TransForum

News from Argonne's Transportation Technology R&D Center
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Argonne NATIONAL LABORATORY

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Shown here
Bloom and Javier Bareño prepare a sample of battery materials for testing in the Post-Test Facility.

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New Facility Investigates Battery Wear and Tear

With Argonne's new Battery Post-Test Facility (PTF), scientists have the unique ability to dissect, harvest and analyze battery materials to gain a better understanding of exactly what changed, so they can improve the performance, life and safety of batteries.

An X-ray photoelectron spectrometer (XPS) is integrated into the Post-Test Facility's large, central glove box. The XPS is used to gather information regarding the electronic structure of materials.

NEW FACILITY INVESTIGATES BATTERY WEAR AND TEAR

Argonne scientist Nancy Dietz Rago analyzes results in the Post-Test Facility. After a battery sample is characterized in the large glove box, it is transferred without exposure to air to the scanning electron microscope for detailed, microstructural characterization.

Argonne's new Battery Post-Test Facility (PTF) will allow scientists to help battery developers and manufacturers identify the exact mechanisms that limit the life of their battery cells. In the past, the cause of performance degradation could only be inferred.

"Post-test analysis is a natural extension of the battery testing that Argonne has been doing for many years," said Argonne chemist Ira Bloom, who will run the PTF. "As a battery ages during use or testing, performance degrades and changes occur in the battery materials. Post-test analysis lets us see what physical changes occurred."

Bloom and his team will use the PTF to dissect, harvest and analyze battery materials to gain a better understanding of exactly what changed, so they can improve the battery's performance, life and safety. Using new, aged and abused batteries, the researchers will characterize factors such as remaining electrode capacity, surface chemistry, electrolyte chemistry; and electrode morphology, composition and phase distribution.

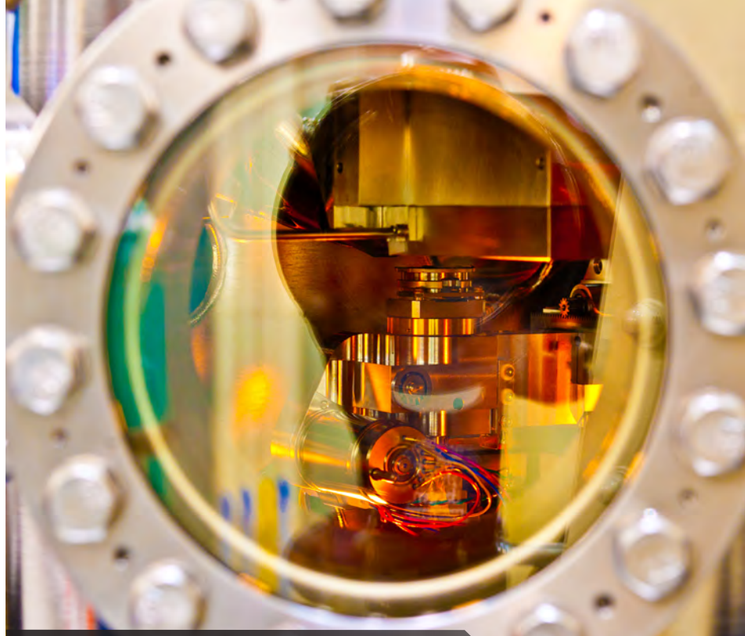
The PTF, which opened in late 2011, is one of the few known facilities in the world capable of conducting this kind of research and the only one doing work at this scale. The new Argonne lab can handle cells up to 300 Ah, while other facilities like this are typically limited to about 1-2 Ah. Cells of commercial interest are in the range of 10-100 Ah.

Bloom believes the PTF's capabilities will appeal to battery developers looking for answers about performance degradation.

Another unique aspect of the PTF is that all work, from dismantling the cell to harvesting and analyzing its components, is performed in one glove box.

"All the materials that we handle in the PTF are air-sensitive, meaning that they will degrade or decompose on contact with air or moisture," said Bloom. "The advantage of doing everything in one glove box is that it keeps the samples pristine and intact, yielding more information about what's really going on in later stages of characterization and analysis."

Argonne scientist Ira Bloom prepares to open a lithium-ion cell. Prior to opening the cell, a thermocouple is attached to provide information on cell temperature.



A view of the heart of the X-ray photoelectron spectrometer unit, showing the servo-motor and the stage that it moves.

Performing this work in an inert atmosphere also guarantees that observed changes in battery chemistries or materials are due to electrochemical operation, rather than sample manipulation.

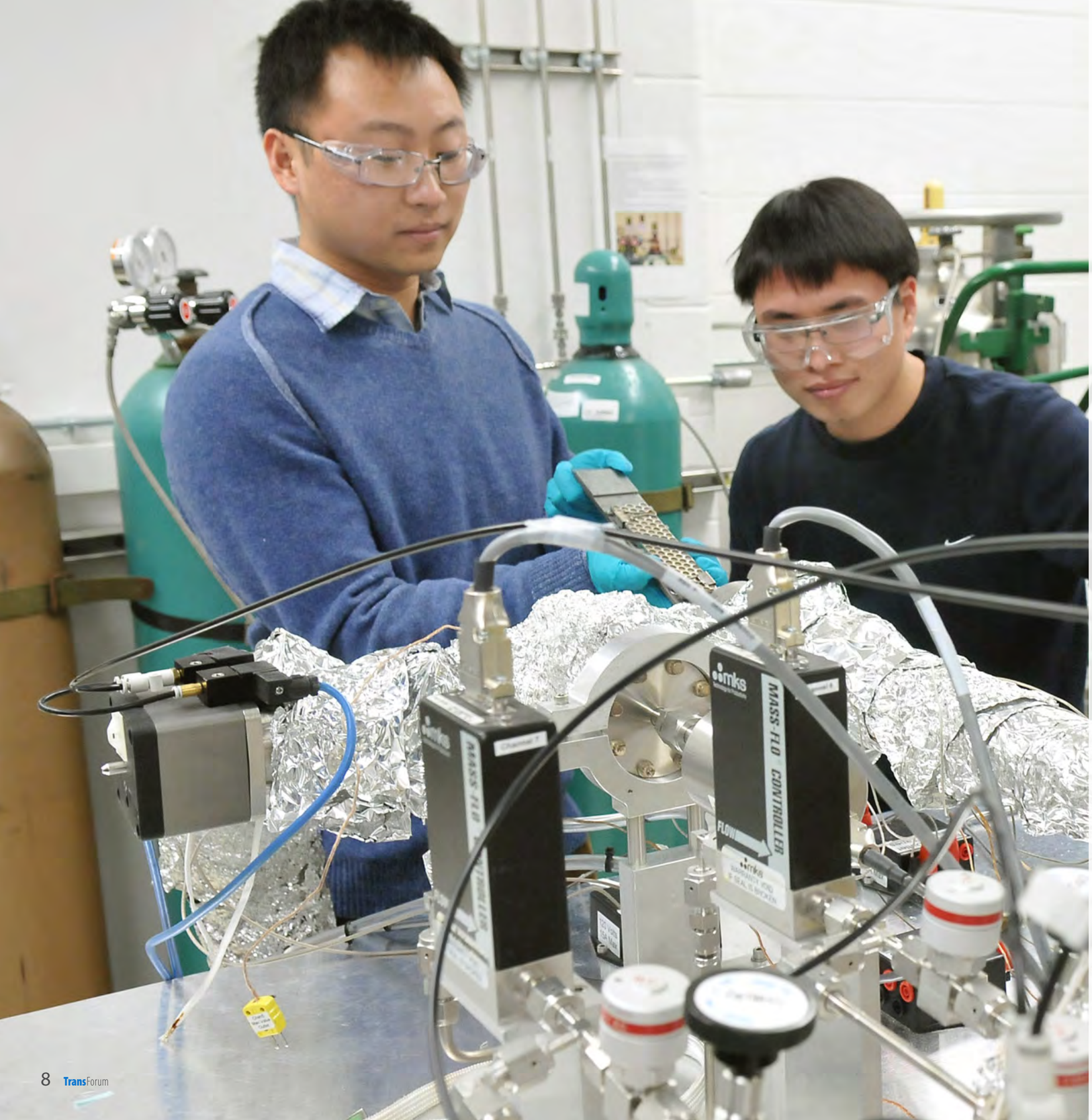
> The PTF is one of the few known facilities in the world capable of conducting this kind of post-test battery research and the only one doing work at this scale.

