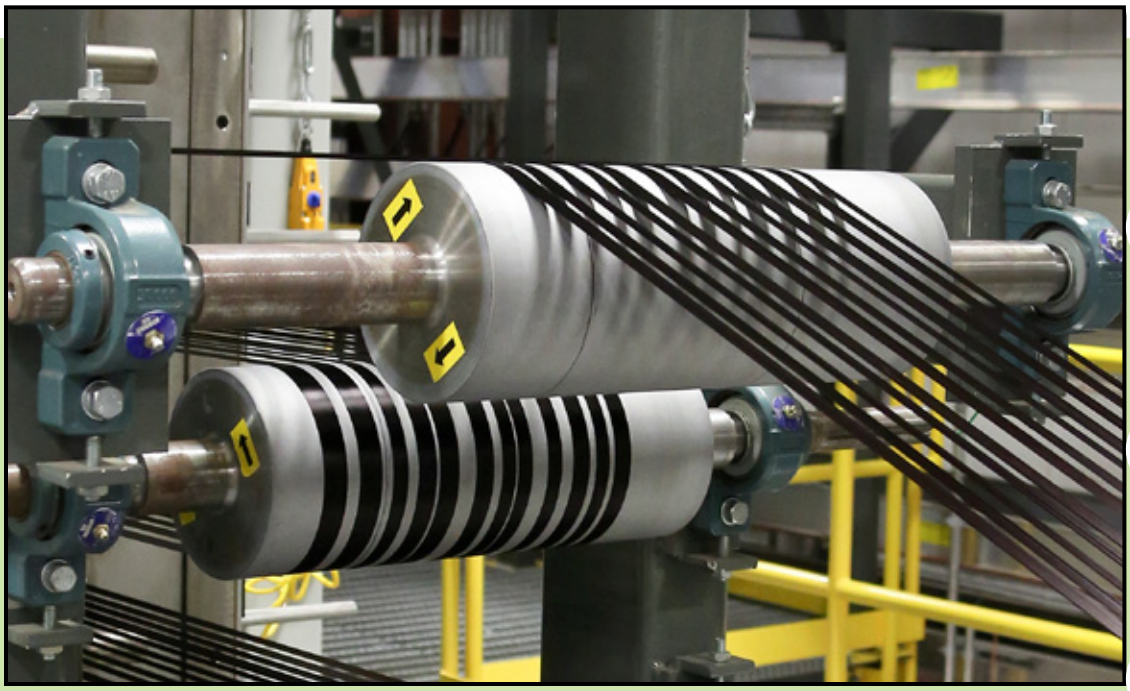
cleanenergy

No. 1 • 2013

NEWSLETTER OF *Oak Ridge National Laboratory's Energy and Environmental Sciences Directorate*

Advanced Manufacturing

Building a Better Tomorrow Demands a Better Set of Tools



ORNL's new Carbon Fiber Technology Facility, an advanced manufacturing facility, researches and develops low-cost carbon fiber—a lightweight substitute for steel that can be used in clean energy and automotive applications.

Advanced manufacturing uses new materials and manufacturing technologies to rapidly supply high-quality products to meet market demands. Although advanced manufacturing applies to a host of consumer goods, the Department of Energy (DOE) and Oak Ridge National Laboratory (ORNL) are interested in advanced manufacturing for clean energy technologies.

In light of an expanding global population that must make the most of available resources, DOE supports research and development in technologies that use renewable energy derived from the sun, water, wind, and plants, or in methods and materials that improve the energy-efficiency of current technologies, such as lighter car parts to cut down on fuel consumption.

Manufacturing is the step that makes these goals possible on a national scale. The Energy and Environmental Sciences Directorate (EESD) at ORNL brings researchers from a range of science and engineering programs together to improve manufacturing materials and methods.

Advanced manufacturing relies on processes that use heat, magnetism, and other physical forces to make metals

(continued on page 1)

Climate Change Science Institute
Predicts more cash might get sucked into severe weather damages by 2050

National Transportation Research Center
Streamlines engine and transmissions R&D at new Vehicle Systems Integration Lab

Environmental and Biosciences Divisions
Discover genes tied to toxic mercury in aquatic food chain

Buildings Technologies Research and Integration Center
Talks energy-efficient buildings with delegations from China

Measurement Science and Systems Engineering
Works with Spallation Neutron Source to get in-demand instrument back on track

BioEnergy Science Center
Reaches 500 publications and counting

OAK RIDGE National Laboratory

director's letter

Martin Keller at the FIRST robotics competition kickoff in January

Associate Laboratory Director for Energy and Environmental Sciences Martin Keller

The global market for clean energy technologies has grown fivefold within the last decade. Today, investments in the industries that produce our solar panels, wind turbines, energy-efficient electronics, and energy-saving building materials, in addition to many other applications, reach as much as $269 billion worldwide as governments, businesses, and individuals embrace these technologies on a larger scale.

The fundamental science that drives these technologies ranges from the biochemistry of plants and microbes that store and release energy; to the physical science that explains what makes a material stronger, lighter, or more corrosion-resistant; to the computational science that analyzes and packages information to help us understand the environment around its use.

To shorten the time it takes to get an idea from the laboratory to the factory floor, DOE is challenging its national laboratories to innovate and improve manufacturing methods so American industries can compete in the global clean energy market. ORNL and EESD have played a pivotal role in demonstrating how science and industry can accelerate advances in clean energy.

When DOE Assistant Secretary for Energy Efficiency and Renewable Energy David Danielson announced the department's new Clean Energy Manufacturing Initiative (CEMI) in March, he chose the backdrop of EESD's Carbon Fiber Technology Facility (CFTF), the latest DOE manufacturing demonstration facility, which produces low-cost carbon fiber through new precursor materials and processing methods.

CEMI is focused on boosting US competitiveness in the clean energy sector not only by advancing manufacturing methods but also by delivering these methods to industry leaders through partnerships and research and development collaboration. Facilities such as the CFTF and ORNL's Manufacturing Demonstration Facility—the first of its kind—are designed to streamline scientific research into the materials and manufacturing technologies that industry partners will want to use when designing new products. Further, promising prototypes can be evaluated for manufacturing scalability in the very facilities that spurred their development.

EESD is uniquely positioned to provide the backbone of scientific research required by these facilities and their research and development programs. With research areas spanning bioenergy, advanced manufacturing, environmental sciences, genetics, climate science, renewable energy, and energy-efficient technologies (including building, transportation, and industrial technologies), EESD runs the gamut of basic to applied science.

The directorate's relationships with other leading research facilities at ORNL provide an unmatched concentration of resources. With ORNL's Spallation Neutron Source, the most powerful of its kind in the world, users can gain extraordinary insight into the structure of a material, allowing researchers to determine the processing technologies—such as those that apply heat, magnetism, or chemical compounds—which will enhance a material's performance. Through the Oak Ridge Leadership Computing Facility, which houses the 27-petaflop supercomputer Titan, as well as through other scientific computing facilities at the lab, users can analyze new technology and product designs before time or money is spent building prototypes. High-resolution computer simulations also monitor the performance of a material or process on the most relevant scale, from the atom to the supply chain.

Among directorates at ORNL and other DOE labs, EESD has a highly collaborative culture that reaches across these different disciplines and stages of scientific development to meet a single objective: clean energy.

Through the new issues of our directorate newsletter, we hope to update you on our successes.

cleanenergy

Produced by Creative Media at Oak Ridge National Laboratory for the Energy and Environmental Sciences Directorate

Team Leader
Suzy Fowler

Publication Director
Katie Elyce Jones

Editors
Deborah Counce
and Charlie Horak

Graphic Designer
LeJean Hardin

Newsletter Committee and Contributing Writers
Meghan Drake, Lori Frye, Penny Humphreys, Katie Elyce Jones, Jennifer Palmer, Tamara Rogers, and Sara Shoemaker

Photographers
Curtis Boles, Genevieve Martin, and Jason Richards

Additional Images
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in the spotlight

Sudarsanam Suresh Babu, new Governor's Chair for Advanced Manufacturing

New Advanced Manufacturing Governor's Chair

Babu to lead materials innovation, industry collaboration

Sudarsanam Suresh Babu, an expert in advanced manufacturing from materials development to production, began his appointment as the new University of Tennessee–Oak Ridge National Laboratory Governor's Chair for Advanced Manufacturing on July 1.

Formerly a professor in the Welding Engineering Program in the Department of Materials Science and Engineering at The Ohio State University, Babu's research focuses on the design and processing of structural materials and metals with particular implications for the accelerating field of additive manufacturing (3D printing).

