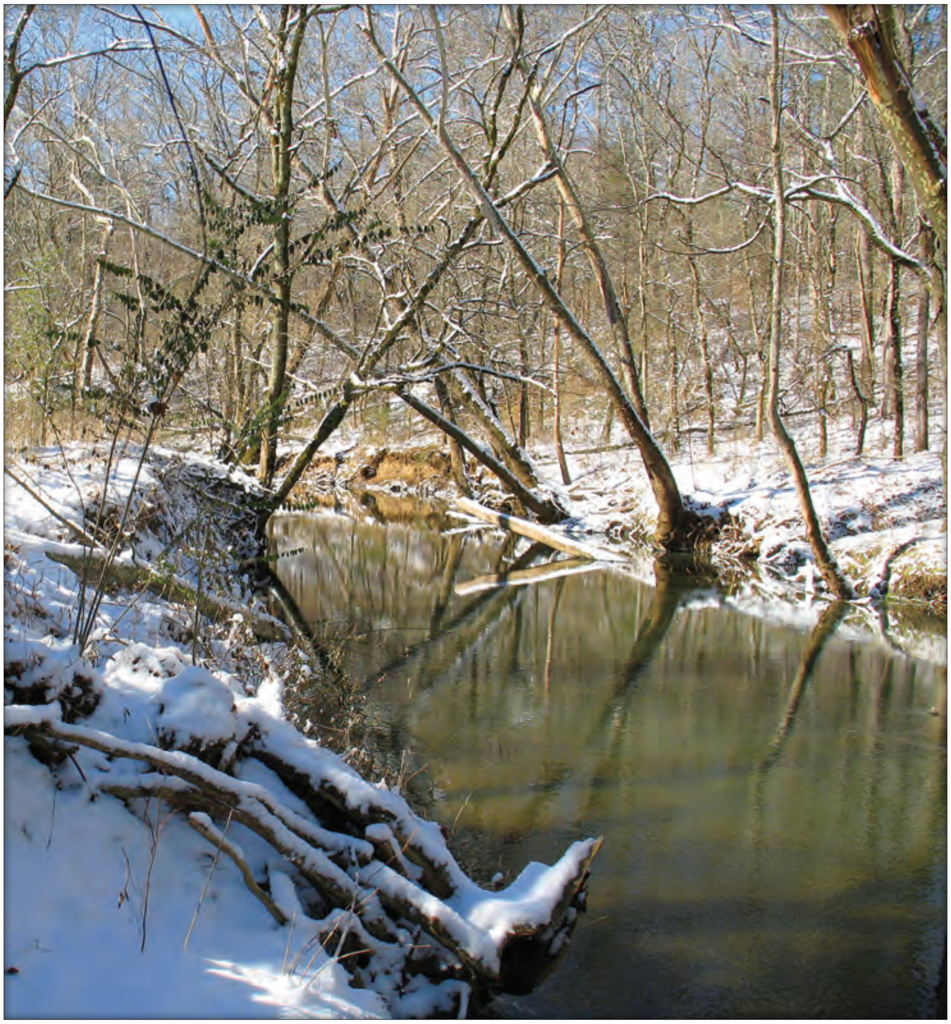
"To be fair, the world has been looking for a solution to remediate mercury contamination for a long time," Brooks said.

ORNL's collaborative culture has accelerated understanding of mercury.

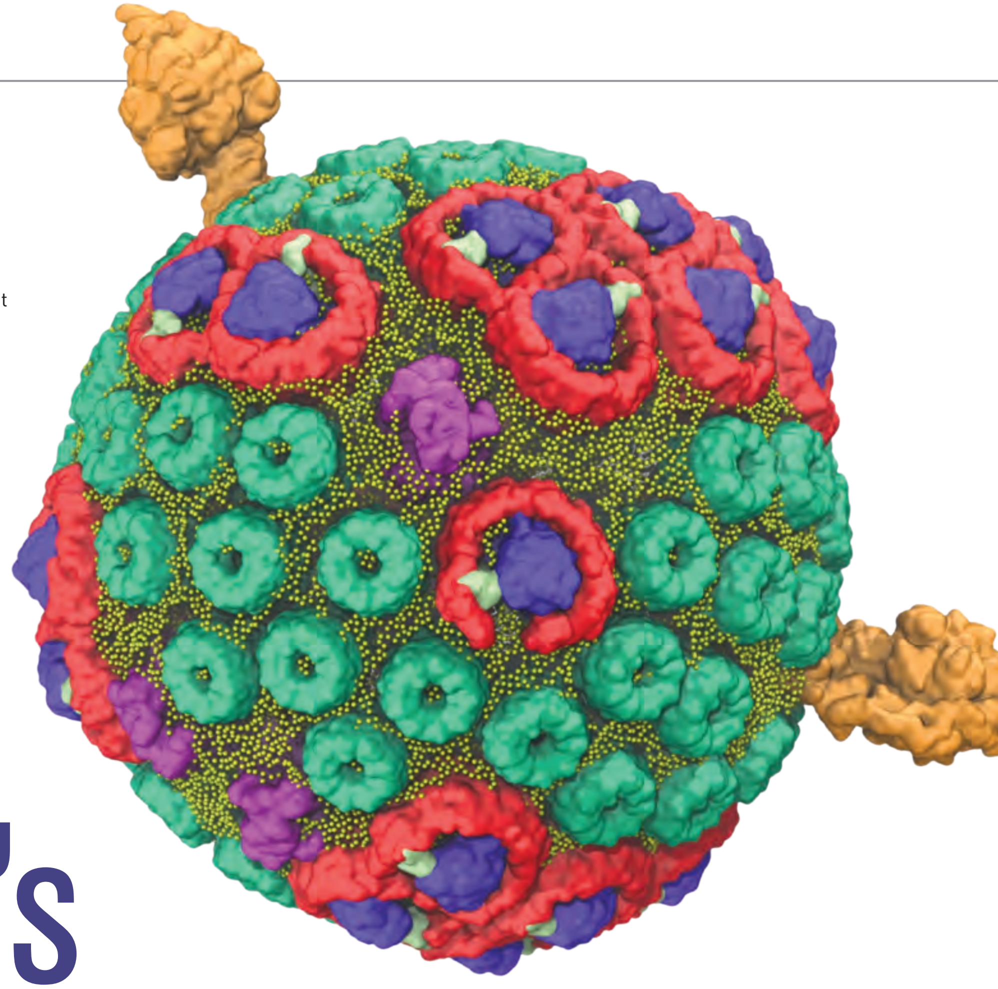
"Without the partnerships we have at ORNL, I couldn't conduct my research as effectively," says Mathews.