The PTF complements Argonne's Electrochemical Analysis and Diagnostics Laboratory, where batteries from both private and government-funded initiatives have been tested for more than three decades.

While its current focus is lithium-ion batteries, the PTF is highly flexible; its equipment can characterize materials from any type of battery, from lead-acid (found in most of today's cars) to cutting-edge technologies, such as lithium-air.

Funding for this work is provided by the U.S. Department of Energy's Vehicle Technologies Program.

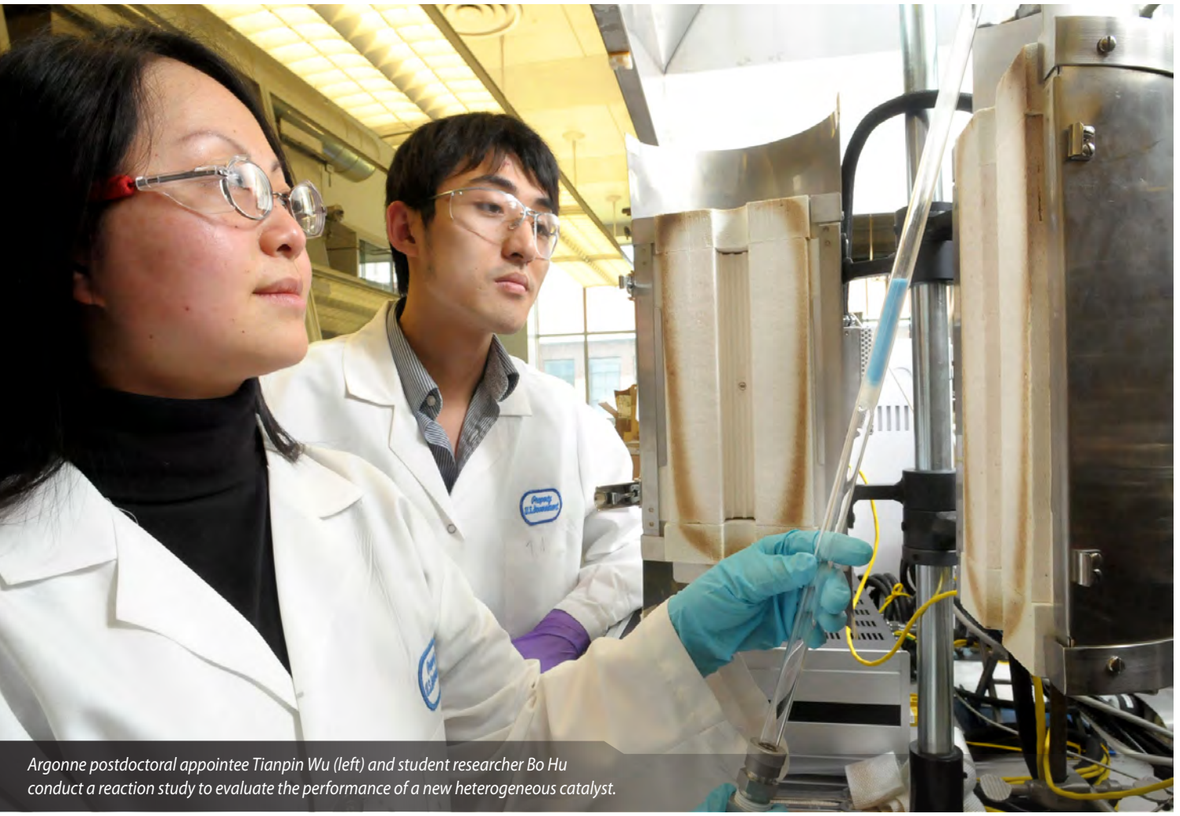
For more information, contact Ira Bloom, ira.bloom@anl.gov



Unlocking the Door to Better Biofuels through Catalysis

Biofuels—derived from biomass such as plants—are often seen as one of the best solutions for reducing our nation's dependence on petroleum. While nature does a good job of creating fuel from plant matter using enzymes, so far there are no ideal man-made methods that replicate this efficient natural process.

Argonne postdoctoral appointees Yu Lei (left) and Junling Lu load a catalyst sample into one of the laboratory's atomic layer deposition systems.



Argonne postdoctoral appointee Tianpin Wu (left) and student researcher Bo Hu conduct a reaction study to evaluate the performance of a new heterogeneous catalyst.

Enter the Institute for Atom-efficient Chemical Transformations (IACT), a multi-institutional, multi-disciplinary Energy Frontier Research Center based at Argonne and funded by the U.S. Department of Energy. IACT's primary focus is advancing the science of catalysis to improve the efficiency of producing fuels from biomass.

"We face a real challenge in the catalysis and conversion process, which is that nature and evolution have already fashioned far better catalysts than we could create on our own—namely enzymes," said IACT director Christopher Marshall. "In order to aid the transition away from a petroleum-based economy, we have to take our cues from the catalysts that have existed for millions of years."

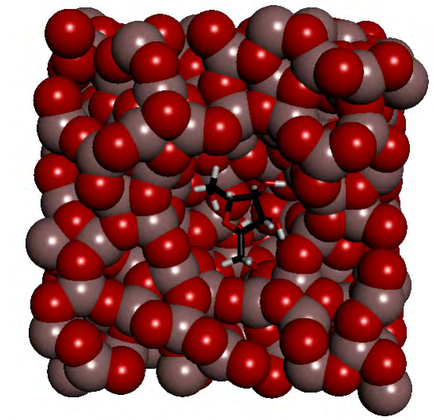
Instead of enzymes, modern industrial approaches to biofuels production depend on catalysis, which transforms materials through chemical reactions. Unfortunately, modern commercial catalytic methods require large amounts of hydrogen, which is produced using high-energy, petroleum-based feedstocks. The challenge for IACT scientists lies in identifying biologically inspired approaches to catalysis that can extract hydrogen directly from plant matter as part of the biofuels manufacturing process.

"The current methods of getting the hydrogen we need to do the conversion require the input of just as much energy as we'd get out of the fuels we'd be trying to create," Marshall said. "In order to really get biofuels to take off, we first have to tackle the problem of where we're going to get all the hydrogen we need."

> IACT seeks to advance the science of catalysis to improve the efficiency of producing fuels from biomass.

IACT brings together some of the world's best scientists at Argonne, Northwestern University, the University of Wisconsin-Madison, Purdue University and Brookhaven National Laboratory to solve the difficult challenges associated with catalysis for biofuels. The primary tasks for IACT researchers are identifying and advancing self-sustaining catalytic methods that draw their inspiration from nature.

Along those lines, IACT researchers are exploring ways to better apply a traditional element in the catalytic production of biofuels—precious metals—through methods that render the metals more catalytically productive. They are constructing complex "nanobowls" that appear to be very effective catalytic structures.



Nanobowls such as the one shown in the middle of this image can serve as the heart of large-scale, energy-efficient, and environmentally benign chemical transformations. They can stabilize more active nanosized metals and create bifunctional sites similar to those seen in enzymes.

According to Marshall, "while scientists know that small metal particles can be more effective than larger particles for catalysis, IACT researchers have determined that maintaining the small size of those particles throughout the catalytic process is even more important. IACT researchers have found that atomic layer deposition (ALD), a process that deposits precious metal nanoparticles on a substrate and then adds protective walls around the metal, appears to boost the metals' catalytic capabilities. This facilitates creation of nanobowls that can serve as the heart of large-scale, energy-efficient and environmentally benign chemical transformations."

As for the hydrogen question, IACT researchers have made great progress in creating platinum-molybdenum alloys that are very effective for aqueous reforming of biomolecules (glycerol, for example) to hydrogen at moderate temperatures.

"This process is an important key to deriving hydrogen directly from biomass, a self-sustaining reaction that's needed to make the creation of biofuel from biomass a viable alternative to petroleum-based fuels," said Marshall.