Babu's current research team analyzes the performance of new and transformed materials during fabrication and manufacturing. First, they use characterization tools such as atom probe field ion microscopy and neutron diffraction sources in order to understand the effects of temperature, chemistry, magnetic fields, and mechanical forces on materials processing. They further advance new materials and manufacturing methods through high-performance computer modeling that shrinks the research and development workload for industry partners, expediting the manufacture and availability of new products.

As part of his appointment in EESD and the Advanced Manufacturing Program, Babu's experience will underpin the technology being developed by the Manufacturing Demonstration Facility to innovate new materials and product designs, compelling strong Lab and industry partnerships. He will also serve as professor in both the UT departments of Mechanical, Aerospace, and Biomedical Engineering, as well as Materials Science and Engineering.

Babu received his bachelor of engineering degree in metallurgy from PSG College of Technology, Coimbatore, India; his master of technology in industrial metallurgy-welding from the Indian Institute of Technology, Chennai, India; and his doctoral degree in materials science from the University of Cambridge.

He is the eleventh Governor's Chair, a position that bridges research efforts between UT and the Lab in areas of importance to US energy, security, and prosperity, such as advanced materials, computational science, neutron sciences, among others.

(continued from cover)

stronger and more resistant to corrosion, coatings and sealants more resistant to water, or insulating materials more resistant to heat. Studying the large-scale production of biofuels and biotechnologies also draws from the directorate's range of biological and environmental science resources.

EESD centers such as the Building Technologies Research and Integration Center and the National Transportation Research Center connect scientists and engineers to industry leaders to collaborate on more energy-efficient materials and designs, and ORNL's advanced manufacturing facilities—the Manufacturing Demonstration Facility and the Carbon Fiber Technology Facility—develop ways through manufacturing tools and processes for industries to readily adopt new materials and technologies.

ORNL and EESD's goal for advanced manufacturing is not only to make clean energy technologies available that release fewer greenhouse gases or have longer life cycles than their counterparts but also to ensure that the raw materials and energy that goes into manufacturing these technologies is used efficiently.

Strong, lightweight fiber tow bands exit furnace at the Carbon Fiber Technology Facility.

Climate change scientist predicts US weather-related losses could double by 2050

US economic losses from extreme weather could at least double by 2050, according to an article by ORNL's Benjamin Preston, deputy director of the Climate Change Science Institute, which was published in April's issue of Global Environmental Change. Preston studied historical data from 1960 to 2009 on more than 3,000 US counties to establish regional trends in severe weather (such as hurricanes and wildfires) and population growth (an indicator of urban development vulnerable to large-scale weather damages). He then applied predictive modeling to project resulting economic losses into 2054.

Predictions suggest counties in the Southeast and Southwest could experience the most rapid growth in wealth and exposure, while those in the already densely populated Northeast and West Coast will become exposed to risk increases more slowly. Using two accepted models for projecting loss, Preston forecasts that current annual US disaster losses of $10 billion to $13 billion could increase by a factor of 1.8 (double current losses) or by as much as 3.9 (quadruple current losses). He said these results show a pressing need for more research to improve cost projections and to prepare communities for escalating costs associated with extreme weather.

In 2012, Superstorm Sandy cost hundreds of lives and billions of dollars. A recent Climate Change Science Institute study predicts that as US cities and populations grow, future extreme weather events could cost even more.

Experimental prototype of whole-ecosystem enclosure, located at ORNL, including warming technologies like those under construction at the SPRUCE research site in northern Minnesota.

Climate project accelerates warming of sensitive ecosystem to study impact

An ORNL-led climate change project known as SPRUCE, for the Spruce and Peatland Responses Under Climatic and Environmental Change, is constructing specially designed warming technologies that will mimic global warming scenarios in one of Earth's most sensitive ecosystems. The target boreal peatland forest in northern Minnesota is representative of an ecosystem type common throughout Canada, northern Europe, and Russia.

A cold, damp earth rich in carbon from the mix of slowly decomposing vegetation, boreal peatland forests are "carbon sinks" because organic carbon that would normally be released as the greenhouse gas carbon dioxide in warmer, dryer forests is trapped in wet and cold bog conditions. Warming temperatures threaten to release these carbon stores that are more than 1,000 years old in the form of the carbon dioxide and methane, another greenhouse gas associated with climate change.

SPRUCE will use the whole-ecosystem warming technologies currently under construction in northern Minnesota to modify air and soil temperatures for glimpsing a range of possible future conditions. The warming treatments will be repeated under elevated carbon dioxide levels. Treatments are set to begin in the 2014 fiscal year. In the past year, ORNL supported construction of local access roads, installation of more than three miles of electrical supply lines, and the placement of extensive "dock" boardwalks to service experimental plots. The project, which began development and prototype design in 2010, is set to run for 10 years.

New lab analyzes powertrains and advanced components from cars to big rigs

The Vehicle Systems Integration (VSI) Laboratory became fully operational this summer, offering unique capabilities to evaluate and simulate engines, electric motors, and transmissions in conventional and hybrid powertrain configurations from light-duty cars to heavy-duty trucks.

Growing transportation costs and future regulations have increased the focus on vehicle fuel efficiency and emissions control. The VSI Lab can address these concerns by performing prototype research and characterization of advanced systems on a research cell level, which is particularly convenient for manufacturers of Class 8 trucks (tractor-trailers) who can bring individual parts to the lab to analyze and leave the big rig at the factory.

"We can take specific components through virtually any driving scenario—simulating or emulating various road conditions—to glean the most realistic results. Industry partners can use this kind of data to adjust their vehicle designs accordingly to help them meet federal regulations and address the country's demand for cleaner, more efficient powertrains," said David Smith of ORNL's Energy and Transportation Science Division and manager of the Advanced Vehicle Systems Research program.

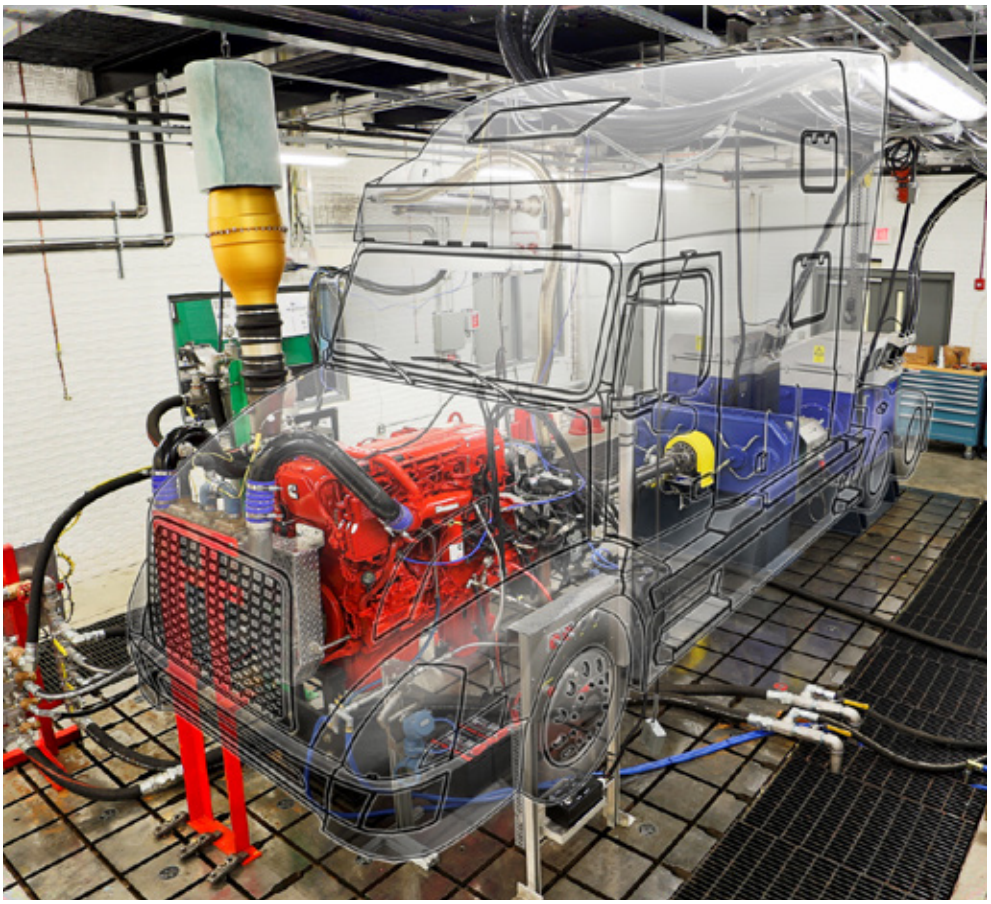
Located at ORNL's National Transportation Research Center, the VSI Lab comprises a powertrain test cell with twin AVL 500 kW AC transient dynamometers and a component test cell—both share energy storage system emulation and dSPACE hardware-in-the-loop real-time platform capabilities. The VSI Lab also features "X"-in-the-loop hardware evaluation of powertrain components or subsystems in virtual vehicle environments, where "X" represents any experimental component or subsystem.

