

JCESR Named the DOE Batteries and Energy Storage Hub

A multipartner team led by Argonne National Laboratory has been selected for an award of up to \$120 million over five years to establish the new U.S. Department of Energy (DOE) Batteries and Energy Storage Hub. The Hub, to be known as the Joint Center for Energy Storage Research (JCESR), will be led by Argonne and combines the R&D firepower of five DOE national laboratories, five universities and four private firms in an effort aimed at achieving revolutionary advances in battery performance.

Argonne physicist Mahalingam Balasubramanian loads an *in situ* lithium-ion battery into the low-energy resolution inelastic X-ray (LERIX) system at the Advanced Photon Source. This multi-element X-ray scattering instrument is helping Argonne researchers understand the fundamental mechanisms that limit the performance of batteries.

NEW BATTERIES AND ENERGY STORAGE HUB



The large-scale, innovative research and transformational new battery systems that will result from this venture will mean more effective, lower-cost and longer-life energy storage technologies with real-world applications for anything that can use a rechargeable battery.

Advancing next-generation battery and energy storage technologies for electric and hybrid cars and the electricity grid are critical parts of President Obama's "all-of-the-above" energy strategy to reduce America's reliance on foreign oil and lower energy costs for U.S. consumers.

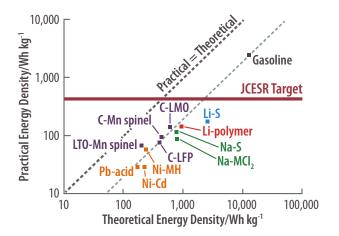
"This is a partnership between world-leading scientists and world-leading companies, committed to ensuring that the advanced battery technologies the world needs will be invented and built right here in America," said U.S. Secretary of Energy Steven Chu. Illinois Governor Pat Quinn and Chicago Mayor Rahm Emanuel joined Secretary Chu in making the announcement on November 30, 2012.

"Based on the tremendous advances that have been made in the past few years, there are very good reasons to believe that advanced battery technologies can and will play an increasingly valuable

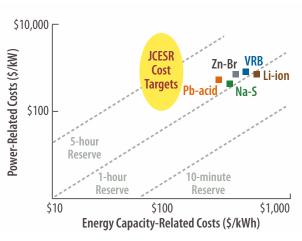
role in strengthening America's energy and economic security by reducing our oil dependence, upgrading our aging power grid, and allowing us to take greater advantage of intermittent energy sources like wind and solar," Chu continued.

The ambitious JCESR initiative builds on Argonne's long history of innovative and successful research in advanced battery technologies

Sited at Argonne National Laboratory, JCESR (pronounced "J-Caesar") brings together a dream team of high-powered global leaders in energy storage R&D with a staff of top-tier researchers and provides them with the unique suite of world-class scientific user facilities for characterization, computing and experimental validation; and the scientific and engineering tools for battery research, materials scale up and testing. Their combined expertise







Capital costs of various energy storage systems with the JCESR Cost Target.

spans the full innovation ecosystem—mission-driven basic research, innovative engineering, technology development, entrepreneurial experience and commercialization. JCESR's industrial partners have the resources and market reach to swiftly commercialize revolutionary energy storage technologies.

Argonne's partners in JCESR include national laboratories Lawrence Berkeley National Laboratory, Pacific Northwest National Laboratory, Sandia National Laboratories and SLAC National Accelerator Laboratory. University partners include Northwestern University, University of Chicago, University of Illinois-Chicago, University of Illinois at Urbana-Champaign and University of Michigan. Four industrial partners have also joined to help clear a path to the marketplace for the advances developed at JCESR, including Dow Chemical Company; Applied Materials, Inc.; Johnson Controls, Inc.; and Clean Energy Trust.

"The JCESR Batteries and Energy Storage Hub gives us a new collaborative, inter-institutional R&D paradigm in which to develop the energy storage technologies that transform both the electricity grid and transportation and so reduce our dependence on foreign oil," said Eric Isaacs, Director of Argonne National Laboratory.

Selected through an open national competition with a rigorous merit review process that relied on outside expert reviewers, JCESR is the fourth Energy Innovation Hub established by the U.S. Department of Energy (DOE) since 2010. Other hubs are devoted to modeling and simulation of nuclear

reactors, achieving major improvements in the energy efficiency of buildings, and developing fuels from sunlight. A fifth hub focused on critical materials research was announced earlier this year and the application process is still under way.