IACT is an Energy Frontier Research Center supported by the U.S. Department of Energy, Office of Basic Energy Sciences.

Argonne postdoctoral appointee Junling Lu evaluates a sample in one of Argonne's catalyst testing systems.

For more information, contact Christopher Marshall, marshall@anl.gov

IACT website:
www.iact.anl.gov

IACT video:
http://www.youtube.com/watch?v=Rq2dOsU_pKY

Nanofluids Improve Performance of Vehicle Components

Argonne researchers are working with two industrial partners to create nanofluids that improve the cooling of power electronics in hybrid electric vehicles.

These new coolants can lessen the need for heat exchangers, which could result in smaller cooling systems and lighter vehicles.

"Fluids containing nanoparticles have a proven ability to increase thermal conductivity and heat transfer and hence reduce the size, weight and number of heat exchangers for cooling power electronics," said Argonne researcher Jules Routbort.

Using silicon carbide nanoparticles from partner Saint Gobain, Routbort and his colleagues have created an ethylene glycol/water nanofluid that carries heat away 15 percent more effectively than conventional fluids. And working with industrial partner Valvoline, they've developed a graphite-based nanofluid that has an enhanced thermal conductivity 50 percent greater than the base fluid, which would, under specific conditions, eliminate the need for a second heat exchanger for cooling power electronics.

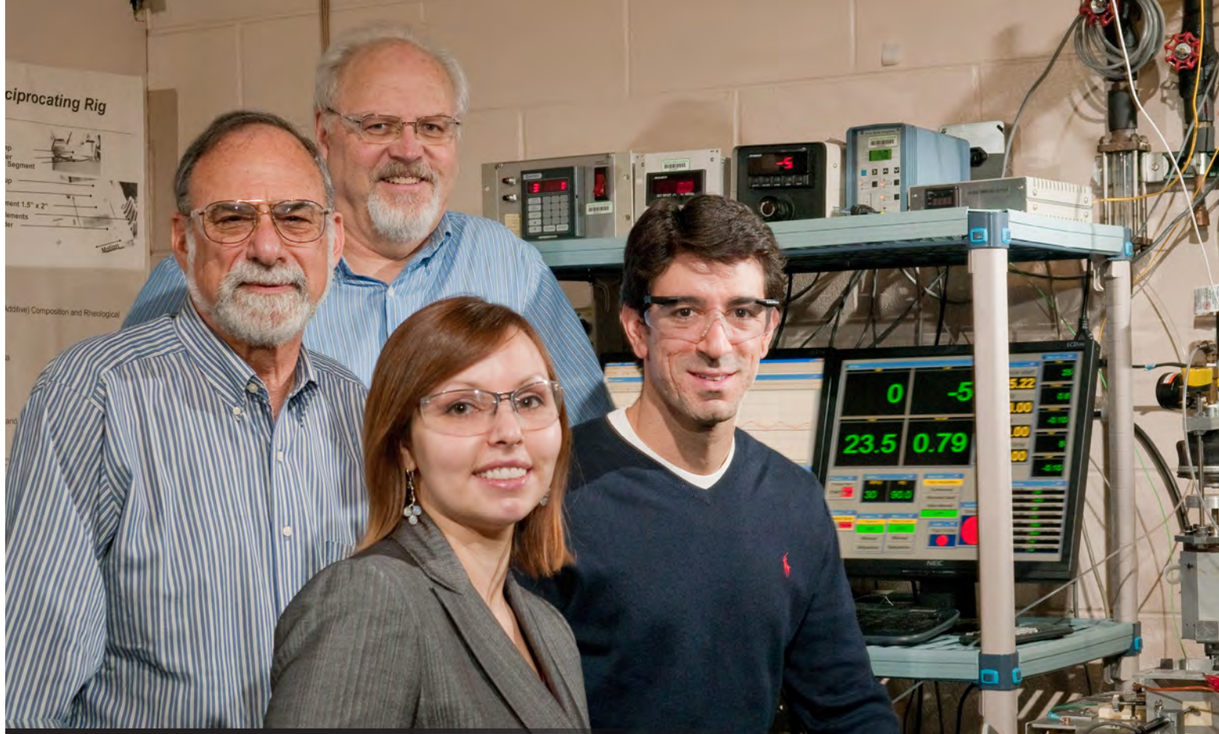
> Working with Valvoline, Argonne developed a graphite-based nanofluid that enhances thermal conductivity.

To develop nanofluids for heat transfer (i.e., cooling), the Argonne team used a systems engineering approach. Rather than looking at each individual property of the system (e.g., nanoparticle material, concentration, shape, size, etc.), the scientists analyzed the behavior of the whole system to study how nanofluid systems work. Using this scheme, they discovered that particle size and concentration were key to designing nanofluid systems.

Part of the current research effort focuses on a nanolubricant based on poly-alpha-olefin (or PAO). When combined with nanoparticles of molybdenum disulfide (MoS_2) and a surfactant, the resulting lubricant shows reduced friction and wear, thus increasing the lifetime and fuel efficiency of vehicle components.

Using Raman spectroscopy, Routbort's team showed that the interaction between the nanoparticles and rubbing surfaces produced a very thin film between contacting parts. This film is responsible for the improved properties.

Argonne chemist Elena Timofeeva conducts a quality control evaluation of thermal nanofluids.



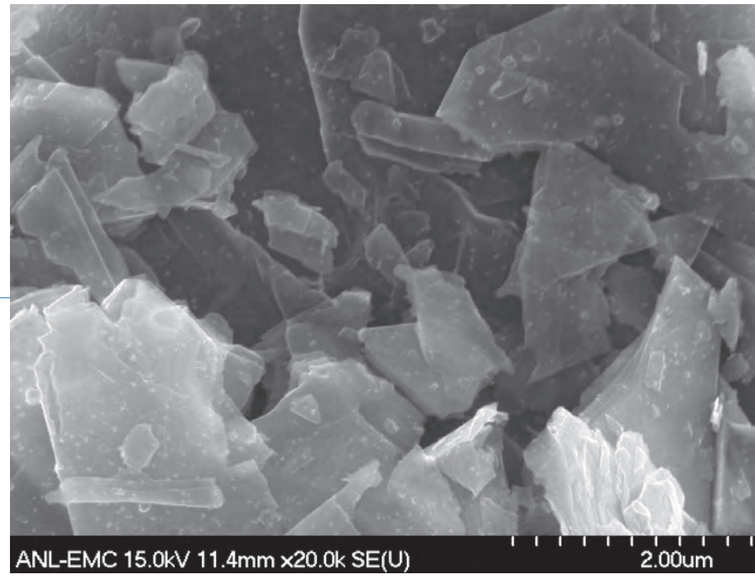
Argonne's nanofluid research team (clockwise from left) Jules Routbort, George Fenske, Nicholaos Demas and Elena Timofeeva.

Future work will concentrate on further development of carbon-based nanofluids for hybrid electronic cooling that result in higher heat transfer coefficients while keeping the viscosity low.

Funding for this work is provided by the U.S. Department of Energy, Energy Efficiency and Renewable Energy, Vehicle Technologies Program and Advanced Manufacturing Program.

For more information, contact
George Fenske, fenske@anl.gov

Our colleague, Jules Routbort, passed away suddenly just as this issue was going to print. He was an esteemed scientist at Argonne for 44 years, and a dedicated and enthusiastic mentor who taught many young researchers the joy of doing important work. His integrity, creativity, dedication and sense of humor will be deeply missed. Argonne and the world of science have suffered a great loss.



Scanning electron microscope image of MoS_2 powders, which are used in the Argonne-developed nanolubricant. Particle sizes range from 50 nanometers up to 2 microns.

Electric Vehicle-Smart Grid Interoperability Center Established at Argonne

As the U.S. home of a new Electric Vehicle-Smart Grid Interoperability Center, Argonne National Laboratory will play a key role in supporting global standardization activities to ensure that future electric vehicles (EVs) and charging stations worldwide will work together seamlessly.