Pierce agrees. "Mercury contamination is really a global issue. We are working together to understand how it works and how to remediate it."

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



East Fork Poplar Creek. Image credit: ORNL



This chromatophore model contains about 16,000 lipids and 101 proteins, including the five major types of protein that contribute to the conversion of light energy to the cellular fuel ATP. Image credit: Abhi Singharoy and Melih Sener, University of Illinois at Urbana–Champaign

Building bacteria's

photosynthetic engine

by Jonathan Hines
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Since its inception, computational biophysics has sought to simulate an entire living organism, atom by atom.

Though we're not there yet, recent work from Klaus Schulten of the University of Illinois at Urbana–Champaign demonstrates that this goal is much more than a dream.

Schulten and colleagues used ORNL's Titan supercomputer to carry out the largest biomolecular simulation ever—more than 100 million atoms. Their work is helping us better understand the fundamental process of photosynthesis in purple bacteria—basic research that could one day lead to better solar energy technology.

The project marks a shift in the field from simulating individual cell parts (e.g., a single protein) to simulating specialized cell systems, or organelles (e.g., hundreds of proteins working together to carry out an autonomous function). This is a major milestone on the path to simulating a complete organism.

Single-celled purple bacteria, thought to be one of the first photosynthetic organisms on Earth, possess simple organelles called chromatophores that convert light energy to food. Using experimental data and the molecular dynamics code NAMD, Schulten's group solved an atomistic model of the soccer ball-shaped system made up of 16,000 lipids and 101 proteins.

With a stable model, the team was able to study the remarkable processes of the chromatophore in unprecedented detail, with atoms moving and coordinating within an active energy-conversion system.

"For years, scientists have seen that cells are made of these machines, but they could only look at part of the machine. It's like looking at a car engine and saying, 'Oh, there's an interesting cable, an interesting screw, an interesting cylinder,'" Schulten said. "Titan gave us the fantastic level of computing we needed to see the whole picture. For the first time, we could go from looking at the cable, the screw, the cylinder, to looking at the whole engine."

For more information: http://go.usa.gov/3zSKR

Shining a light on subsurface flows

by Eric Gedenk
gedenked@ornl.gov

We can assume "out of sight, out of mind" is a sentiment rarely voiced by geoscientists. Learning how materials interact below the Earth's surface is of the utmost importance.

Studies of oil production, subsurface contamination, carbon sequestration, and other research fields share a common thread—they deal with multiphase flows, where materials flowing close together may be solids, liquids, or gases. In some cases, the materials refuse to mix even when they are in the same phase (think oil and water).

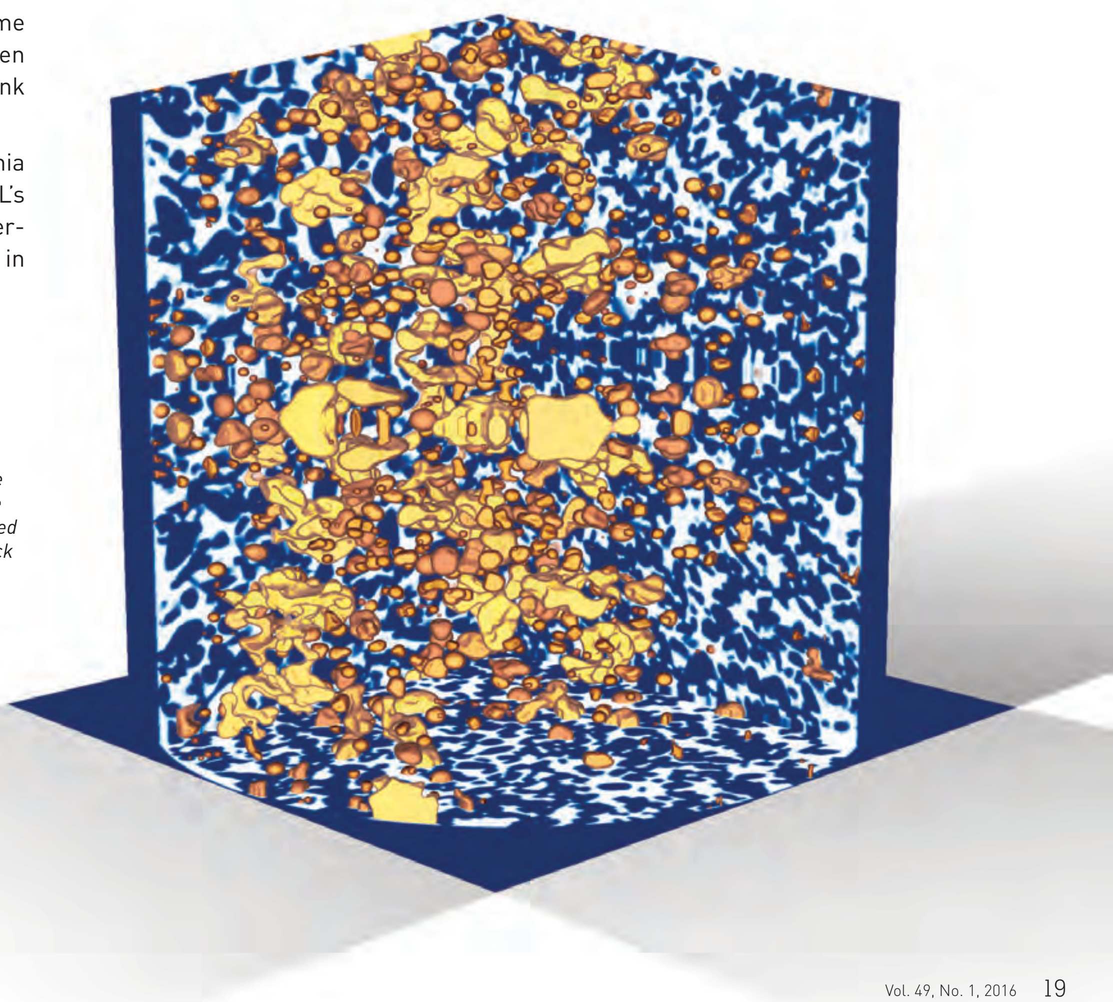
A research team led by Virginia Tech's James McClure is using ORNL's Titan supercomputer to improve understanding of transport phenomena in multiphase systems.

The team's code takes full advantage of Titan and the GPUs that make it the second fastest supercomputer in the world. In fact, the ability to use GPUs has transformed the team's simulations. McClure said that the team does its calculations entirely on Titan's GPUs and uses the system's CPUs for data analysis.