Energy Innovation Hubs are major integrated research centers with researchers from many different institutions and technical backgrounds that combine basic and applied research with engineering to accelerate scientific discovery in critical energy areas. They are modeled after the strong scientific management characteristics of the Manhattan Project; the Lincoln Lab at MIT that developed radar; AT&T Bell Laboratories that developed the transistor; and, more recently, the highly successful Bioenergy Research Centers established during the Bush Administration to pioneer advanced techniques in biotechnology, including biofuels.

Over the decades, DOE national laboratories and DOE-funded university research programs have been responsible for some of the most important advances in battery technology. For example, key battery improvements developed at Argonne helped make the Chevy Volt battery possible.

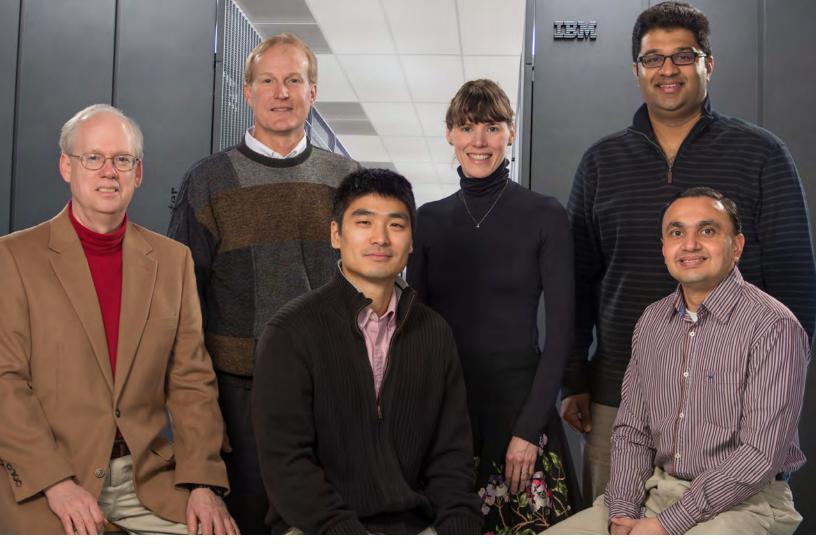
For more information on JCESR:

www.anl.gov/articles/department-energy-awards-120-million-battery-Hub-argonne-led-group www.jcesr.org

For more information on DOE's Energy Innovation Hubs: http://energy.gov/articles/what-are-energy-innovation-Hubs

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From left, Argonne researchers Raymond Bair, Doug Longman, Oingluan Xue, Marta Garcia, Shashi Aithal (seated) and Sibendu Som are part of a multidisciplinary team working to advance diesel and spark engine modeling and simulation tools into the high-performance computing realm.

High-Performance Computing Enables Huge Leap Forward in Engine Development

When we turn the key in our car's ignition, we usually don't think about the combustion process that takes place inside the engine that enables the car to go. We just know that it works.

But, what actually takes place inside the engine? How do fuel injectors, turbulent mixing and combustion chemistry impact the fuel efficiency of a vehicle? And how do engine manufacturers improve these hidden-from-view processes to increase engine efficiency?

The answers lie in computer modeling and simulation tools. Automotive and engine manufacturers are becoming increasingly reliant on computers to aid in the development of next-generation engines. Modeling and simulation software offers a cost-effective way to optimize the complex fuel spray and combustion processes, and do so over a wide range of operating conditions using a variety of fuels (e.g., gasoline, diesel, biodiesel and fuel blends).

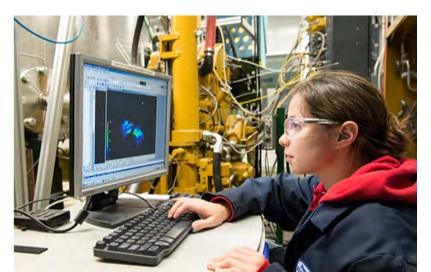
Simulations provide unprecedented insights into the complex processes taking place inside engines

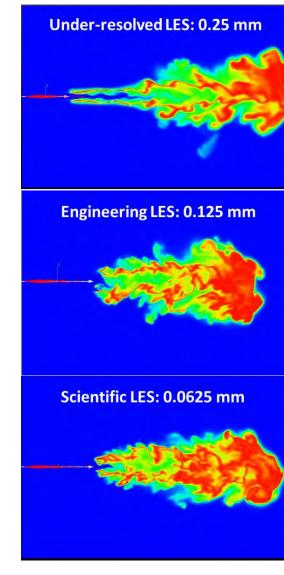
High-performance computing (HPC) will elevate these tools to new heights, providing industry with an improved path for designing more fuel-efficient and clean automotive engines.