In November, the U.S. Department of Energy (DOE) and the European Commission's (EC) Joint Research Centre (JRC) announced plans to establish two Electric Vehicle-Smart Grid Interoperability Centers, with the European center to be housed at JRC facilities in Ispra, Italy.

Achieving interoperability between EV and electric vehicle supply equipment (EVSE) will require standards for connectivity and communication that ensure that (1) all EVs can recharge at any charging station, and (2) EVs and/or EVSE can communicate with the utility/grid operator to enable billing or more sophisticated interactions, such as two-way communication and load management.

The goals of the international partnership are to develop and test vehicle-grid interface technologies, support data-driven standards refinement and development, and take on projects that enhance interoperability. The Argonne center will build upon the laboratory's ongoing efforts to develop technologies and standards related to the grid and electric-drive transportation.

> Standardizing between the U.S. and Europe will allow a multinational company to build components here that will be applicable there, and vice versa.

Argonne's Keith Hardy (center) discusses EV-grid interoperability issues with DOE Secretary Steven Chu (left) and DOE Assistant Secretary of Policy and International Affairs David Sandalow at the Transatlantic Economic Council meetings on Nov. 28-29 in Washington D.C. (Photo courtesy of the U.S. Department of State).

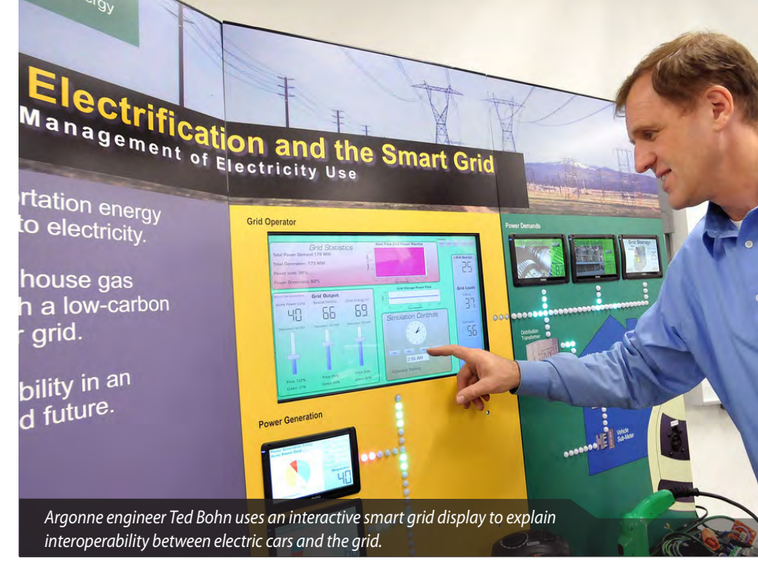
Keith Hardy, a senior technical advisor at Argonne, believes the partnership can help accelerate the deployment of electric cars by minimizing the engineering, development and manufacturing costs for automotive and component companies.

"Working with Europe is a perfect opportunity," Hardy said. "We share an automobile industry. We share a supplier industry. So this situation is targeting standardization between the U.S. and Europe to allow a multinational company to build components here that will definitely be applicable there, and vice versa."

"Pressure to standardize has increased because global automotive manufacturers and suppliers are evaluating technical solutions and must make investment decisions to support production of plug-in vehicles for the 2014 model year," he added.

In addition to helping industry, efforts to harmonize standards are expected to boost consumer confidence in electric cars by paving the way for an EV infrastructure that would make recharging a battery as simple and convenient as refilling a gas tank. Global standardization will allow seamless operation of EVs and EVSE across borders and service areas of different utilities.

In Argonne's Power Electronics Lab, researchers are evaluating communication technologies for vehicle-grid connectivity to validate standards, while plotting a deployment path for charging infrastructure.



Argonne engineer Ted Bohn uses an interactive smart grid display to explain interoperability between electric cars and the grid.

A DOE-JRC task force is being formed to prepare a work plan for the two interoperability centers outlining common goals and final targets.

Funding for this work is provided by the U.S. Department of Energy, Energy Efficiency and Renewable Energy, Vehicle Technologies Program.

For more information, contact Keith Hardy, khardy@anl.gov

Argonne researcher Glenn Keller charges a test vehicle using the laboratory's solar-powered charging station.

Argonne's Vehicle Data Resource is Online

Using Argonne National Laboratory's Downloadable Dynamometer Database (D3), you can now access data critical to the development and commercialization of next-generation vehicles. This data resource is available free to the public and other researchers worldwide via a page on Argonne's transportation website.

At Argonne, one of the tasks of its Advanced Powertrain Research Facility (APRF) is to measure and collect the numbers that reveal important information on performance, fuel economy, energy consumption and emissions output. The data—which you can access from the D3—results from vehicle benchmarking and testing activities conducted by transportation researchers using the facility's two-wheel drive (2WD) and four-wheel drive (4WD) dynamometers and state-of-the-art instrumentation.

The D3, located at www.transportation.anl.gov/D3, offers easy and fast access to data from all kinds of makes and models of vehicles including hybrid electric vehicles, plug-in hybrid electric vehicles, electric cars, and alternative and conventional fuel vehicles. To view available data, simply click on a vehicle's photo and you will be able to download test cycles (UDDS, HWYx2, USO6x2, SS Stairs and more), levels 1 and 2 testing reports and presentations, signal lists and long-term mileage factsheets. Information may vary per vehicle and new data is being added all the time.

"We had a previous version of the D3, but it was hard to use and maintain. We decided to redo the database with a point-and-click set up so that more researchers could get to it and use it easily," said Glenn Keller, a principal project engineer behind the D3. "With our state-of-the-art facilities and a wide range of vehicle expertise, we're ideally positioned to collect this data, and we want to share it with everyone. Our research here is helping facilitate more widespread adoption of alternative fuels and advanced vehicle powertrains."

Vehicle data is used to develop advanced technology.

Vehicles are put through all their paces and more, as each component and powertrain aspect is rigorously studied. At the APRF, researchers are able to:

- Simulate road load and tractive effort of vehicles using 2WD and 4WD dynamometers (vehicles with weight of 12,000 and 14,000 pounds, respectively);
- Measure fuel usage and criteria emissions of advanced technology vehicles, including super ultra-low emission vehicles;
- Instrument components using innovative techniques that measure a full inventory of power and energy flows through vehicle powertrains; and
- Design and implement *in-situ* vehicle torque sensors to determine the precise efficiency of the major components in the entire driveline system.

Working with the U.S. Department of Energy (DOE) and the automotive industry, APRF research helps provide solutions to significantly improve vehicle fuel efficiency and emissions. In addition to providing unbiased research findings to researchers and stakeholders, vehicle data obtained in the APRF is used to support DOE's transportation goals and policies, to help develop advanced technology and push it into the marketplace, and to show the benefits of alternative fuels and technology.

Argonne researcher Mike Kern takes a vehicle through city and highway driving cycles at the Advanced Powertrain Research Facility (APRF). The APRF's dynamometers allow researchers to simulate real-world driving conditions in a controlled laboratory environment.

Argonne researchers Henning Lohse-Busch (left) and Eric Rask prepare for vehicle benchmarking tests.

The D3 and APRF are funded by the U.S. Department of Energy, Energy Efficiency and Renewable Energy, Vehicle Technologies Program.

Argonne researcher Neeraj Shidore prepares a plug-in hybrid electric vehicle (PHEV) battery for testing on the laboratory's Battery-in-the-Loop system.

For more information, contact Glenn Keller, gkeller@anl.gov

Downloadable Dynamometer Database (D3) website: www.transportation.anl.gov/D3

Advanced Powertrain Research Facility (APRF) website: http://www.transportation.anl.gov/facilities/aprf.html

GREET Evaluates New Fuels and Sources for Bigger Impacts

Algae and fast-growing grass are some of the more unusual sources of alternative fuels for tomorrow's world. Argonne's GREET (Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation) model now takes these into account by offering even more ways to analyze the energy and emission impacts of producing alternative fuels and their use in advanced vehicles.

The GREET team, led by senior scientist Michael Wang, recently released an updated version of the model named GREET1_2011, which adds shale gas, jet fuels and algal fuels—along with a host of other new features—to a model that is used worldwide and already considered by many to be the "gold standard" for life-cycle analysis.