Working with the Oak Ridge Leadership Computing Facility, McClure has developed simulation tools that allow researchers to take the information from a three-dimensional microcomputed tomography image—essentially a 3-D X-ray image—and put it into motion.

With this approach, the team can study interfacial dynamics and other aspects of the system behavior quantitatively at various spatial scales. The team can predict rocks' properties—such as relative permeability—from first principles to measure the resistance to flow that controls the movement of fluids at the reservoir scale. These results are vital for situations where the mobility of trapped, non-wetting phases—in this case, oil or liquid carbon dioxide—is important in areas such as carbon sequestration, oil recovery, and contaminant transport.

For more information:
http://go.usa.gov/3Jqj4



This simulation on Titan tracks oil ganglia (yellow) mobilized in experimentally imaged sandstone (the solid part of the sandstone is in blue). Much can be gained by knowing when oily phases can be removed from subsurface rock or placed permanently in rock structures. Image credit: James McClure

Cataloging drug candidates at the petascale

Multi-institution team creates virtual clinical trials

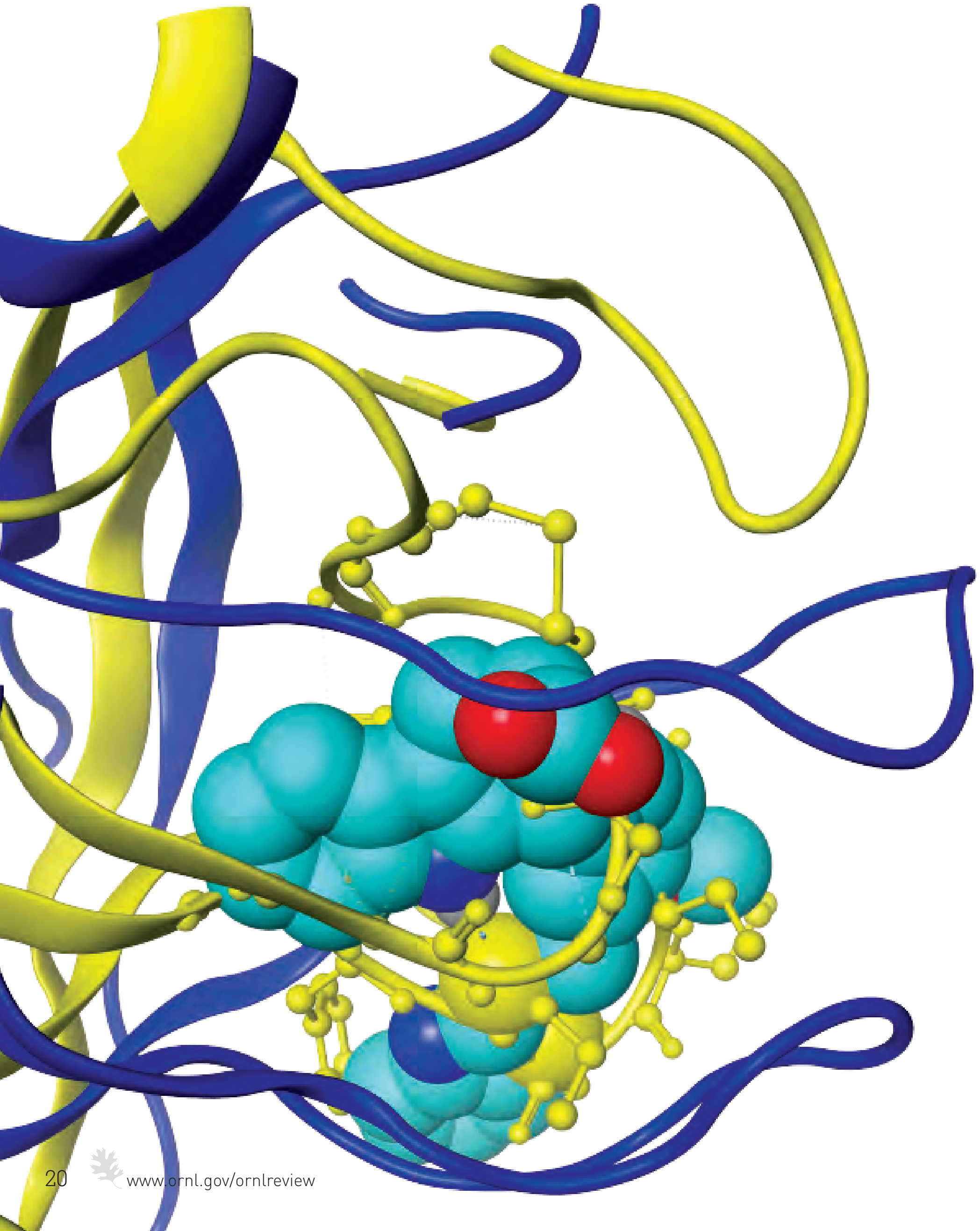
by Eric Gedenk
gedenked@ornl.gov

Developing new pharmaceuticals is a long, expensive process with success far from guaranteed. In fact, almost 99 percent of drug candidates never make it to market.

"Our particular project deals with how we can improve the abysmally low rate of success in the drug discovery pipeline," said Jerome Baudry, associate professor at the University of Tennessee, Knoxville. Baudry leads a team dedicated to using supercomputers to expedite clinical trials for drug candidates, saving pharmaceutical companies years of work and millions of dollars.

Baudry, who also holds a research position at ORNL, works with collaborators from Georgetown and Howard universities as well as Jeremy Smith's group at the Center for Molecular Biophysics at ORNL.

Since 2009, the team has explored drug interactions at the cellular level using Oak Ridge Leadership Computing Facility supercomputers, most recently Titan. At a peak speed of 27 petaflops, or 27 million billion calculations each second, Titan



The superposition of the protein crystal structure (yellow) with a molecular dynamics (MD) snapshot (blue). The predicted drug-candidate only binds to the MD snapshot where the loops open up to expose the binding pocket. Image credit: Jerome Baudry, University of Tennesse is the second most powerful supercomputer in the world.

"The main problem is that drug candidates fail late and fail expensive," Baudry said. Typically, researchers spend a couple of years doing test tube experiments to observe how certain compounds interact with specific proteins in the body. Then, if tests are encouraging, companies move to testing on animals and, finally, humans. These final two stages are called preclinical and clinical trials, respectively.

For a drug to work correctly, the substance must effectively bind to specific proteins, or receptors, in the body. During preliminary testing, drug companies try to make sure the target drug molecule binds to the target protein receptor.