The VSI Lab pulls from core transportation research capabilities across ORNL to handle analysis requests related to conventional and hybrid powertrains, including advanced combustion engines, fuels and emissions, power electronics and electric machinery research, and medium and heavy truck duty cycle databases.

Through the VSI Lab's first industry Cooperative Research and Development Agreement partner, Meritor Inc., Smith and his team—Paul Chambon, Dean Deter, Norberto Domingo, Steve Whitted, and PT Jones—are able to bridge modeling, simulation, analysis, and controls development of prototype hardware in transient operation of the Meritor Class 8 tractor hybrid electric powertrain.

Other significant collaborations with the VSI Lab include the DOE; US Environmental Protection Agency; International Council on Clean Transportation; Cummins, Inc.; Eaton Corporation; California Air Resources Board; National Renewable Energy Laboratory; Argonne National Laboratory; and SAE International. The VSI Lab is sponsored by the DOE Vehicle Technologies Office.

Industry partners can use VSI Lab research data to help determine vehicle design adjustments that can help meet federal regulations and address the country's demand for cleaner, more efficient powertrains.



Cracking a 40-year mystery: ORNL scientists discover genes tied to toxic methylmercury production

A research team with members from the Biosciences and Environmental Sciences divisions has identified two genes present in bacteria responsible for converting mercury into the harmful neurotoxin methylmercury. Their work is featured in the journal Science.

People are exposed to methylmercury—which is especially harmful to fetuses, infants, and small children—primarily through consumption of fish and shellfish. Scientists have known for more than 40 years that certain strains of bacteria take up inorganic mercury from the environment and convert it to its more harmful form through methylation. However, they have not had the tools to determine the genetic triggers for this process until the genome sequencing of key, methylating microbes became feasible in the last few years.

As a gaseous pollutant, mercury cycles from the atmosphere through precipitation into waterways and sediment, where it is methylated by bacteria. Methylmercury accumulates in aquatic species through the food chain.

While contaminated fish and other sources of methylmercury are a global concern, ORNL is uniquely suited to study the long-term cycling of mercury in the environment using the local East Fork Poplar Creek (EFPC), which was contaminated with large quantities of the metal as a result of industrial processes at the Y-12 National Security Complex during the 1950s and 1960s. Despite the reduction of direct mercury discharge into EFPC, methylmercury concentration in fish remains high.

DOE's Office of Science funded ORNL through a science focus area program to study methylmercury production in the EFPC environment. Liyuan Liang, the program director, assembled a team of scientists from ORNL and collaborating universities, including biophysicists, chemists, geneticists, hydrogeologists, and microbiologists.

"The multidisciplinary nature of our project worked extremely well," said Jerry Parks, one of the lead authors. "Geneticists and microbiologists don't always interact closely with chemists or biophysicists, but maybe they should try to do that more often."

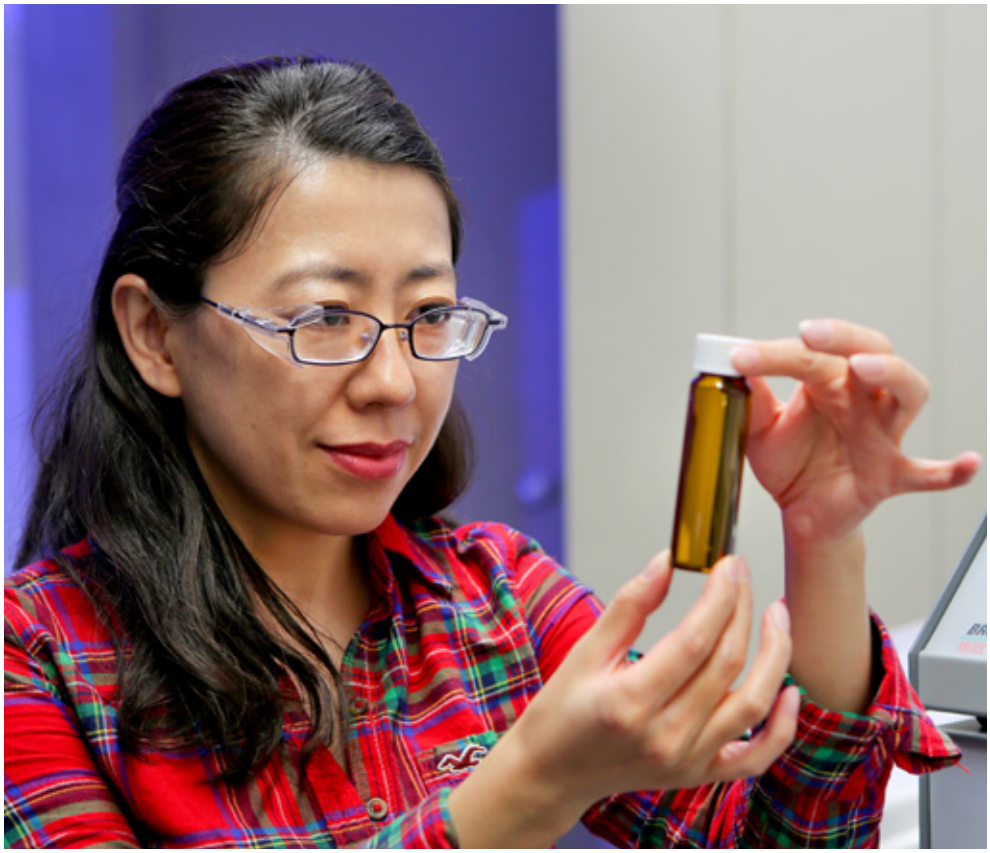
The team—including lead authors Alexander Johs, Mircea Podar, and Parks—used a unique approach combining bioinformatics with experimental evidence to identify the genes that transform mercury into methylmercury. After sifting through a genomic database, they began with a list of candidate genes present in methylating bacteria but absent in non-methylators. To pinpoint the specific genes involved, the team studied the chemical principles underpinning methyl transfer to metal ions.

They narrowed their search to two genes, which they later named hgcA and hgcB. These genes encode proteins that facilitate the transfer of a methyl group to the inorganic mercury taken up by the bacteria, producing methylmercury, as well as proteins that enable the cycle to repeat. Significantly, these two genes are absent in the genomes of several non-methylating bacteria that are closely related to the methylators. After painstaking experiments over several months, the team was able to delete one gene at a time and then both genes at once. In both cases, the deletion strains could no longer make methylmercury. When the genes were re-inserted into the methylators, the bacteria once again produced the neurotoxin, confirming their role in the methylation process.

"We found the two gene clusters in more than 60 strains of microorganisms in four other lineages for which genome sequences are available," Liang said. "This is significant, as the mercury methylators are more widely distributed in microorganisms than previously thought."

The discovery of hgcA and hgcB could eventually lead to the development of biomarkers for detecting organisms that produce methylmercury in the environment.

"We'd like to identify hotspots for mercury methylation," Liang said. "In time, on-site analyses will be possible using biomarker sensors, which could help the engineering communities evaluate the best cleanup strategy."



Yun Qian of the Environmental Sciences Division preps samples for methylmercury analysis.

China delegations visit ORNL building efficiency facility, discuss future collaborations

The ORNL–China National Building Waterproof Association meets at BTRIC's new MAXLAB facility to discuss energy efficiency advancements in commercial and residential building.

Patrick Hughes, director of the Building Technologies Research and Integration Center, hosted two Chinese delegations in the newly opened MAXLAB, a research facility to advance the energy efficiency and durability of building envelopes—walls, roofs, and foundations—equipment, and appliances.

The meetings were designed to build relationships and strengthen collaborations between researchers and industry partners in the US and China engaged in the US-China Clean Energy Research Center for Building Energy Efficiency. Known as CERC BEE, the US-China research center is dedicated to advancing the energy efficiency and reducing the carbon footprint of residential and commercial buildings in both countries. A 33-person delegation from the China National Building Waterproof Association and a 10-person delegation from China's Broad Homes Industrial Co., Ltd. attended. Two representatives from each of three US industry partners (Dow Chemical, ClimateMaster, and Gate Precast) also participated with Broad Homes.

China estimates that 60% of the urban building floor space anticipated to be in its country by 2030 has yet to be built, so they have a far greater focus on new construction than the US. How energy efficient China's construction execution turns out to be will have global climate ramifications. The construction style in China is almost exclusively poured-in-place concrete or pre-cast concrete panels. Broad Homes has demonstrated an innovative way to construct high-rise buildings from groundbreaking to occupancy in 100 days using pre-cast concrete panels.