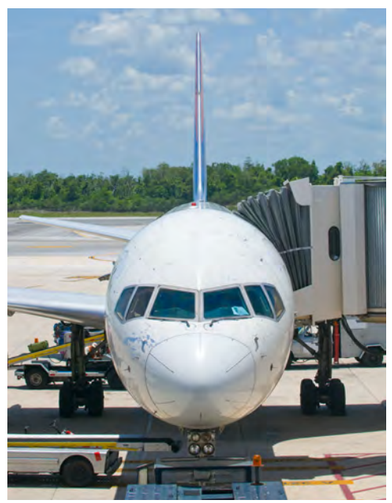
"We've added shale gas because it is perceived as a game-changing resource, which could permit expanded natural gas usage," said Amgad Elgowainy, one of the chief developers of GREET. "In addition, the interest in low-carbon jet fuels and algae-based fuels motivated us to examine their impacts on the planet."

Other new items in GREET's menu include production of liquid fuels, more like gasoline and diesel, from fast pyrolysis (thermal decomposition) of biomass, and options for including energy uses and emissions associated with the construction of petroleum and natural gas wells, as well as coal mines.

> GREET — used worldwide and considered by many to be the "gold standard" for life-cycle analysis

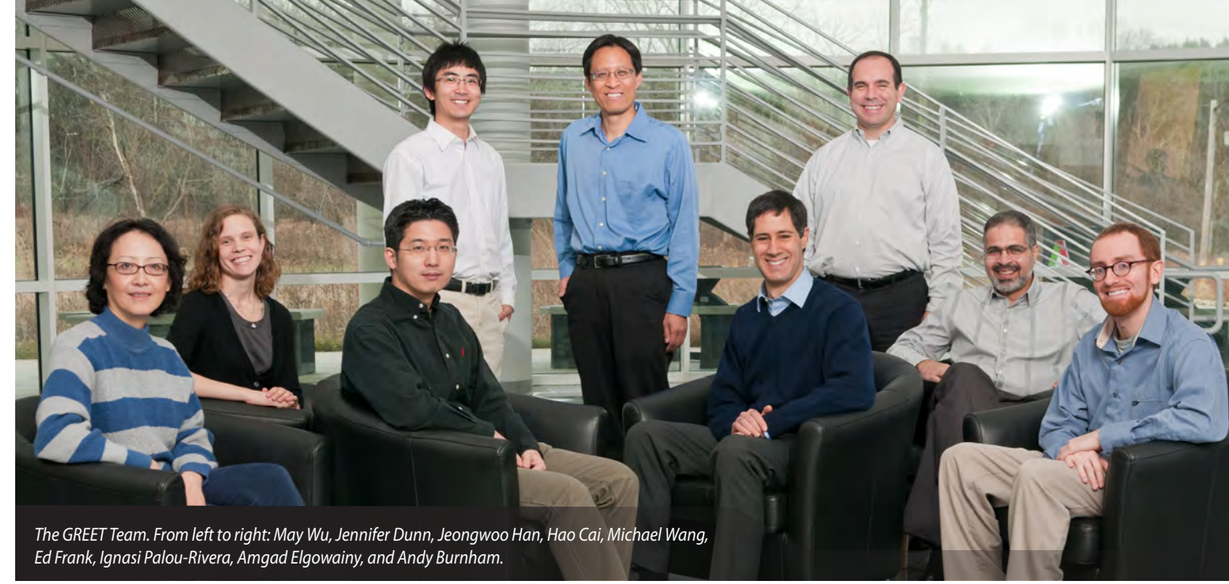
Shale gas, located under and between shale rocks, has become an important source of natural gas in the United States. It is predicted that by 2030, about half of all U.S. natural gas could come from shale gas. GREET notes this importance with its new shale gas analysis, which includes well drilling, gas recovery and processing. Associated gas, carbon dioxide and methane emissions from flaring, methane leakage, transportation and distribution variables are sources of greenhouse gas emissions. The study, "Life Cycle Greenhouse Gas Emissions of Shale Gas, Natural Gas, Coal and Petroleum," by Argonne researcher Andy Burnham and others fully describes the impact of shale gas.

Micro-algae is being explored as a source of biofuels because it creates a huge amount of biomass per acre compared to other bio-feedstock sources. The oil in the algae can be converted into fuels as a viable alternative to petroleum diesel and gasoline. So GREET has now added algae pathways to its lineup. The pathways explore options for the production of bio-oil, including algae growth, dewatering and oil extraction, as well as algae-growth nutrient and energy needs. The new pathways in GREET are accompanied by a new Algae Process Description (APD) tool to dynamically link different algae pathway stages together. The algae study is described in "Life-Cycle Analysis of Algal Lipid Fuels with the GREET Model," an Argonne report authored by Ed Frank and others.

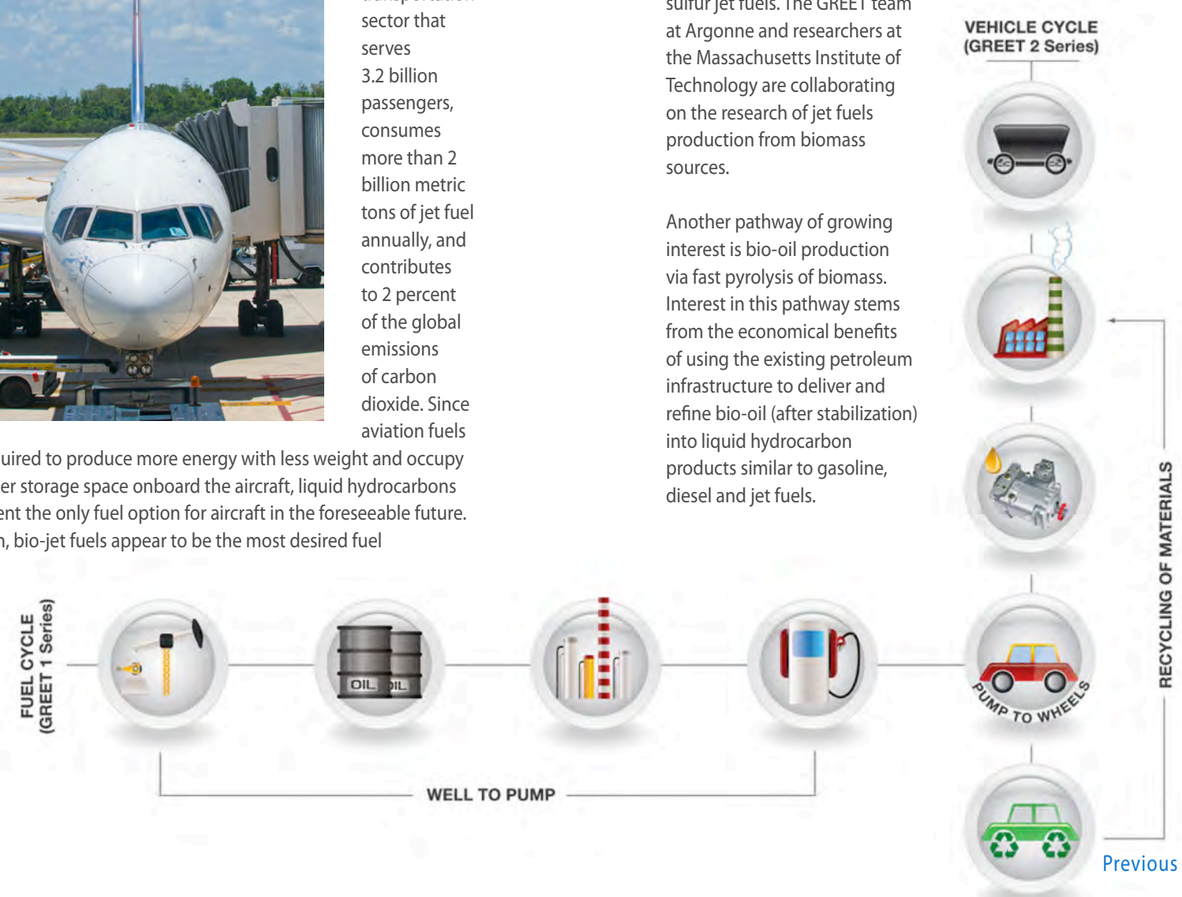


Aviation is a fast-growing transportation sector that serves 3.2 billion passengers, consumes more than 2 billion metric tons of jet fuel annually, and contributes to 2 percent of the global emissions of carbon dioxide. Since aviation fuels are required to produce more energy with less weight and occupy a smaller storage space onboard the aircraft, liquid hydrocarbons represent the only fuel option for aircraft in the foreseeable future. As such, bio-jet fuels appear to be the most desired fuel product from a limited biomass feedstock source. The aviation fuel pathways in the new version of GREET include the refining of conventional petroleum and hydro-treating of pyrolysis oil to produce jet A and ultra-low sulfur jet fuels. The GREET team at Argonne and researchers at the Massachusetts Institute of Technology are collaborating on the research of jet fuels production from biomass sources.