Once a drug candidate reaches the clinical trial stage, though, two major obstacles remain. During clinical trials, researchers often find drug candidates that bind to so many receptor proteins that the drug does not effectively address a person's medical condition—this is a problem of specificity. In other cases, the protein interacts with the target receptor, but its interactions with other receptors can make a person sick in different ways—this is called drug toxicity.

Wrangling receptors

In an attempt to help pharmaceutical companies identify likely failures before testing begins, the team is working to create virtual clinical trials.

Baudry credits the Georgetown and Howard collaborators for providing anonymous clinical data. This data helps the team work on creating more individualized, precision medicines. Further, getting data from multiple locations allows the team to broaden its research database. "All of these institutions have unique cases in terms of public health," Baudry said. "That's what this project aims at integrating. It is translational medicine, which means developing new concepts in medicine that can be applied to the clinical field as early as possible."

The computational approach works somewhat like a telephone operator's switchboard. The Baudry team has a gigantic list of drug candidate molecules and a giant list of protein receptors. They take these data sets, put them into Titan, and let the matchmaking begin. Titan then does millions of relatively simple calculations to match molecules with receptors and then allows researchers to see how that protein will behave after binding to the drug molecule.

"There are a lot of small operations that have to be done that, individually, wouldn't necessarily need Titan," Baudry said. "But the complexity that emerges from those many calculations is what drives new science insights, and Titan allows us to do not just more of the same, but to generate a new level of biocomplexity."

"The main problem is that drug candidates fail late and fail expensive,"

—Jerome Baudry, associate professor, the University of Tennessee, Knoxville.

That new level of biocomplexity has led to enhanced productivity. All of the team's simulations have identified a good drug candidate for further development, and the team is just getting started.

Baudry says that within two years, his team should be able to identify not only good drug candidates based on how effectively they bind to protein receptors, but also candidates that won't be toxic. These insights come by sifting through mountains of data, though.

Data-driven drug development

In the early days of the team's research, Baudry noted that the most significant hurdle came from understanding how to take full advantage of a supercomputer's power. Now the team has an efficient code in place that generates extreme amounts of data—so much, in fact, that transporting, processing and analyzing the data is now the most difficult part of the research.

Thankfully, the OLCF offers researchers more than just the nation's fastest computer—it offers world-class data management resources.

"In supercomputing, we can produce more 'books' than we can read," Baudry said. "It doesn't matter how good a book is if no one reads it. If a book has a solution to your problem, but you don't read it for 20 years, you negate the advantage of reading the book."

Baudry credits the OLCF's analysis resources, specifically the Eos and Rhea clusters and the High-Performance Storage System, for helping his team analyze its data in a timely fashion.

However, these technologies are only as good as the people who use them. "I would say on a higher level, beyond the machines, there are the people who help us access the machine and facilitate how we can use the machine efficiently," Baudry said. "We get this fear of becoming obsolete for the next machine every five years, but thanks to those who are supporting us at the OLCF, we can focus on the science."

As ORNL prepares for its next-generation supercomputer, Summit, Baudry can see his team's ability to run comprehensive, efficient clinical trials reaching new heights.

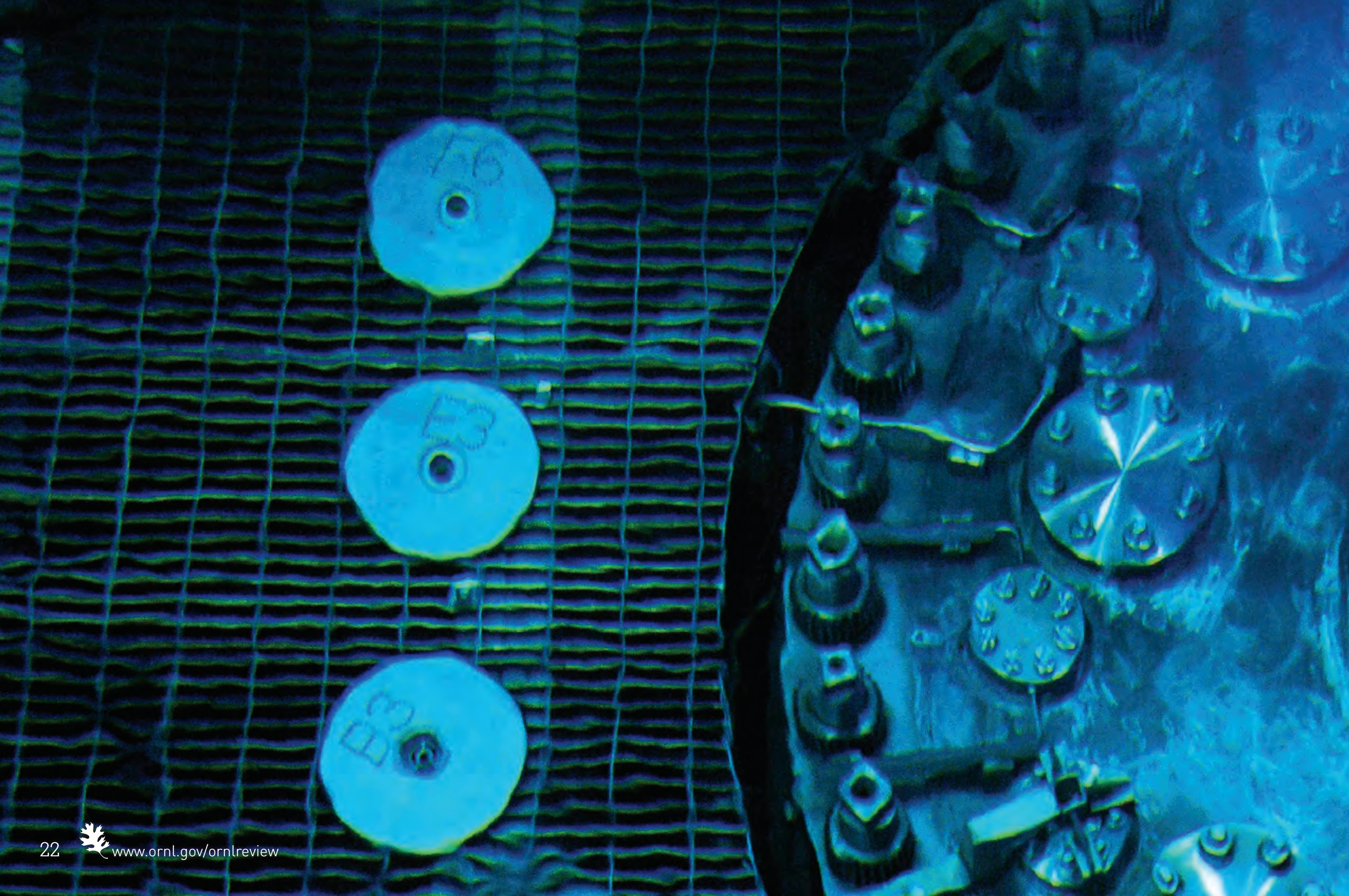
"Summit will be a production machine," Baudry said. "It will allow us to say, 'Here is the probability that this drug will succeed or fail in a clinical trial,' and we will be able to better individualize the risks of side effects. In effect, we will not simulate what happens in test tubes, but what happens in individuals, and even more, populations. It will achieve our translational goal."