The delegation from China's Broad Homes Industrial Co., Ltd. visits BTRIC's new MAXLAB facility.

China-side industry participants in these visits expressed strong interest in becoming collaborators on ORNL's three CERC BEE projects lead by Diana Hun (spray-on liquid flashing for water and air sealing), Scott Hunter and Mengdawn Cheng (spray-on superhydrophobic cool roof coating resistant to soiling and microbial growth), and Xiaobing Liu (advanced decentralized ground-source heat pump system).

Division wins three R&D 100 awards for clean technologies

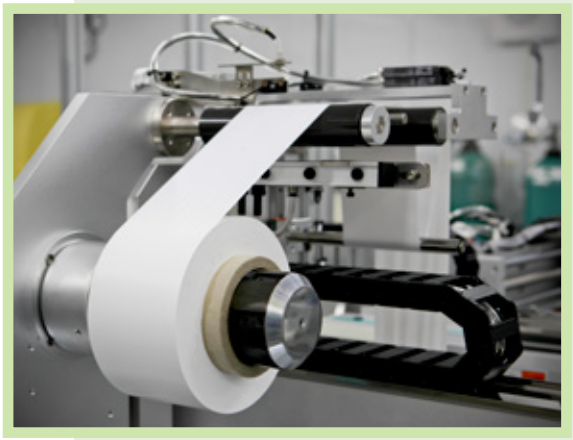
Energy and Transportation Science Division (ETSD) researchers contributed to three out of six R&D 100 awards from ORNL. The awards for the 100, top technology products of the year are selected by R&D Magazine from a survey of university, government and private sector technology developments.

Ed Vineyard, Moonis Ally, Jeffrey Munk, Bo Shen, Keith Rice, Van Baxter, and Anthony Gehl, of ETSD, for the ClimateMaster Trilogy 40 Q-Mode Geothermal Heat Pump, developed by ClimateMaster and ORNL through a cooperative research and development agreement. This water-to-air packaged heat pump provides significantly lower energy costs, reduces peak demand for electricity, and provides environmental benefits, especially through reductions in greenhouse gases and pollutants. Using the earth as its heat source and sink rather than outdoor air, homeowners and small businesses can reduce energy costs by up to 65%.

David Wood III, Claus Daniel, Jianlin Li, and Curt Maxey, of ETSD, who worked with colleagues in the Physical Sciences Directorate, for the SYMMETRIX HPX-F Nanocomposite Separator for Improved Lithium Ion Battery. Jointly developed by Porous Power Technologies LLC and ORNL, SYMMETRIX HPX-F addresses market demands by lowering lithium-ion battery costs and improving safety through the replacement of polymer separators. This breakthrough membrane technology could affect electric vehicles, grid storage applications, portable electronic applications, filters, barrier fabrics, transdermal drug delivery, and toxic chemical absorption.

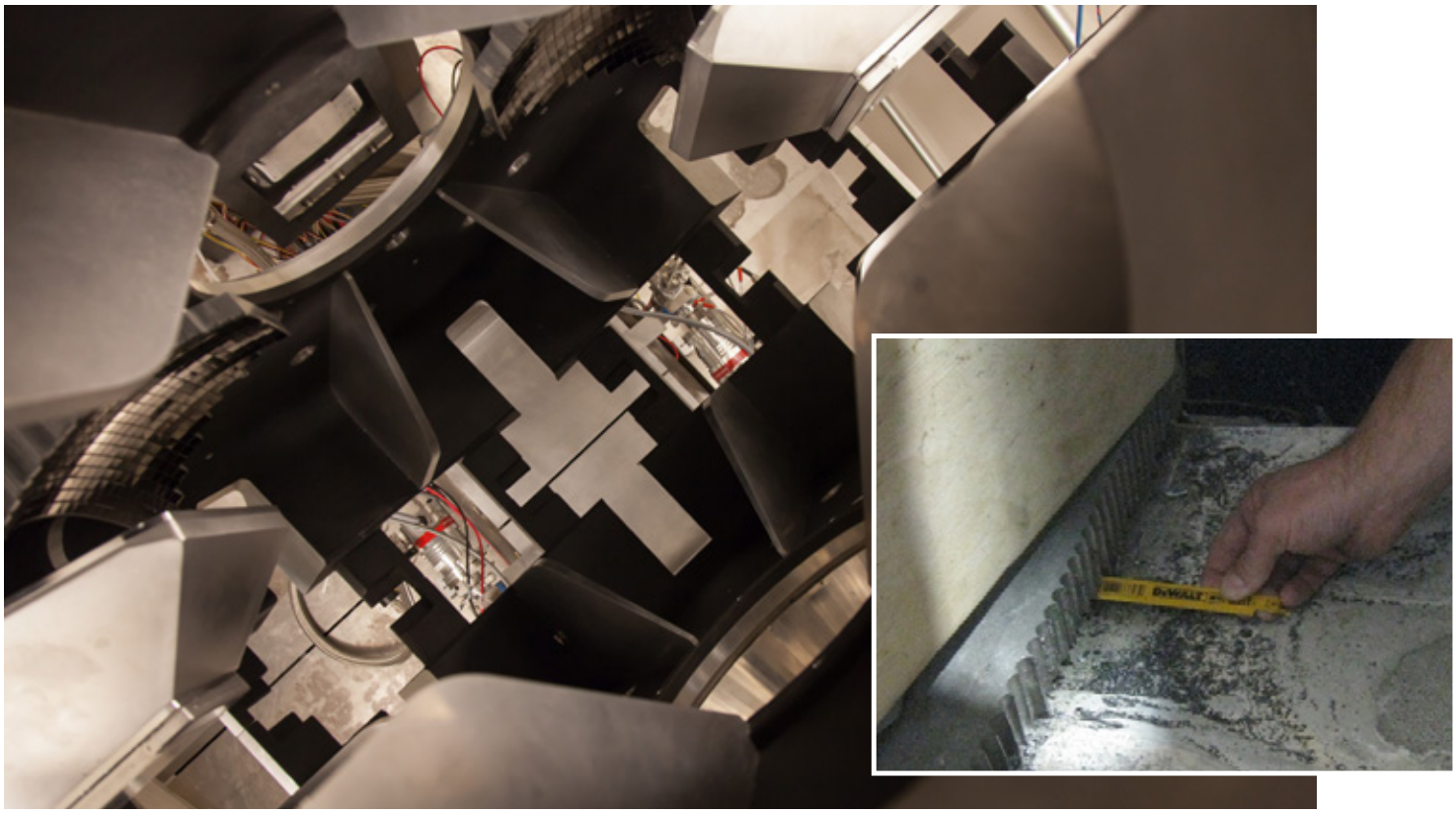
James Parks and William Partridge, of ETSD, who worked with David Sims of the Science and Technology Partnerships Directorate, for the Da Vinci Fuel-in-Oil, or DAFIOTM, Measurement System. Developed and jointly submitted by Da Vinci Emissions Services Ltd., Cummins Inc., and the ORNL team, the DAFIOTM system uses a fiber-optic probe to obtain real-time measurements of oil in an operating engine to quantify the fuel dissolved in the lubricant oil. The DAFIOTM technology enables combustion engineers to rapidly assess any issues related to fuel dilution of oil during development of efficient, clean, and reliable engines.

The creators of the ClimateMaster Triology 40 Q-Mode Geothermal Heat Pump stand with the R&D 100 award-winning technology, from the left, Van Baxter, Ed Vineyard, Jeffrey Munk, Anthony Gehl, Moonis Ally, Keith Rice, and Bo Shen.



SYMMETRIX HPX-F addresses market demands by lowering lithium-ion battery costs and improving safety through the replacement of polymer separators.

The Da Vinci Fuel-in-Oil Measurement System, which uses a fiber-optic probe to obtain real-time measurements of oil in an operating engine, is demonstrated in the laboratory.



(Inset) An unbounded baseplate on Spallation Neutron Source's (SNS's) VISION beam line caused excessive vibrations, which were diagnosed by MSSE staff and corrected by SNS engineering and technical staff.

The VISION beam line detects molecular vibrations in a wide range of materials at energies up to 500 MeV.

MSSE helps remove vibration from SNS beam line

Experts from the Measurement Science and Systems Engineering (MSSE) Division helped correct excess shaking in the VISION beam line of ORNL's Spallation Neutron Source (SNS) recently, thereby allowing the instrument to begin operating as planned.

SNS is the world's premier neutron source. The VISION beam line and instrument are used to analyze the molecular vibrations in a wide variety of materials, both crystalline and disordered, and over a broad energy range, from under 5 to more than 500 MeV.