Another pathway of growing interest is bio-oil production via fast pyrolysis of biomass. Interest in this pathway stems from the economical benefits of using the existing petroleum infrastructure to deliver and refine bio-oil (after stabilization) into liquid hydrocarbon products similar to gasoline, diesel and jet fuels.



The GREET Team. From left to right: May Wu, Jennifer Dunn, Jeongwoo Han, Hao Cai, Michael Wang, Ed Frank, Ignasi Palou-Rivera, Amgad Elgowainy, and Andy Burnham.



Producing environmentally sustainable fuels that are compatible with existing fuel infrastructure and vehicle technologies could satisfy society's growing need for energy and avoids the risk of investment associated with new developments. GREET examined the fast pyrolysis of corn stover and forest residue, as well as the stabilization and upgrading of pyrolysis oil to produce renewable gasoline, diesel and jet fuels. This study is described in "Well-to-Wheels Analysis of Fast Pyrolysis Pathways with GREET," an Argonne report authored by Jeongwoo Han, Amgad Elgowainy, and others.

Historically, GREET has been created in Microsoft Excel. Efforts are now underway to finalize the development of GREET into a new, dynamic platform. Interactive GREET software has been designed from the ground up and will be developer- and user-friendly, more adaptable to future expansion and will better serve user needs. The new platform is currently being tested by select GREET users and is expected to debut in the Fall of 2012.

GREET is a public domain model available to everyone, free of charge, from Argonne's GREET website, greet.es.anl.gov. Technical publications can also be downloaded from the site. GREET has 18,000 registered users worldwide.

Funding for GREET is provided by several offices within the U.S. Department of Energy.

For more information, contact Michael Wang, mqwang@anl.gov

GREET website: greet.es.anl.gov

GREET Publications:
http://greet.es.anl.gov/publications

Fastrax

Mike Duoba

JANUARY 2012

Mike Duoba and **Thomas Wallner** both received the 2012 McFarland Award for their work on the Society of Automotive Engineers' Advanced Power Sources (APS) Committee. As an organizer of the Advanced Hybrid Vehicle Powertrains Session at the SAE World Congress, Duoba and his co-organizers succeeded in growing the session to one of the largest of the committee with outstanding attendance and feedback from conference attendees. Through Duoba's extraordinary commitment and dedication, the organizers were able to handle the large numbers of papers submitted. Wallner has been one of the most active members of the APS committee for years, before becoming a Vice-Chair and subsequently a Chair of APS in 2010. His enthusiasm, energy and organizational skills make him an effective leader, always ready to offer innovative solutions. In addition to his own contributions, Wallner helped engage a number of volunteers from the national labs in the work of the APS.

Thomas Wallner

NOVEMBER 2011

Argonne's Chemical Sciences and Engineering Division introduced **BatPaC**, *A Lithium-Ion Battery Performance and Cost Model for Electric-Drive Vehicles.* This project represents the only public domain model that captures the interplay between the design and cost of Li-ion batteries for transportation applications. To learn more about BatPaC, visit http://www.cse.anl.gov/BatPaC/.

Argonne signed a letter of intent with the EU to establish facilities to develop and test vehicle-grid interface technologies, support data-driven standards refinement and development, and undertake projects to enhance the interoperability of electric vehicles, electric vehicle supply equipment and smart grids. (See story on page 14.)

Tijana Rajh

A team of Argonne researchers, led by nanoscientist **Tijana Rajh** and battery expert **Christopher Johnson**, discovered that nanotubes composed of titanium dioxide can switch their phase as a battery is cycled, gradually boosting their operational capacity. Laboratory tests show that new batteries produced with this material could be recharged up to half of their original capacity in less than 30 seconds.

OCTOBER 2011

Kuilin Zhang chaired the session, "Dynamic Traffic Assignment Models and Their Applications to Integrated Corridor Management," at the 2011 IEEE Intelligent Transportation Systems (ITS) Conference held in Washington, D.C., October 5-7.

Linda Gaines was the session chair for "Transportation Options for the Future: Using Nuclear Power to Fuel Our Vehicles," at the American Nuclear Society Annual Meeting held in Washington, D.C., October 31-November 3.

Jules Routbort was an invited speaker, session chair and moderator for a session on nanofluids at the Carbon Nano Materials and Applications Workshop held October 30-November 1 in Rapid City, South Dakota. The event was sponsored by NASA, the U.S. Department of Defense and the National Science Foundation. Routbort presented the talk, "Thermal Properties of Ceramic-based Nanofluids," which was co-authored by **Elena Timofeeva**, **Dileep Singh**, **Wenhua Yu** and **David France**. After the workshop, Routbort was interviewed and appeared on a local television affiliate of NBC.

Romesh Kumar and **Shabbir Ahmed** helped facilitate the Natural Gas and Hydrogen Infrastructure Opportunities Workshop hosted at Argonne on October 18-19. The event, which was sponsored by the U.S. Department of Energy's Fuel Cell Technologies (FCT) Program, included discussions led by plenary speakers, expert panels, and break-out sessions concerning R&D needs, regulatory and environmental barriers, and innovative approaches to accelerating the use of natural gas and hydrogen technologies in the United States, with emphasis on end-use infrastructure for transportation and stationary applications of these gaseous fuels. Workshop participants included Energy Efficiency and Renewable Energy Deputy (EERE) Assistant Secretary Steve Chalk and FCT Program Manager Sunita Satyapal.

Jun Lu

Jun Lu, an Argonne postdoctoral appointee, was awarded the U.S. Department of Energy's EERE Postdoctoral Fellowship. He will be mentored by Argonne battery expert Khalil Amine. As a recipient of this award, Lu will have the opportunity to continue his education and training by participating in research projects related to vehicle research. Lu's proposal, "Develop New Non-aqueous Electrolytes for Rechargeable Li-Air Battery Application," details his plan to develop new siloxane-based electrolyte systems that can resist oxidation at high voltage. The objective of the EERE Postdoctoral Fellowships is to create the next generation of scientific leaders in energy efficiency and renewable energy by attracting the best scientists and engineers to pursue breakthrough technologies in a highly prestigious postdoctoral research program.

Dow Chemical Company and **Argonne** signed a Memorandum of Understanding for a multi-year research collaboration to jointly develop the next generation of materials for advanced battery technologies. The two organizations will be collaborating on several new materials with the intent to improve the performance, cost competitiveness and adoption of these advanced materials in the energy storage industry.

Western Lithium USA Corporation signed an agreement with **Argonne** as a step toward the commercialization of lithium carbonate from the company's Kings Valley Lithium Project located in Humboldt County, Nevada. Under the agreement, Argonne will analyze and develop the Western Lithium's lithium carbonate products for battery applications.

Research Results

Patents and Technologies Available for Licensing

Available for licensing

Redox Shuttle Electrolyte Additive. Argonne has developed a way to make commercially viable lithium-ion (Li-ion) batteries that are safer, will last longer, and cost less than current Li-ion batteries for plug-in hybrid electric vehicles and electric vehicles. Argonne researchers, **Khalil Amine** and **Zonghai Chen**, accomplished this goal by making only a small change to the Li-ion chemistry. The scientists are testing a new molecule based on boron and fluorine as an additive in the electrolyte of Li-ion batteries. By adding a small amount of this substance to battery cells, they found that they can keep individual cells in the battery from reaching unsafe voltage levels. Read more about this licensing opportunity at http://techportal.eere.energy.gov/technology.do/techID=600.