"We're taking advantage of the amazing computational power at Argonne to create more robust fuel spray and combustion models for predictive engine simulations," said Sibendu Som, Argonne mechanical engineer. "These simulations provide unprecedented insights into the complex processes taking place inside

As an example, high-fidelity simulations allow researchers to peer inside a virtual combustion chamber to see how injected fuel, air and combustion products intermingle when the engine is fired up. These interactions produce the primary breakup of the liquid fuel, which is followed by atomization and secondary

Argonne engineer Anita Ramirez performs dynamometer tests on a one-cylinder Caterpillar engine to validate data for the modeling and simulation efforts.





The temperature distribution inside the combustion chamber of a diesel engine obtained using high-fidelity simulations and a robust, large-eddy simulation model.

breakup of the fuel into drops. These drops then vaporize and combust, resulting in the heat release that ultimately powers internal combustion engines.

This complicated process involving fluid dynamics, chemistry and combustion determines engine performance and emissions characteristics, but it would be impossible to observe and understand without the aid of computer models.

With expertise in automotive engines and combustion chemistry, and state-of-the-art transportation and high-performance computing facilities, Argonne is one of the few places in the world with the ability to rapidly advance modeling and simulation tools into the HPC realm for more intelligent engine design.

Som is part of a multidisciplinary team using some of the world's most powerful computers at the Argonne Leadership Computing Facility (ALCF) and Argonne's Laboratory Computing Resource Center (LCRC) to develop improved predictive modeling capabilities for engines using computational fluid dynamics (CFD) tools.

The Argonne team is currently collaborating with Convergent Science, Inc., and Caterpillar Inc. to scale up the CONVERGE code, a CFD software program widely used by industry, to run on much larger computers without any technical glitches.

According to Som, simulations with high temporal and spatial resolutions combined with Argonne's advancements in spray and combustion modeling have necessitated the use of HPC to ensure quick turnaround times, which is of paramount interest in the industry.

The current state-of-the-art for most manufacturers involves running engine simulations with up to 50 processors. With this project, Som and his colleagues are scaling up CONVERGE to run on more than 1,000 processors.

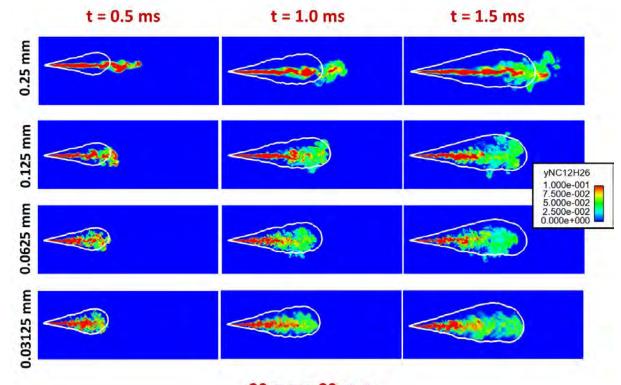
The team's huge leap forward was made possible by the development and implementation of an improved load-balancing algorithm called METIS (original algorithm developed at University of Minnesota). This enabled the researchers to perform the largest diesel engine simulations run to date.

"Implementation of METIS has enabled the effective use of highperformance computing resources for engine simulations," said Keith J. Richards, vice-president and co-founder of Convergent Science, Inc. "METIS will be available in the next version of the CONVERGE code so that other original equipment manufacturers can also realize the benefits."

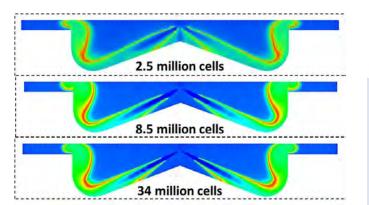
The massive simulations also successfully demonstrated gridconvergence (i.e., when simulations, results are independent of the chosen numerical parameters such as grid- and time-step size).