The excess vibration was associated with the T_0 Chopper, which helps scientists fine-tune their experiments by blocking fast neutrons.

Being true to their name, fast neutrons reach the chopper nearly instantaneously once a proton hits the SNS mercury target. The chopper is responsible for swinging a 400-pound mass of neutron-absorbing material into place to intercept these fast neutrons, then swinging it out of the way in time to allow slower neutrons to pass by. The forces created in the process are enough to tax even the best-designed equipment.

In this case, the chopper created excessive vibration on the beam line, preventing it from reaching full capacity and preventing scientists from using a secondary chopper. The vibration also threatened to shorten the working life span of the T_0 chopper itself.

MSSE staff were able to diagnose the problem and provide engineering guidance in its solution. Using operation deflection shape techniques, they were able to show that the chopper and the base mounting points were moving together—in phase and at the same relative amplitude—during the run-up to full speed, which is an indication of severe looseness.

SNS engineering and technical staff redesigned the baseplates and removed the existing plate. As seen in the accompanying photo, the concrete grout failed to bond over a significant portion of the original steel plate, allowing it to move.

The case of the unbonded baseplate is not the only instance in which MSSE staff have helped out their SNS colleagues. MSSE is also supporting upgrades to instrument software and hardware systems at SNS.

In addition, MSSE is working alongside SNS colleagues to develop new, one-of-a-kind neutron imaging capabilities. Two major efforts are research and development of neutron microscopy methods using a coded source technique and development of a neutron imaging instrument named VENUS.

The coded source microscopy project is a DOE early career award project of Philip Bingham's, interim group leader for MSSE's Imaging, Signals, and Machine Learning, which is led by MSSE with a goal of neutron radiographic imaging at 1 μm resolution using magnification.

VENUS is a neutron radiography instrument that is being proposed for development at SNS. Initial designs for the instrument have been developed, and a port at SNS has been identified for the instrument.

Currently the VENUS team is working to secure funding to build the instrument.

EESD sparks public interest in clean energy and manufacturing through STEM

Science, technology, engineering, and mathematics (STEM) education can inspire the next generation of scientists and engineers. STEM education initiatives are an important part of professional life at ORNL and within EESD.

BESC teaches about biofuels through museum activities, lesson plans

In collaboration with the Creative Discovery Museum of Chattanooga, Tennessee, the BioEnergy Science Center has developed a set of "Farming for Fuels" lesson plans aimed at fourth-, fifth-, and sixth-grade levels to educate students about the basics of energy production and use. These lessons include basic renewable energy concepts, such as the carbon cycle, lignocellulosic biomass for the production of biofuels, and obstacles to a bio-based fuel economy. The expanded outreach program has now reached teachers and parents nationally by partnering with museums and centers in Tennessee, Georgia, Texas, Michigan, Illinois, Florida, New York, Oklahoma, and Arizona. Another part of this outreach is a series of "science night" programs offered to students and the general public through local schools and museums, which include a number of portable experimental workstations and activities to inform the general public about bioenergy. Last year, 68 science nights were presented nationwide. To date, this program reached more than 60,000 students, teachers, and parents.

The center has also developed a software-based game kiosk called "Road Trip Challenge" to teach students different strategies for transportation energy use. Students design their own cars and select types of fuel for travel to several destinations. The game incorporates lessons to explore fuel efficiency, fuel availability, and environmental impact. A prototype is in use at the Creative Discovery Museum.

UT-Battelle and Advanced Manufacturing support FIRST robotics competition

Four area high school teams supported by UT-Battelle were winners in the FIRST robotics Smoky Mountains Regional Competition at the Knoxville Convention Center in March. Local teams Hardin Valley Academy, Oak Ridge High School, and Halls High School netted the championship title at the regional event, which qualified them, along with Roane County High School, to compete in the national finals. Many ORNL employees dedicated time and expertise to mentor students for the challenge.

Also, thanks to the support of DOE's Advanced Manufacturing Office and Manufacturing Demonstration Facility (MDF) staff, ORNL opened the MDF to local teams as a building and educational space. Several teams took advantage of the opportunity to learn about cutting-edge manufacturing techniques such as additive manufacturing and carbon fiber composites, which they applied to building their robots.

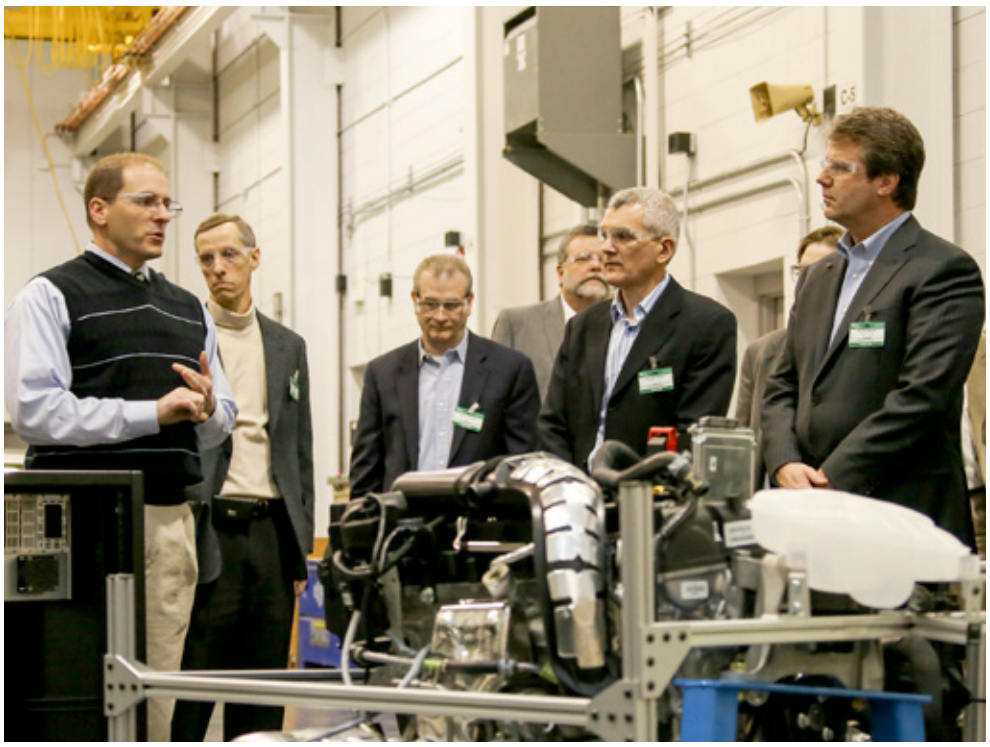
The FIRST robotics competition gives high school teams six weeks to design, build, and program a complex robot that can meet the intense demands of the year's game. Throwing discs and climbing pyramids were among the challenges of the 2013 regional game called "Ultimate Ascent."

Hardin Valley Academy team members react to winning the Smoky Mountains Regional Competition.

Finding New Ways to Reach Students with STEM

Road Trip Challenge is now available as a free application compatible with the Apple iPad. The app teaches the user about switchgrass, ethanol, biofuels, and alternative energy sources as they complete a cross-country road trip that rewards responsible environmental choices with energy credits.

Museum visitors play "Road Trip Challenge" to learn about transportation energy.



Inside the Fuels, Engines, and Emissions Research Center, ORNL's Shean Huff (left) discusses with Ford visitors the catalyst, engine, and vehicle roles in forming the connection between the chemical laboratory, combustion research, and production vehicle applications.

Ford's top management visits ORNL, reviews wide range of R&D capabilities

ORNL hosted a two-day visit for Ford Motor Company's senior managers interested in reviewing current research projects ongoing between the lab and the automaker, as well as exploring the breadth of science and research capabilities available at ORNL. Tour stops included demonstrations by scientists and engineers who specialize in cutting-edge research methods that address some of the greatest challenges facing the automotive industry today.

Project examples given at each tour stop focused on Ford's specific interests in carbon fiber and composites, computational modeling, manufacturing methods and products, engine research and development (R&D), materials characterization, and advanced battery technology. Information gleaned from these areas of research is expected to aid Ford's progress on pressing issues surrounding fuel economy, low emissions, alternative fuels, and electric vehicles.

ORNL's ties with Ford span more than three decades, more recently through a DOE Energy Efficiency and Renewable Energy-funded project in collaboration with Dow Chemical Company to develop low-cost, lightweight carbon fiber composite materials that could be used in vehicle bodies, wind turbines, and other industrial products. Ray Boeman, EESD Strategic Partnerships, presented Ford representatives with a detailed look at ORNL's R&D efforts with Dow and Ford to develop and scale up polyolefin-based carbon fiber that offers the potential for a less expensive alternative to most of today's carbon fiber. The group also toured the new Carbon Fiber Technology Facility, which was commissioned in March.