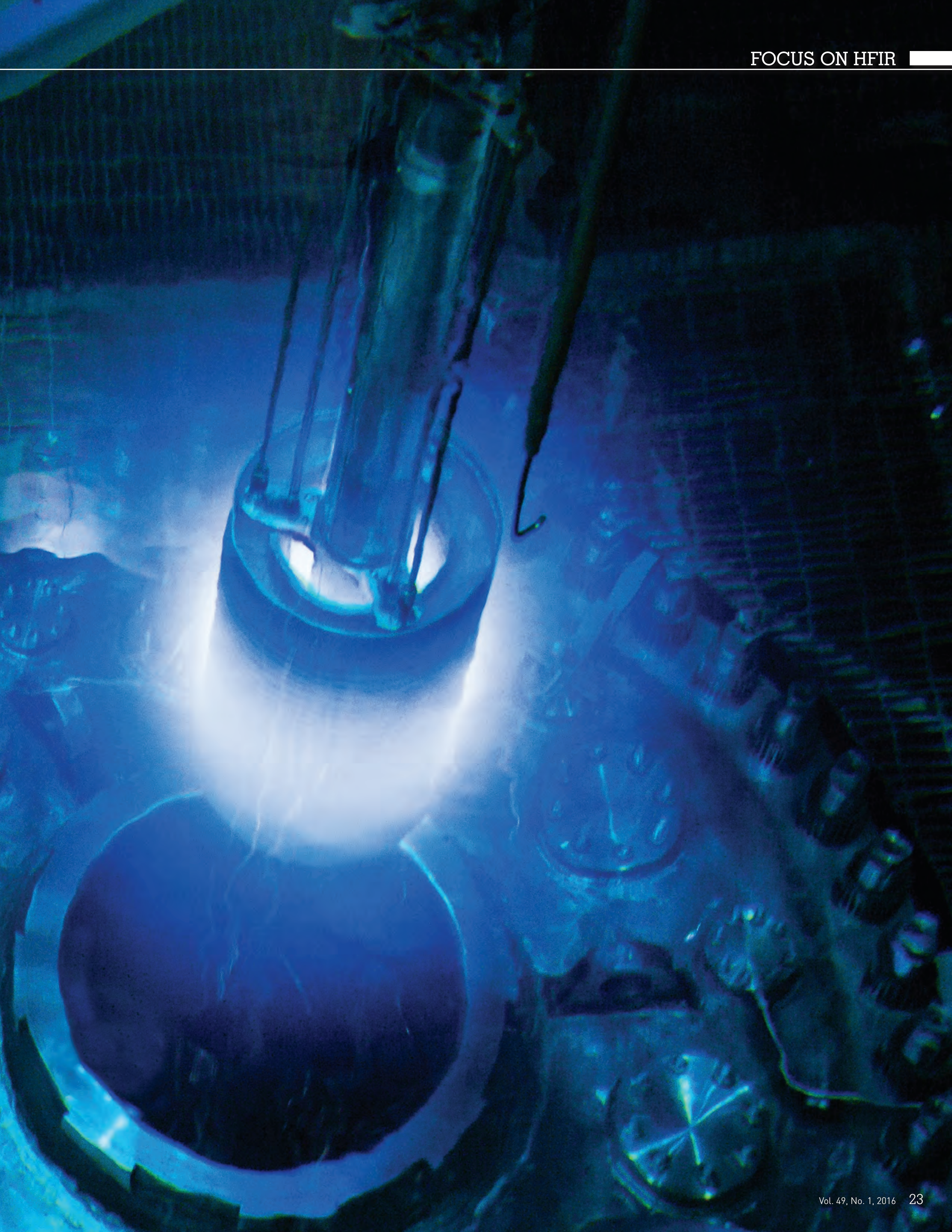
Beautiful refueling

It produces more than 2 million billion neutrons each second through an area less than half the size of a dime, providing researchers with the Western world's highest reactor-based neutron flux. Its neutron scattering stations allow scientists to better understand the structure and dynamics of matter. It produces medical isotopes for the treatment of cancer patients, powers deep space missions for NASA, and made the rare berkelium-249 isotope that enabled the recent discovery of element 117. It even determined whether our 12th president, Zachary Taylor, was poisoned with arsenic. (He wasn't.)

Not only is ORNL's High Flux Isotope Reactor going strong after 50 years, it is as indispensable a research tool now as when it began operation in the summer of 1965. As an added benefit, as long as it continues to be well cared for, HFIR has another good 50 years of operation, says Tim Powers, director of ORNL's Research Reactors Division.

This photo shows HFIR during routine refueling in July 2015. The blue glow comes from Cherenkov radiation, caused when electrons emitted by the spent fuel travel through water faster than light does.
Image credit: Genevieve Martin, ORNL





Frances H. Arnold is the Dickinson Professor of Chemical Engineering, Bioengineering, and Biochemistry at the California Institute of Technology. She is a pioneer of "directed evolution," which mimics Darwinian evolution in the laboratory to create new biological molecules. Her research is particularly focused on how enzymes evolve new catalytic functions.

She delivered the Eugene Wigner Distinguished Lecture Nov. 2, 2015, on the topic "Innovation by Evolution: The Expanding Enzyme Universe." We asked her about the accelerated evolution of proteins and the application of these methods to clean energy technology and health care.

Distinguished

Frances H. Arnold

1. You pioneered methods to accelerate the evolution of proteins for a variety of uses. How do you go about directing protein evolutions?

It's actually simpler than you can imagine. The tools of molecular biology developed in the last 30 years have given us an unprecedented ability to manipulate DNA sequences any way we want. The problem is we don't know what to write out in the DNA to solve a problem. So we use evolutionary algorithms of mutations, recombination—molecular sex, so to speak—to create new DNA sequences. And then bacteria read those and start making proteins. And the human being, the breeder of molecules, has to come in and decide which ones have the properties of interest. Those become the parents for the next generation. So, in a sense, it's like breeding cats. You don't really understand what's happening at the level of DNA, but you choose the parents, you choose the progeny that you're interested in, and you can breed over multiple generations to solve a particular problem.