Olivine Phosphate Composite Cathodes. Argonne has developed a family of lithium iron composite materials with unique electrochemical features that enable the high energy and power performance of olivine cathodes without the use of carbon coatings. These materials have excellent rate capability when used as the active material in a Li-ion battery. More specifically, Argonne describes the synthesis and characterization of composite materials that include $LiFePO_4$ for use in, but not limited to, electrode materials for lithium-ion batteries. The materials have been made, characterized and fully tested. Read more about this licensing opportunity at http://www.anl.gov/techtransfer/pdf/Profile_olivine_phosphate.pdf.

New patents

"Compact Electrochemical Bifunctional NO_x/O_2 Sensors with Internal Reference for High Temperature Applications;" **Dileep Singh**, **Jules Routbort**, **Prabir Dutta**, **John Spirig**, **Jiun-Chan Yang**; US Patent No. 8,012,323; issued September 6, 2011.

"High-Temperature Potentiometric Oxygen Sensor with Internal Reference;" **Jules Routbort**, **Dileep Singh**, **Prabir Dutta**, **Ramamoorthy Ramasamy**, **John Spirig**, **Sheikh Akbar**; US Patent 8,057,652; issued November 15, 2011.

"Processes for Making Dense, Spherical Active Materials for Lithium-Ion Cells;" **Sun-Ho Kang**, **Khalil Amine**; US Patent No. 8,062,792; issued November 22, 2011.

"Porous Polymeric Materials for Hydrogen Storage;" **Luping Yu**, **Di-Jia Liu**, **Shengwen Yuan**, **Junbing Yang**; US Patent No. 8,076,382; issued December 13, 2011.

"Manganese Oxide Composite Electrodes for Lithium Batteries;" **Christopher Johnson**, **Sun-Ho Kang**, **Michael Thackeray**; US Patent No. 8,080,340; issued December 20, 2011.

"Method for the Separation of Overlapping Density Porous Materials from Less Porous Materials;" **Joseph Pomykala**, **Bassam Jody**, **Edward Daniels**, **Jeffrey Spangenberger**, **Scott Lockwood**; US Patent No. 8,083,067; issued December 27, 2011.

For more information, contact
Argonne's Technology Development and Commercialization Office at 800.627.2596

Recent Papers and Presentations

"Recent progress in CFD modeling and challenges," **Sibendu Som**, Indo-US Science and Technology Forum Workshop on Liquid Atomization, Indian Institute of Technology at Madras, Chennai (India), December 19, 2011.

"Recycling of Lithium-Ion Batteries," **Linda Gaines**, U. Illinois Urbana-Champaign, November 15.

"Life-Cycle Greenhouse Gas Emissions of Shale Gas, Natural Gas, Coal, and Petroleum," **Andrew Burnham**, **Jeongwoo Han**, **Corrie Clark**, **Michael Wang**, **Jennifer Dunn** and **Ignasi Palou-Rivera**, Environ. Sci. Technol., November 2011.

"A reduced mechanism for biodiesel surrogates with low temperature chemistry for compression ignition engine applications," **Sibendu Som** and **Doug Longman**, Combustion Theory and Modeling, 2011.

"Recycling of LiFePO4 Batteries," **Linda Gaines**, 7th International Symposium on Inorganic Phosphate Materials, November 9.

"Effect of Battery Components on Safety and Ways of Mitigating the Thermal Runaway in Lithium Batteries," **Khalil Amine**, College de France, November 7.

"Convective Heat Transfer of Nanofluids in Turbulent Flow," **Wenhua Yu**, Carbon Nano Materials and Applications Workshop, October 30.

"Engineering Nanofluids for Efficient Heat Transfer," **Jules Routbort**, Institute of Physics of the Chinese Academy of Sciences, October 23.

"Three Dimensional Simulations of Diesel Sprays Using n-Dodecane as a Surrogate," **Sibendu Som** and **Doug Longman**, Eastern States Section of the Combustion Institute Fall Technical Meeting, October 10.

"A High-Temperature Model for the Combustion of Methylbutanoate," **Raghu Sivaramakrishnan**, **Wei Liu**, **Michael Davis**, **Sibendu Som** and **Doug Longman**, Eastern States Section of the Combustion Institute Fall Technical Meeting, October 10.

"Cold-Start Performance and Emissions Behavior of Alcohol Fuels in an SIDI Engine Using Transient Hardware-In-Loop Test Methods," **Andrew Ickes** and **Thomas Wallner**, Directions in Engine- Efficiency and Emissions Research (DEER) Conference, October 6.

"Evaluating Benefits of Idling Restrictions in a Large Northern City," poster by **Linda Gaines**, Directions in Engine-Efficiency and Emissions Research (DEER) Conference, October 3.

"Simulating Flame Lift-off Characteristics of Diesel and Biodiesel Fuels Using Detailed Chemical-kinetic Mechanisms and LES Turbulence Model," **Sibendu Som** and **Doug Longman**, ASME Internal Combustion Engine Division Fall Technical Conference, October 2.

"Alternative Fuels and Propulsion Systems: A U.S. Perspective," **Thomas Wallner** and **Mike Duoba**, Working Process of the Internal Combustion Engine Symposium, September 22.

"Lithium-Ion Battery Issues," **Linda Gaines**, IEA Workshop on Battery Recycling, September 26-27.

"Alternative Fuels for Transportation—The Quest for the Silver Bullet...," **Thomas Wallner**, ICE2011 - 10th International Conference on Engines & Vehicles, September 14.

Note: Some papers/presentations had additional contributing authors; only Argonne authors are noted here.

Visit our website to download copies of these papers and presentations:
http://www.transportation.anl.gov/publications/papers_presentations.html

Media Highlights

September to December 2011

***Ferret* website, September 19.** GreaseMax lubricators will be released in the U.S. market with Nanotech synthetic diamond lubricants later this year. This is a new range of nanolubricants developed by the U.S. Department of Energy's Argonne National Laboratory. The lubricants incorporate an exceptionally low coefficient of friction. Read more at http://www.ferret.com.au/c/Delta-Distribution/Nano-lubricants-to-be-used-in-GreaseMax-lubricators-n1826728.

Henning Lohse-Busch

***WTTW* television station, October 4.** Henning Lohse-Busch of Argonne explains hybrid and electric vehicles in a video highlighting the arrival of electric cars and their infrastructure to Chicago, Ill. Watch the video at http://chicagotonight.wttw.com/2011/10/04/electric-cars.

***TEDx* conference, October 11.** Don Hillebrand and Jeff Chamberlain talk about advanced batteries in their presentation, "A Little Can of Sunshine," presented at the University of Illinois. Don Hillebrand is the director of Argonne's Center for Transportation Research, and Jeffrey Chamberlain is the leader of Argonne's laboratory-wide Energy Storage Initiative, which is developing solutions for both electric cars and the power grid. Watch a video of their talk at http://www.youtube.com/watch?v=88BPZrZoKU4.

***Washington Monthly* magazine, November 1.** Argonne Lab Director Eric Isaacs wrote a review of the Seth Fletcher book, "Bottled Lightning: Superbatteries, Electric Cars, and the New Lithium Economy." In the review, Isaacs states, "As the director of a National Laboratory, I have a deep-seated personal and professional interest in the future of energy research. And—like Fletcher—I see increasing reason for optimism about the potential of lithium-based batteries to transform our energy economy." Read more of Isaacs' views on the book at www.washingtonmonthly.com/magazine/november_december_2011/on_political_books/assault_on_battery032975.php.