The tour continued with short presentations highlighting ORNL's recent achievements and ongoing research for the automotive industry. The group visited the High Temperature Materials Laboratory, the National Transportation Research Center, the Oak Ridge Leadership Computing Facility (OLCF), the Spallation Neutron Source, and the Manufacturing Demonstration Facility.

At NTRC, the tour group visited the Fuels, Engines, and Emissions Research Center (FEERC). FEERC has a long-standing relationship with Ford which includes research in combustion, fuels, and emissions controls.

"This exposure broadens Ford's view of ORNL's unique scientific research tools that could foster additional opportunities to address their key challenges in the near- and mid-term, as well as for longer-range objectives," said Ron Graves, director of the Sustainable Transportation Program.

At OLCF, Ford managers saw early results from an ORNL and Ford collaboration created to investigate further stretching the efficiency of internal combustion engines. In particular, the project team taps the lab's massive high-performance computing resources to understand the effects of higher exhaust gas recirculation rates on the combustion process.

Ford's group of ten top research executives, including Paul Mascarenas, chief technical officer and vice-president of Ford Research and Innovation, also met with ORNL director Thom Mason; Jim Roberto, associate director of Science and Technology Partnerships; and Martin Keller, associate laboratory director for EESD.

(Foreground, from left) DOE Assistant Secretary for Energy Efficiency and Renewable Energy David Danielson joined Council on Competitiveness CEO Deborah Wince-Smith, Congressman Chuck Fleischmann, and Governor Bill Haslam for the dedication of the Carbon Fiber Technology Facility.

Carbon fiber facility opens at pivotal time for clean energy science and US manufacturing

The opening of ORNL's new Carbon Fiber Technology Facility (CFTF) on March 26 was exceptionally timely for DOE as the US competes for a leading role in the global clean energy market and for ORNL as it aims to see its cutting-edge science rapidly transformed into commercial technologies. Established under the American Recovery and Reinvestment Act, the facility is also timely for the American manufacturing sector, which has been damaged by the worldwide recession and is striving to restore economic growth and jobs.

The CFTF, a semi-production-scale pilot plant for the scale-up of low-cost carbon fiber, is an example of how these challenges can be addressed—from the early stages of basic scientific research to the manufacture of a finished product.

Ninety percent of carbon fiber currently on the market is reduced from the petroleum-based precursor material polyacrylonitrile, or PAN. The stringy, white PAN fibers undergo processing where time, temperature, and tension convert them into very strong, black carbon fibers.

Carbon fiber composites are so durable they can substitute for steel and aluminum in vehicles and airplanes yet weigh less than steel and aluminum parts. But PAN-based carbon fiber is also expensive. Spools of the stuff can cost as much as $15 per pound or more, making it cost-prohibitive for most manufacturers.

At the opening of the CFTF, David Danielson, DOE's Assistant Secretary for Energy Efficiency and Renewable Energy (EERE), advocated carbon fiber for its ability to reduce vehicle weight by 50% and improve fuel efficiency by up to 35%. He also cited its applications in clean energy technologies, such as its use as a lightweight material for wind turbine blades.

If the cost of carbon fiber could be cut to five or seven dollars per pound, key industries like automotive could afford to use it on a larger scale, said Lee McGetrick, CFTF director. And with the knowledge, tools, and precedent, that market could be based in the United States.

"We translate basic science into the innovation that creates jobs," ORNL Director Thom Mason said at the CFTF ribbon-cutting, "and our new facility will help the US establish a leadership position in the growing carbon fiber manufacturing sector."

The $34.7 million facility, funded through EERE, has a twofold mission: to find cheaper precursor materials than PAN for making carbon fiber and to enhance processing and manufacturing methods so that industry partners can quickly introduce carbon fiber into their products.

The 42,000-square-foot facility houses a one-of-a-kind carbon fiber conversion line that can produce up to 25 tons of carbon fiber per year and is capable of processing a variety of lower-cost precursor materials. The 390-foot conversion line includes a conveyor belt that feeds mat-format precursor materials through large oxidation ovens and carbonization furnaces.

The oxidation process relies on heat and oxygen to chemically alter the precursor material's chemical structure, preparing it for carbonization. Carbonization takes place in high-temperature furnaces that strip the oxidized precursor material down to its carbon atoms.

"The oxidation process is really where the chemistry takes place and is the most critical step in the conversion process," McGetrick said. "Oxidation is an exothermic process and must be precisely controlled. In this phase the material is cross-linking and forming new chemical combinations so that once it reaches the carbonization phase everything but the carbon molecules will burn off."

The CFTF is specially designed to scale-up research that ORNL has been performing over the last decade using lower-cost precursor materials. One of these potential precursors is a compound found in the cell walls of woody plants known as lignin, a common byproduct of the paper and biofuels industries that is much less expensive and more abundant than PAN.

But like the plants from which it is derived, lignin's molecular structure comes in many varieties.

"The chemical composition of lignin varies depending on things like plant type and growing conditions," McGetrick said. "So our biologists, chemists, and materials

scientists are working together to figure out which lignins are best-suited for carbon fiber production and how to optimize the conversion process for lignin-based carbon fibers."

Another precursor researched at the facility is polyolefin, which has a higher carbon yield than PAN and would also be a cheaper alternative, but its performance doesn't yet match PAN-based carbon fiber.

"The carbon fibers we produce are tested for tensile strength, modulus, and other indicators of performance against the expensive carbon fiber already on the market," McGetrick said.

ORNL researchers are currently developing advanced conversion technology based on plasma and microwave-assisted plasma processing technologies. Provisions have been made at the CFTF for the future construction of an advanced technology line—similar in scale to the conventional conversion line—when the technologies are ready for semi-production-scale demonstration.

The CFTF is also partnering with Roane State Community College's Advanced Materials Training Education Center—which is located in ORNL's Science and Technology Park on the main campus—on a workforce development program targeting carbon fiber and composites. Half of the facility's technicians are trained through the center and make up a small, starting class of skilled carbon fiber technicians in the country.

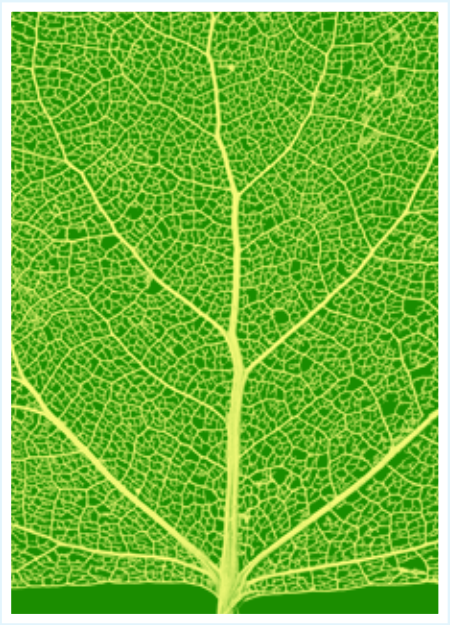
To ensure that the facility's developments in low-cost carbon fiber are practical for American manufacturers, ORNL is working closely with industry to overcome commercialization and manufacturing barriers and realize the strength and energy saving benefits of these new materials. The Oak Ridge Carbon Fiber Composites Consortium, with more than 45 member companies, is just one example which enables these public-private partnerships that provide an important perspective on what is needed to transform R&D results into commercial application.

Additionally, ORNL is now accepting proposals from companies that want to try low-cost carbon fiber to develop new products and tap markets in areas such as transportation, energy production, and infrastructure. Proposals are accepted under a federal business opportunity issued by ORNL's Manufacturing Demonstration Facility.

Taking a Closer Look at Lignin

Recycling biofuels byproducts to make carbon fiber

A joint team of ORNL and UT Center for Renewable Carbon researchers is testing enzymatic and organic solvent extraction protocols on unique Populus trichocarpa (black cottonwood poplar) clones with various lignin precursors. The project will establish an optimal lignin purification protocol and identify lignin characteristics that determine carbon fiber quality, which will hopefully result in new carbon fibers from renewable sources with improved performance characteristics. Led by Tim Tschaplinski and including ORNL's Jonathan Mielenz, Jerry Tuskan, and Amit Naskar, the effort is part of ORNL's integrated Laboratory Directed Research and Development (LDRD) portfolio of lignin-based carbon fiber projects led by Tom Rogers and Naskar.



Regenerable carbon fiber-based filters for indoor air would cut energy waste

The current practice to maintain indoor air quality is to dilute polluted indoor air with fresh outside air, using ventilation rates set by the American Society of Heating, Refrigerating and Air-conditioning Engineers, at a heavy heating and cooling energy penalty. Researchers in the Materials Science and Technology Division (MSTD) have a concept they believe will deliver healthy indoor air through filtration, which will reduce ventilation rates and wasted energy.