2. Your work earned you a National Medal of Technology and Innovation in 2011 for pioneering research on biofuels and chemicals. How can these techniques promote clean energy?

It turns out that bacteria or other microbes are these incredible chemical factories. They can take renewable resources like carbon dioxide, biomass, even garbage and convert it into more microbes. Now imagine if you could rewrite the DNA so that instead of turning those renewable resources into microbes, they turned it into fuels or chemicals. They have all the catalysts that could do that, and you can string them together in new ways, or even add whole new catalysts in the form of new DNA sequences. So we were interested in how you would rewrite the DNA of a microbe to become an advanced clean chemical factory.

3. How can they also lead to advances in health care?

There are many health care applications. They can be used to discover new drugs, and they can be used to make better drugs. Many of the drugs we use to treat diseases, from cancer to arthritis, are proteins themselves. Imagine that you would be able to improve the lifetime of a protein in the bloodstream, or its ability to withstand the immune system. We can envision properties that we would like to confer on biological systems, and then use directed evolution to obtain those properties.

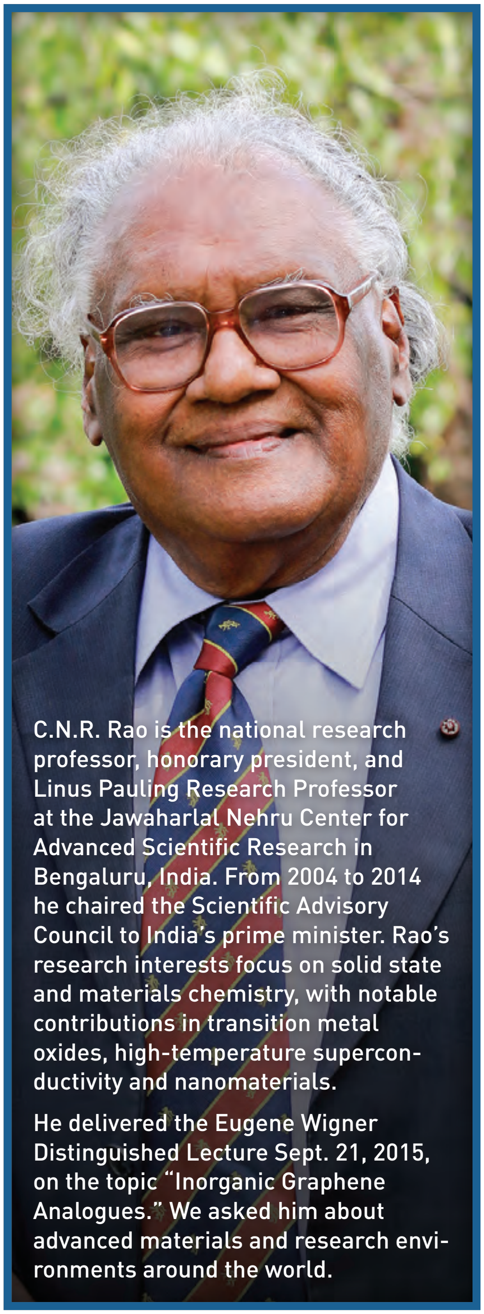
4. Why was it important to visit ORNL, meet with researchers here, and participate in the Wigner Lecture Series?

As a former national laboratory employee myself, I understand the critical role that the national laboratories play in bringing science to society and in solving difficult problems that reach across multiple disciplines. Academia is great for solving individual problems, maybe even inventing some new technologies. But somebody has to integrate this all and tackle the really challenging problems for the future. I really enjoy coming to Oak Ridge and learning about some of the impossible problems that you're tackling.

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.

Lecturers

C.N.R. Rao



C.N.R. Rao is the national research professor, honorary president, and Linus Pauling Research Professor at the Jawaharlal Nehru Center for Advanced Scientific Research in Bengaluru, India. From 2004 to 2014 he chaired the Scientific Advisory Council to India's prime minister. Rao's research interests focus on solid state and materials chemistry, with notable contributions in transition metal oxides, high-temperature superconductivity and nanomaterials.

He delivered the Eugene Wigner Distinguished Lecture Sept. 21, 2015, on the topic "Inorganic Graphene Analogues." We asked him about advanced materials and research environments around the world.

1. Over a long, illustrious career, you have worked with a wide variety of advanced materials, including superconductors, carbon technology, nanotechnology and others. What strikes you as most promising at this time?

There are many areas, particularly in nanotechnology. For example, graphene has possibilities in electronics, medicine and a number of areas. The same is true of other areas of nanomaterials. Nanomedicine is going to be a very big thing, for example, in finding a cure for cancer or creating artificial organs.

The second, of course, would be energy technologies, where we have to find substitutes for existing traditional energy sources. There I expect a lot of interesting things to happen.

2. You have worked with scientific institutions around the world as well as in your home country of India. How would you compare the research environment in India and, for example, the United States?

I came to this country 60-odd years ago to do a Ph.D. India was just coming up. We had just got freedom at the time, and we were in a very poor condition. There were hardly any institutions which could give the facilities for a proper Ph.D.

But today there are a large number of institutions providing good facilities for undergraduate and graduate training. In spite of that, when it comes to the quality of science being done, India doesn't figure anywhere near America. America is still the No. 1 country and is doing the top-quality research.

In quantity of research, India is doing a lot. But in quality, nobody can beat the United States. Sixty percent of the top research in the world is done in the United States today. India probably does 1 or 2 percent. In India, we are building institutions. Things are looking better. We are funding science. But still we have a long way to go.

3. You also have much experience working with colleagues at American national laboratories. Where do you believe DOE should focus its efforts in materials research?

I feel that the Department of Energy should increase their international activities a bit more. They should give international fellowships for bright young people from elsewhere coming and working here. And this kind of thing may, in fact, lead to greater results in crucial areas. I think we should have much more of an international component to research funded by DOE.

Secondly, I think they should create joint programs between institutions—for example, a good institution in India and a good institution here working together jointly on some problems.

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

For those who come from my generation, Oak Ridge has been very well known. In science, they're a name to contend with. In the old days of the Manhattan Project, Oak Ridge was very important—a key center for atomic research. I've always had the highest regard for someone like Wigner, who was codirector of this place.

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.

Melissa Allen

Postdoc, Computational Sciences and Engineering Division
Ph.D., Energy Science & Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Longmont, Colorado

What are you working on at ORNL?