***Green Car Congress* website, November 14.** A project led by Thomas Wallner from Argonne National Laboratory has optimized a spark-ignited direct injection combustion system for a hydrogen engine. The engine delivers peak brake thermal efficiency (BTE) levels of 45.5% and 33.3% BTE at the worldwide mapping point, and 14.3 bar brake mean effective pressure (BMEP). These results exceed the U.S. Department of Energy 2010 efficiency goals (45% peak, 31% BTE at the worldwide mapping point). Read more at http://www.greencarcongress.com/2011/11/wallner-20111114.html.

***Naperville Sun* newspaper, November 15.** Naperville resident Steve Lottes wants to start a revolution. A research scientist at Argonne National Laboratory, Lottes believes that change isn't about numbers, it's about just one person stepping up and hoping to make a difference. And for Lottes, changing the world started with buying a car. Read more about Steve and his Chevrolet Volt at http://napervillesun.suntimes.com/news/7968490-418/charged-up.html.

***Naperville Sun* newspaper, November 26.** When the Green Fuels Depot in Naperville, Ill. is up and running, the device will convert shredded yard debris picked up curbside into electricity, hydrogen and ethanol, all of which can be used to run cars and small trucks in the city fleet. About two tons of biomass can be processed per day, producing up to 60 kilowatts of power, enough to serve about a dozen homes, and more will be possible in the future. The depot is a collaborative effort of the city, Packer Engineering, Argonne National Laboratory and the College of DuPage. Read more at http://napervillesun.suntimes.com/news/8977280-418/innovative-fuel-plant-goes-public-at-naperville-launch.html.

Forrest Jehlik

***NewsGnomes* website, November 29.** In "Xtreme Research: Interesting Places and Unusual Challenges," Argonne researcher Forrest Jehlik and other panelists discussed their research and more at Fermi National Accelerator Laboratory during the fourth in a series of joint speaker events for University of Chicago faculty and Argonne National Laboratory and Fermilab scientists, researchers and engineers. Read more at http://news.gnom.es/news/exploring-the-world-of-extreme-science and watch a video at http://www.wbez.org/blog/clever-apes/2011-12-05/top-hair-raising-research-moments-94614.

***Reuters* website, December 15.** The Society of Automotive Engineer's (SAE's) International Executive Nominating Committee named Donald Hillebrand as its candidate for 2013 SAE International President. Hillebrand is Director of the Center for Transportation Research at Argonne National Laboratory. Read more at http://www.reuters.com/article/2011/12/15/idUS227504+15-Dec-2011+PRN20111215.

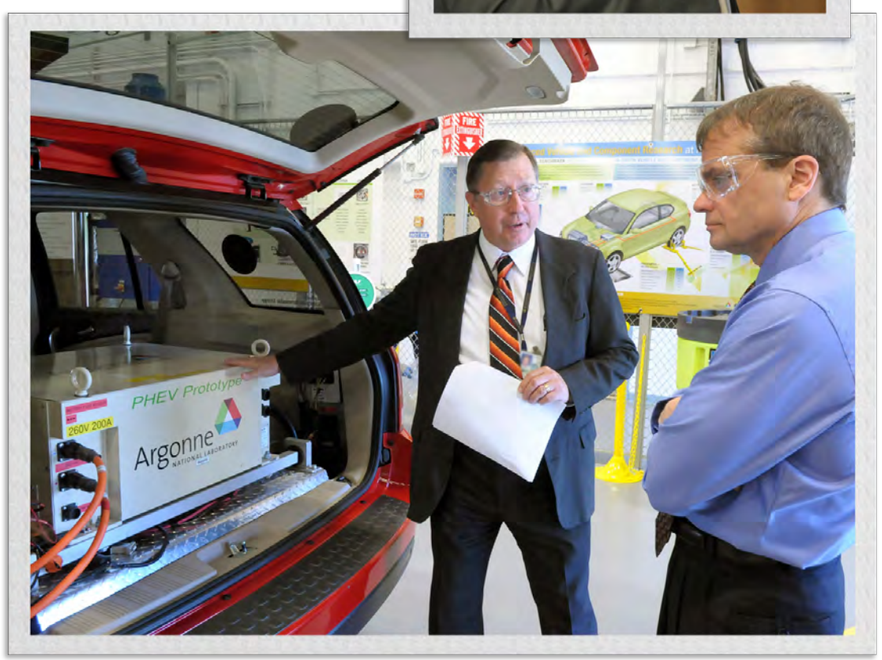
***Bridges* online magazine, December 16.** Thomas Wallner, a mechanical engineer by training and a principal investigator at Argonne's Center for Transportation Research, has been "in hydrogen for the last 12 years," as he puts it. Wallner is doing research in the area of alternative fuels, with a special focus on hydrogen internal combustion engines, a technology that should eventually pave the way for fuel cell cars. Read more at http://www.ostina.org/content/view/6131/1570/.

For complete Argonne transportation research press coverage, visit http://www.transportation.anl.gov/media_center/press_coverage.html

Parting Shots

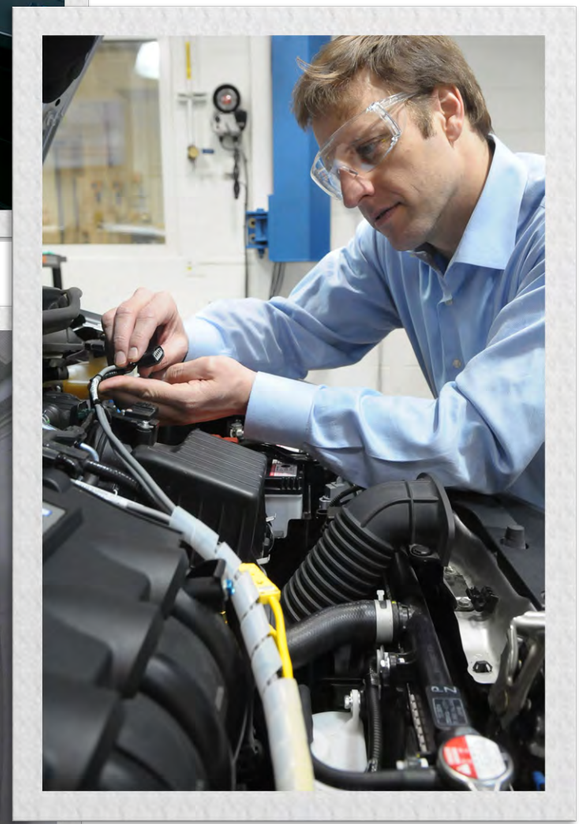
Left: Argonne researchers developed the Green Racing Simulator to be a fun outreach tool to educate consumers on the benefits of alternative fuels and advanced technologies.

Right: Steve Chalk, DOE Deputy Assistant Secretary for Energy Efficiency and Renewable Energy, gave the opening plenary talk at the Natural Gas and Hydrogen Infrastructure Opportunities Workshop, hosted at Argonne on October 18-19, 2011. The workshop was sponsored by DOE's Fuel Cell Technologies Program.



Above: Argonne researcher Glenn Keller (left) explains Argonne's work with electric vehicles to Illinois Congressman Mike Quigley.

Below: Engineer Mike Duoba prepares a vehicle for testing at Argonne's Advanced Powertrain Research Facility.



Left: Here's a first look at the Advanced Powertrain Research Facility's thermal upgrade. The new and improved facility allows researchers to test vehicles and components under extreme hot and cold temperature conditions. More on this in the next issue of TransForum.

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WORKING WITH ARGONNE

Industrial technology development is an important way for the national laboratories to transfer the benefits of publicly-funded research to industry to help strengthen the nation's technology base. The stories highlighted in this issue of **Trans**Forum represent some of the ways Argonne works with the transportation industry to improve processes, create products and markets, and lead the way to cost-effective transportation solutions, which in turn lead to a healthier economic future.

By working with Argonne through various types of cost-sharing arrangements, companies can jump-start their efforts to develop the next generation of transportation technologies without shouldering the often prohibitive cost of initial R&D alone. Argonne has participated in dozens of these partnerships and has even been involved in helping to launch start-up companies based on the products and technologies developed here.

If working with world-class scientists and engineers, having access to state-of-the-art user facilities and resources, and leveraging your company's own capabilities sound like good business opportunities to you, please contact our Technology Development and Commercialization Division and see how we can put our resources to work for you.

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