A low-cost, regenerable carbon filter material would remove volatile organic compounds (VOCs) from heating, ventilation, and air–conditioning (HVAC) systems in non-residential buildings. Removing VOCs from HVAC systems by molecular filtration could save 0.5 quads of energy annually. The low-cost activated carbon fibers for the proposed VOC filter will be made from lignin precursors, and the system design will enable them to be regenerated periodically.

Collaborative research between MSTD and the Energy and Transportation Science Division's Building Technologies Research and Integration Center has been proposed to the LDRD committee to verify the concept so that outside funding can be attracted for the next steps.

Chad Duty (right), Deposition Science and Technology group leader, describes additive manufacturing to Secretary of Energy Ernest Moniz (left) and Congressman Chuck Fleischmann (center) during a tour of the Spallation Neutron Source.

New Secretary of Energy Moniz praises ORNL facilities during tour

Newly appointed Secretary of Energy Ernest Moniz selected ORNL for his first lab tour as secretary. On June 2–3, Moniz visited the High-Flux Isotope Reactor and the Spallation Neutron Source (SNS), where he praised ORNL for its scientific capabilities for conducting in-depth research on the structure of materials. At SNS, DOE lab directors and Moniz also learned about the Manufacturing Demonstration Facility and its work with industry in neutron scattering to understand residual stress in additive manufacturing. A physicist, Moniz headed the MIT Department of Physics and the Bates Linear Accelerator Center before his appointment as secretary, where he was also the founding director of the MIT Energy Initiative and of the MIT Laboratory for Energy and the Environment. From 1997 to 2001, he served as undersecretary of DOE. Moniz has visited ORNL before as former chair of the Consortium for Advanced Simulation of Light Water Reactors, or CASL, a DOE Energy Innovation Hub.

DOE boosts clean energy technologies and manufacturing through new funding initiative

David Danielson, DOE assistant secretary for Energy Efficiency and Renewable Energy, announced the launch of the department's new Clean Energy Manufacturing Initiative (CEMI) during the opening of the Carbon Fiber Technology Facility (CFTF) at ORNL in March. The initiative is focused on strengthening US competitiveness in the production of clean energy technologies and increasing manufacturing energy productivity.

Danielson stressed CEMI's importance in light of the accelerating global investment in the clean energy sector. "We are at a critical moment in the history of energy in our nation," Danielson said. "The clean energy sector has grown fivefold to more than $260 billion, and these markets will grow into the trillions of dollars in the years to come."

David Danielson at Carbon Fiber Technology Facility opening

Through CEMI, DOE is investing in the clean energy market in two initial ways: through $23 million worth of awards in innovative manufacturing research and development projects and through a $15 million funding opportunity to reduce the manufacturing costs of solar energy technology.

The CFTF provided an exemplary stage for the announcement as DOE's new advanced manufacturing facility dedicated to reducing the cost of carbon fiber—a material critical to producing lightweight vehicles, among other clean energy applications.

Two materials developed by ORNL researchers elected as manufacturing game-changers

The popular science magazine *Scientific American* named two EESD initiatives as "materials that will change the future of manufacturing"—the NanoSHIELD super hard coating and the low-cost carbon fiber precursor research under development at ORNL's new Carbon Fiber Technology Facility (CFTF).

ORNL researchers funded through the Advanced Manufacturing Office, in conjunction with Lawrence Livermore National Laboratory, Carpenter Powder Products, the Colorado School of Mines, and others, received an R&D 100 award last year for NanoSHIELD (or Nano Super Hard Inexpensive Laser Deposited) Coatings, a protective coating for disc cutters and other extreme-duty industrial machines. The NanoSHIELD coating is an iron-based, glassy alloy powder fused to a metal surface by laser deposition.

High-strength steel disc cutters on tunnel-boring machines are sidelined as much as 45% of the time because of wear, which can add millions of dollars to a project. NanoSHIELD improves the lifespan of these cutters by up to 20% because the high concentration of precipitates and refined grain structure reduce the overall wear rate at the surface of the cutter.

"The appeal of amorphous metals in most research is that they are usually four times stronger than their crystalline counterparts," said William Peter, associate division director for Materials Behavior and Processing.

These materials can also be more resistant to corrosion because of their homogenous nature. Amorphous or glassy materials do not possess long-range order, like highly ordered crystalline materials. Compared with conventional steels, the NanoSHIELD iron-based, glass-forming compositions are synthesized into amorphous powders with additional carbon or boron content dissolved in solution. The amorphous powders are then fused to steel components using lasers where the applied material devitrifies. By initiating with an amorphous steel powder and using a fast-cooling process such as laser fusing, the steel devitrifies into sub-micron-sized grains composited with a high concentration of well-dispersed nanocrystalline borides and carbides. The ability to engineer mechanically superior formations and desired nanostructures is possible.

NanoSHIELD protective coating

"More recently we've worked on the chemistries of these coatings," Peter said. "Laser fusing causes convective stirring, so you pull up some of the substrate material and change the chemistry. We have looked at compositions that increase the overall coating hardness and provide high yields in atomization."

Understanding the chemistry also enables the researchers to determine the best chemical composition for providing corrosion-resistant coatings to be used in harsh environments, such as nuclear waste repositories or petroleum-rich sediment. The more recent chemistries allow for austenitic, or stainless steel compositions that are not acceptable to localized corrosion.

"We're looking at a full range of uses, from rock crushing to down-hole drilling to other types of heavy equipment applications," Peter said.

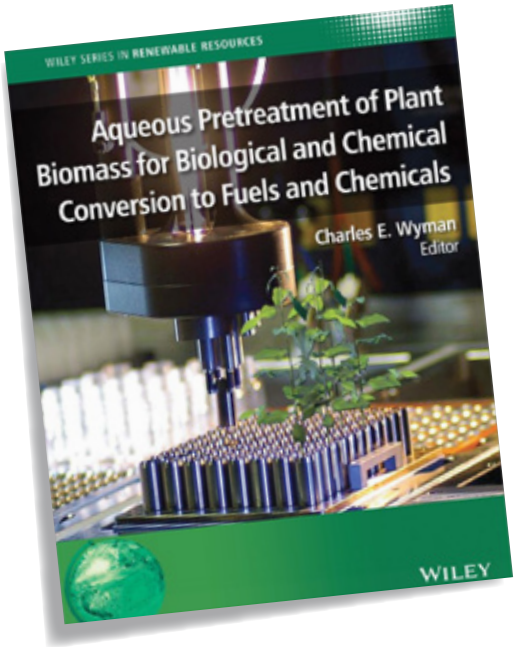
Scientific American also recognized ORNL's CFTF, the site where DOE's new Clean Energy Manufacturing Initiative was announced in March. Low-cost carbon fiber is a technology that is driven, in part, by automotive and aerospace companies looking to improve fuel efficiency with lighter vehicle and aircraft bodies and installations. To read more about the CFTF, see pages 10–11.

Workshop previews emerging advancements in the power grid

More than 100 electricity experts gathered to lay out a research and development roadmap for new power grid technologies at the Advanced Grid Modeling Workshop held in Knoxville on February 5–6. The workshop was co-hosted by EESD's Electricity Technologies Program, represented by organizers Tom King and Penny Humphreys, and the University of Tennessee's Center for Ultra-Wide-Area Resilient Electric Energy Transmission Networks (CURENT).

DOE'S Advanced Grid Modeling program is committed to improving algorithms and computational approaches to shift operational data analytics from a traditionally off-line environment to a fast control, measurement-based environment. The February workshop focused on challenges and advancements in power grid simulation, software tools, and operator platforms.

Victor Zavala of Argonne National Laboratory's Mathematics and Computer Science Division addresses colleagues at the 2013 Advanced Grid Modeling Workshop.



A book co-written by BESC researchers is the 500th publication written or co-written by a BESC author.

Center celebrates 500th publication on its path to improve biofuel production

ORNL's BioEnergy Science Center (BESC) marked its 500th scientific publication in peer-reviewed journals this May during its sixth year of operation. As a DOE Biological and Environmental Research program, BESC is dedicated to researching and eliminating biomass recalcitrance, which is the resistance of plant cell walls to being broken down for fuel production.

The 500th article is one in a collection of articles emphasizing BESC collaborative work in a book, part of the Wiley Series in Renewable Resources, titled "Aqueous Pretreatment of Plant Biomass for Biological and Chemical Conversion to Fuels and Chemicals." The specific 500th publication, an article titled "Xylooligosaccharides production, quantification, and characterization in context of lignocellulosic biomass pretreatment," was co-written by BESC authors Rajeev Kumar, Hongjia Li, and Charles Wyman, the book's editor, with lead author Qing Qing, a former student who is now an assistant professor at Changzhou University in China. Their study reveals important structural information about hemicellulose polysaccharides in plant cell walls and how they are altered during deconstruction to form sugars or other products.