I look at the interfaces between climate, energy, environment and human decision-making. What I've been working on is combining climate models, population dynamics models and agent-based models in a way to look at the climate's impact on urban systems, and vice versa.

What would you like to do in your career?

I'd like to combine scientific inquiry and computational modeling techniques to develop adaptation solutions for worldwide cities at risk. I can see my work as accessible to an eighth-grader or used by decision-makers and other modelers who can collaborate or improve on the science.

Why did you choose a career in science?

My father was a physicist who spent the last few years of his career at ORNL. Weirdly enough, my introduction to atmospheric phenomena was flight training for single-engine airplanes. I got very interested in stuff that pilots wouldn't need to know and thought, "Hmm, maybe that's for me."

Dipanshu Bansal

Postdoc, Materials Science and Technology Division
Ph.D., Materials Engineering, University of Buffalo
Hometown: Palwal, Haryana [state], India

What are you working on at ORNL?

My research involves identifying and analyzing complex interactions between solid-state excitations, such as phonon–phonon, phonon–electron, and phonon–magnon couplings, which are often responsible for unusual material properties. We use neutron and X-ray scattering to investigate the atomic and spin vibrations. Our group is investigating alloys for thermoelectric applications and multiferroics for magnetoelectric devices.

What would you like to do in your career?

In the near future, my focus will be to understand the underlying physics in thermoelectric and multiferroic materials. Further down the line, I'd like to get involved in teaching. Hopefully, I'll be able to interact with younger generations and provide a meaningful contribution to the challenging problems our society is experiencing.

Why did you choose a career in science?

I like exploring new things in life, whether they're mountains, rivers or some strange physics phenomena. A career in science is an aspect of my life that I cherish and enjoy. My career also financially supports my other passions, particularly in sports and nature exploration.

Andrew Lepore

Graduate student, Materials Science and Technology Division
Ph.D. student, Energy Science and Engineering, University of Tennessee, Knoxville (Bredesen Center)
Hometown: Pelham, New Hampshire

What are you working on at ORNL?

I am investigating different catalysts under various reaction conditions. I'm involved in a few collaborative projects, like converting ethanol to hydrocarbons and synthesizing renewable carbon fiber from bioderived propanol. Also, I'm researching how an industrial waste could function as a cheap bio-oil upgrading catalyst.

What would you like to do in your career?

I'm both a scientist and an engineer. My passion is transforming material society has deemed "waste" into something valuable. I intend to keep this big picture theme in whatever work I pursue. I'll consider my career successful if I help develop technology with a positive impact on the world.

Why did you choose a career in science?

I really appreciate the basic understanding chemistry provides. I started college as "premed," but realized with the help of some great professors and several undergraduate research programs that research really intrigued me. With degrees in chemistry and chemical engineering, I hope to apply my knowledge in interdisciplinary energy research.

Larry Millet

Postdoc, Biological Sciences Division
Ph.D., Cell and Developmental Biology, University of Illinois at Urbana–Champaign
Hometown: Rigby, Idaho

What are you working on at ORNL?

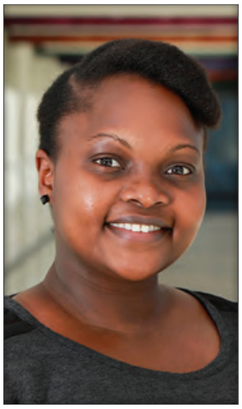
I'm developing micro- and nanotechnological platforms for biological integration studies that resolve chemical signatures of complex biological systems. We're crossing multiple scales—subcellular to multicellular—in biological systems to understand microbial communities: What do they secrete? How do they assemble and behave? We want to measure multiple biological complexities simultaneously.

What would you like to do in your career?

I believe one is fortunate to be happy at work and happy at home. I'm a multidisciplinary scientist who enjoys studying living systems, chemistry, materials and technology. I'm passionate about imaging, microtechnologies and neuroscience, and I'm fortunate to be pursuing technological mycology. I hope to secure a position open to multidisciplinary scientists.

Why did you choose a career in science?

I have a deeply embedded creative and curious nature. When we discover something new, innovative ideas can often emerge from that. That's why I like neuroscience; it's a complex frontier full of opportunity and promise. I love discovery and innovation, and I'm happy when I get to pursue both.



Eva Mutunga

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

What are you working on at ORNL?

I use pulsed-laser melting for assembly of metal nanostructures, which are patterned using electron-beam lithography. This gives highly ordered spatial arrangements of metal nanoparticles on underlying substrates. In addition to making nanoparticles that can be used in electrical, optical and catalytic applications, I'm looking to better understand interactions at the metal–substrate interface.

What would you like to do in your career?

I'll continue in materials research, but I would love to explore where science meets business. As a Bredesen Center student, I've had opportunities to work on technology-based entrepreneurship projects. I've seen how research can be used directly to address a need in the market and how the market drives creativity in the lab.

Why did you choose a career in science?

It's a combination of my interests and encouragement by significant people in my life. My undergraduate mentor introduced me to nanotechnology, which opened up a new world for me. I find the more I learn, the less I know, and the more I want to learn. It's very exciting.

Vinit Sharma

Postdoc, Materials Science and Technology Division
Ph.D., Materials Science, Sukhadia University
Hometown: Jaipur, India

What are you working on at ORNL?

I'm working on computational design of new materials for catalysis, electronic devices and other technological applications. I'm also applying quantum Monte Carlo methods for an accurate theoretical description of electronic properties in strongly correlated systems, where state-of-the-art computational tools aren't always accurate enough to account for electron–electron correlations.

What would you like to do in your career?

I'm fascinated by clean energy technology, like solar cells, solid oxide fuel cells and other energy storing devices. Down the line, maybe I'll lead a research group to look at ongoing scientific challenges on a large scale, such as making electronic devices that stay charged for a very long time.

Why did you choose a career in science?

I got interested in the clean energy initiative because what we have is limited. Even before I got into the field, the power of the scientific principle always fascinated me. Answering questions in a specific, measurable, accurate and realistic way gives a certain freedom to face tough challenges.

Molten Salt Reactor Experiment: Alvin Weinberg's magnum opus

by Tim Gawne
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The Molten Salt Reactor Experiment achieved its first self-sustaining nuclear reaction on June 1, 1965. Three years later, on Oct. 8, 1968, it became the first reactor ever to run on uranium-233.