BESC work has been featured in significant scientific journals including *Nature, Science*, and *PNAS*. The collection of BESC publications has been cited more than 3,000 times in other scientific publications.

Director examines ESD's role in energy security, environmental health for global magazine

An interview in *International Innovation* with Jay Gulledge, Environmental Sciences Division (ESD) director, highlights the research and technology developments advanced by ESD that address critical, national, and international energy challenges. The profile "Oak Ridge National Laboratory: Environmental Sciences Division" appears in the June edition of the magazine titled "Planet in Flux: Exploring the Past, Present and Future of the Earth System."

In the Q&A, Gulledge describes ESD's mission as improving energy security, as well as understanding and mitigating the impacts of energy systems on the environment, through basic science, applied engineering, and environmental systems analysis. He identifies current division priorities as climate change and biogeochemical research that could inform climate and environmental policies.

New developments in environmental science research, such as the dependence on ever-expanding databases and complex climate and ecosystem models, require powerful and specialized tools. Gulledge cites ESD access to ORNL's sophisticated research facilities, including the Titan supercomputer, the Spallation Neutron Source, and monitoring environments (greenhouses, a seafloor process simulator, and aquatic ecology laboratories, among others).

International Innovation is distributed globally to scientific, technical, and research communities. To access the issue featuring ESD, visit http://www.research-europe.com/magazine/REGIONAL/NA13/index.html.

Among research facilities available to ESD are monitoring environments, such as the seafloor process simulator (top) and greenhouses (right).

DOE hub looks to make rare earth market accessible for clean energy technologies

With a June 21 event at ORNL, the Critical Materials Institute (CMI) kicked off a decade-long quest to ease the demand for rare earth materials in the United States.

Rare earth materials are crucial to advancing several clean energy technologies, such as fluorescent lamps containing the scarce elements europium and terbium and a high-efficiency model of wind turbine called a direct-drive turbine.

Martin Keller, associate lab director for EESD and a member of CMI's management oversight committee, introduced keynote speaker and CMI director Alex King. Keller and King addressed researchers on the brink of beginning their missions for CMI.

"Now the hard part starts, because we have to deliver on what we promised," Keller said. CMI aims to create a stable market for rare earth materials by diversifing supply, developing substitutes for rare earth elements, and driving reuse and recycling of materials in manufacturing.

CMI is one of five DOE Energy Innovation Hubs designed to expedite the transformation of research-driven solutions into industrial applications for the nation's most critical energy challenges.

employee excellence

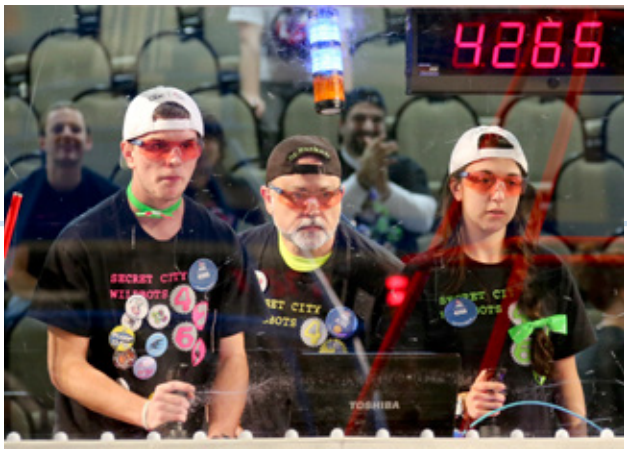
Shahab Sokhansanj, Environmental Sciences Division (ESD), has been elected a Fellow of the Engineers of Canada (FEC). The Association of Professional Engineers of British Columbia and the Canadian Council of Professional Engineers provided the FEC designation to Shahab, citing his achievements and service to the engineering profession.

Carol Wood, ESD's Toxicology and Hazard Assessment Team, has been elected to a four-year term on the Board of Directors of the American Board of Toxicology (ABT). Carol, who was nominated by the president of ToxPath, Inc., and former ABT President of the Board Ernest McConnell, was elected from more than 40 nominees.

David Greene, Energy and Transportation Science Division (ETSD), received an award from DOE's Clean Cities Program in recognition for his contributions as a "Trusted Advisor and Lifetime Mentor to the Clean Cities Program" at their 20th anniversary celebration held in Washington, DC, June 24.

Richard Willems, MSSE, received a Significant Event Award for "Transition to Practice" program technology for the Department of Homeland Security.

Andrea Rocha, Biosciences Division, was selected by the American Society for Microbiology's (ASM) Committee on Microbiological Issues Impacting Minorities to receive a 2013 travel award to attend the ASM general meeting in Denver. Selection of the award was based on letters of recommendation, activities in mentoring, commitment to diversity, and research.



Mark Buckner, MSSE, has received a Woodie Flowers Finalist Award for his work as a FIRST robotics mentor. The award recognizes one adult mentor at each regional FIRST robotics competition who was nominated for his or her ability to "lead, inspire, and empower."

Tom Wilbanks, ESD, will receive Trinity University's 2013–2014 Distinguished Alumni award in January. This award is the highest honor conferred by Trinity University's Alumni Association and is presented to those who have distinguished themselves through exceptional personal or professional achievement. A copy of the award certificate he received as a contributor to the Intergovernmental Panel on Climate Change Nobel Prize in 2007 will be dedicated and displayed in Trinity's new Center for Science and Innovation. Tom received his BA from Trinity University in 1960.

Virginia Dale, ESD, participated in the White House Women's Leadership Summit on Climate and Energy, which brought 100 women leaders together for a dialogue on the President's climate and energy agenda. The gathering provided an opportunity for interaction among women who are leading the nation in outreach, education, and research.

Alan Barker, Measurement Science and Systems Engineering Division (MSSE), has received the Eaton Award in Design Excellence, an early career award, from the Purdue University Electrical and Computer Engineering Department.

Kathy Huczko, ESD, has been named Corporate Secretary for the East Tennessee Chapter of the Project Management Institute.

The Biological and Environmental Research Information System (BERIS) has won two Awards of Excellence in the Society for Technical Communication 2012–2013 International Summit Competition. Awardees are BERIS staff members **Kris Christen**, **Holly Haun**, **Marissa Mills**, **Sheryl Martin**, **Judy Wyrick**, and group leader **Betty Mansfield**; former BERIS member **Jennifer Bownas**; and Creative Media's **Brett Hopwood**. These communication tools were prepared for DOE's Basic Energy Sciences program. The awarded publications are the *Basic Energy Sciences 2011 Summary Report* and the double-sided poster *Powering the Future with a New Era of Science*. Over the past 23 years, the group has received some 75 awards, including three Best of Shows.

New patents show big results for directorate R&D

"Array of Aligned and Dispersed Carbon Nanotubes and Method of Producing the Array," invented by Ilia N. Ivanov (Center for Nanophase Materials Sciences, CNMS), John T. Simpson (Measurement Science and Systems Engineering Division, MSSE), and Troy R. Hendricks

"Method for Morphological Control and Encapsulation of Materials for Electronics and Energy Applications," invented by Ilia N. Ivanov (CNMS) and John T. Simpson (MSSE)

"Variable Waveband Infrared Imager," invented by Scott R. Hunter (MSSE)

"Retinal Instrument," invented by Charles L. Britton (Energy and Transportation Science Division, ETSD), Brian R. D'Urso (MSSE), Edward Chaum (MSSE), John T. Simpson (MSSE), Justin S. Baba (MSSE), Nance Ericson (ETSD), and Robert J. Warmack (MSSE)

"Close-Packed Array of Light Emitting Devices," invented by Ilia N. Ivanov (CNMS) and John T. Simpson (MSSE)

"Mode-Synthesizing Atomic Force Microscopy (MSAFM) and Mode-Synthesizing Sensing (MSS)," invented by Ali Passian (Biosciences Division, BSD), Thomas George Thundat (BSD), and Laurene Tetard

"Optical Backscatter Probe for Sensing Particulate in a Combustion Gas Stream," invented by William P. Partridge (ETSD) and James E. Parks (ETSD)

Oak Ridge National Laboratory
Energy and Environmental Sciences Directorate
P.O. Box 2008
Oak Ridge, TN 37831

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

Two furnaces at the Carbon Fiber Technology Facility heat a precursor material, first for the oxidation process that alters the material's chemical structure, and then for the carbonization process that burns away all but the carbon atoms.