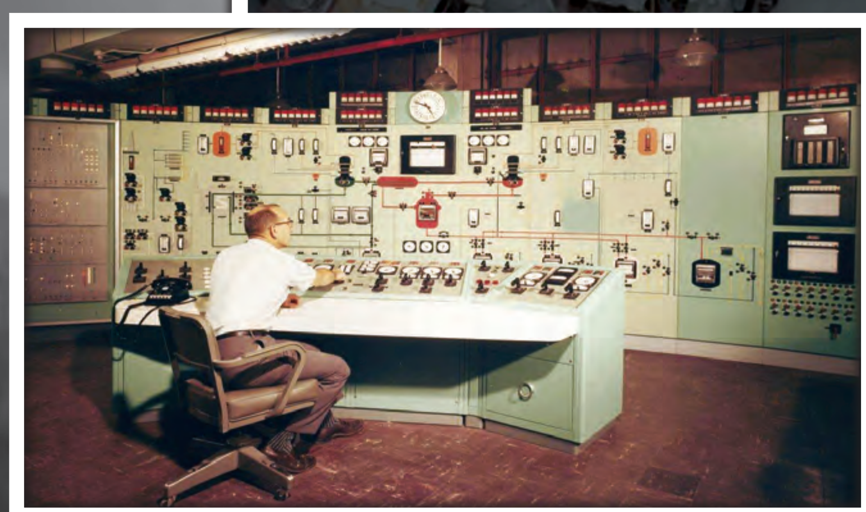
MSRE was noteworthy in at least three respects. Beside running on U-233 and acting as an economic proof of concept for nuclear power, the reactor was fundamentally unlike most modern designs. The fuel did not sit in the reactor core while coolants circulated through; rather, the molten salts acted both as a carrier for the fuel and as a coolant.

Still, liquid-fuel reactors were nothing new; the concept dates from before the end of World War II. Postwar reactor projects were primarily the domain of Chicago's Argonne National Laboratory, but ORNL's Alvin Weinberg met with Argonne's director, Walter Zinn, to carve out a role for the Tennessee lab. That experience included the Homogeneous Reactor Experiment and the Aircraft Reactor Experiment, two fluid-fuel reactors developed in the 1950s that paved the way for MSRE.

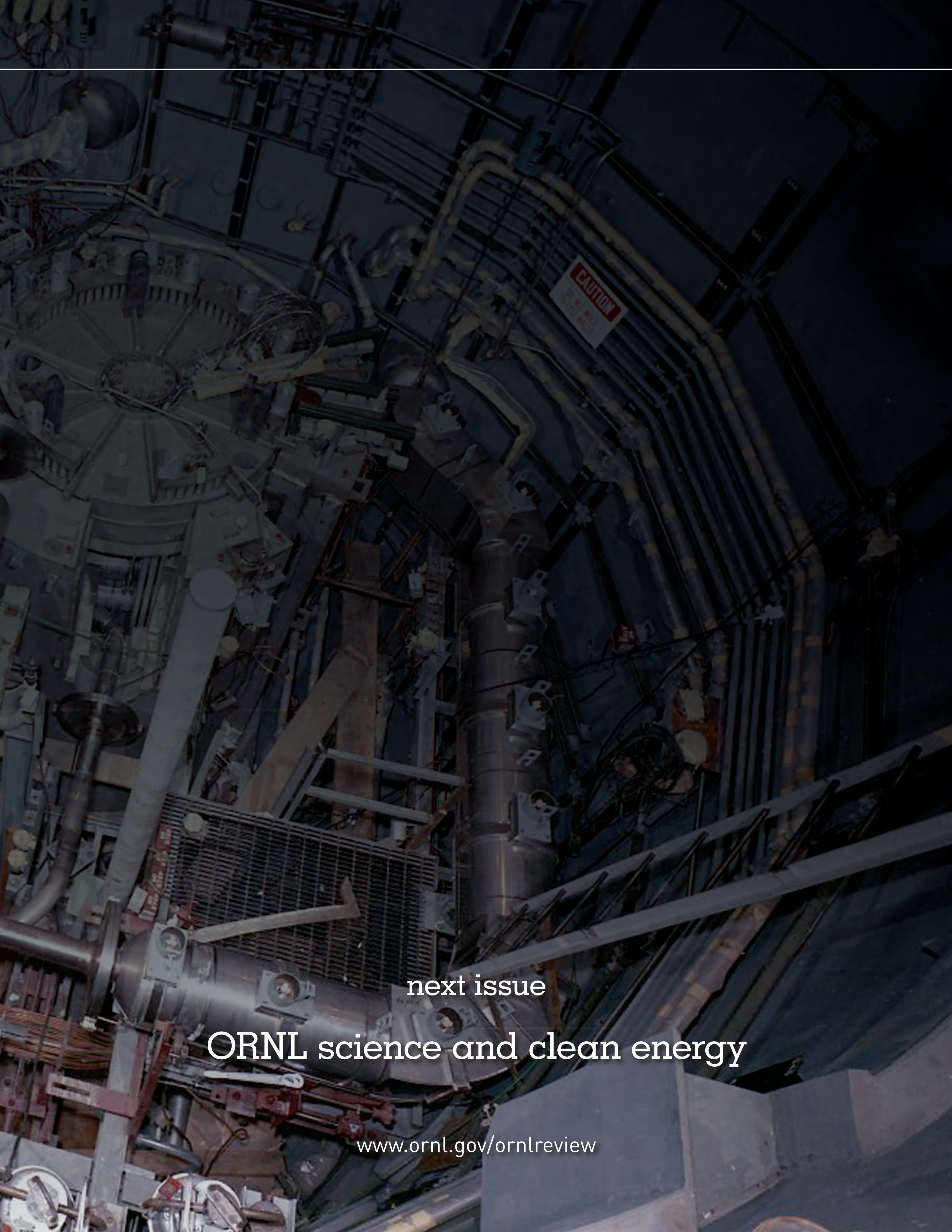
During the 1968 event, Weinberg dubbed MSRE the "Mighty Smooth Running Experiment." As he addressed a gathered crowd, he motioned to nearby barrels containing processed salt carrier and spent fuel. The barrels had no radiological protection and needed none.

The reactor went on to log 11,515 hours of critical operation during its brief run. It was shut down ceremoniously in 1969, having achieved all that was asked of it. The graphite bars that lined the reactor core as its moderator showed little to no damage, whether from heat, radiation or chemical corrosion.

The molten salt program ended in 1973, with the Atomic Energy Commission deciding to focus on other designs. Both government and industry are now reevaluating molten salt technology as an answer to the global energy challenge. It's a conversation built on what Weinberg considered one of ORNL's greatest technical achievements.



[Left] Atomic Energy Commission Chairman Glenn T. Seaborg, left, and ORNL director Alvin M. Weinberg at MSRE. [Above] The control room.



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