"Grid-convergence is a critical step forward towards truly predictive engine simulations. Implementation of METIS, together with Argonne's expertise and computational resources, has enabled us to identify the computational set-up for attaining grid-convergence," said Dr. Peter Kelly Senecal, vice-president and co-founder of Convergent Science, Inc. "This methodology can now be widely applied across the engine manufacturing industry."

These computer-generated images show the fuel distribution inside a combustion chamber (sized 30 by 80 mm) of a diesel engine at different times during the combustion process for four different mesh resolutions ranging from 0.25 mm down to 0.03125 mm. Also shown are the experimentally measured vapor boundaries from Sandia National Laboratories indicated by the white lines.



30 mm x 80 mm



The temperature contours inside the combustion chamber of a diesel engine change when using different numbers of computational cells.

The project has also impacted how Caterpillar approaches its modeling and simulation efforts.

"Working with Argonne researchers has provided us access to the HPC facilities and their expertise in spray and combustion modeling. Through this HPC study, we have learned more about model settings that have improved our simulation practices at Caterpillar," said Marcus Weber, team leader at Caterpillar, Inc.

In the near future, the team plans to use Mira, the ALCF's new 10-petaflop IBM Blue Gene/Q system, to run diesel engine simulations on an unprecedented 20,000 processors. As part of this project, Som and his colleagues will also pursue further model enhancements, such as higher-fidelity turbulence models and improved prediction of turbulence-chemistry interactions.

"With the ability to run more detailed simulations at a faster rate, manufacturers will have valuable new information that will ultimately help them design better engines more quickly and at a lower cost," Som said.

He also believes Argonne's combination of expertise and HPC capabilities will pave the way for new industry partnerships.

Argonne is one of the few places in the world with the ability to rapidly advance modeling and simulation tools

"Most places don't have the kind of resources we have on site at Argonne," Som said. "We're hoping our HPC work will spawn a service for the engine development community."

Funding for this work is provided by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy, Vehicle Technologies Program under Gurpreet Singh.

PreSICE Workshop Identifies Engine Simulation Needs

In 2011, DOE held a workshop with 60 leaders in the engine combustion field from industry, academia and national laboratories to identify research needs and impacts in Predictive Simulation for Internal Combustion Engines (PreSICE).

According to the PreSICE workshop report, current engine design processes that use "build and test" prototype engineering are too slow. Practices must be dramatically accelerated to help improve the fuel economy of the nation's fleet of vehicles, thus reducing U.S. dependence on foreign oil and reducing carbon emissions.

"The use of predictive simulation tools for enhancing combustion engine performance will shrink engine development timescales, accelerate time to market, and reduce development costs, while ensuring the timely achievement of energy security and emissions targets and enhancing U.S. industrial competitiveness," the report states.



Sibendu Som

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EBR: Fuel and Electricity— Anywhere, Anytime

Waste goes in, energy comes out. That's the basic idea behind Argonne's Endurance Bioenergy Reactor ™ (EBR).

Whether it's food waste, agricultural waste (from plants or animals) or human waste, the EBR can quickly turn most carbon-based feedstocks into biofuel that can be used immediately by vehicles or generators.

The EBR concept is built around a groundbreaking photosynthetic bacterium developed at Argonne. A team of scientists led by biophysicist Philip Laible engineered the bacteria to convert biomass into a long-chain alcohol called phytol. The Argonnedeveloped organism uses plant enzymes and light-harvesting machinery normally abundant within the cells to enable the fuel conversion process.

"These hybrid plant-bacterial reactions manufacture fuel molecules that can be sequestered, separated and used in a diesel engine," Laible said.

With chemical and physical properties similar to diesel fuel, phytol is ready for immediate use with no further refinement necessary. It can be used alone or in diesel blends.

A single reactor that could fit easily within a standard shipping container could produce 25 to 50 gallons of fuel per day, but the system's modular nature makes it easy to modify and expand so fuel can be generated on a continual basis.

Waste goes in, energy comes out. That's the basic idea behind Argonne's Endurance Bioenergy Reactor

"One EBR can fuel a generator that can charge up to 60 light- to medium-duty electric vehicles per day," Laible said.

This promising technology provides a viable alternative for operations that require reliable power sources in remote locations that are not near a power grid. By eliminating the need for refining, users can produce fuel or electricity on demand without complicated logistics.

The EBR has generated strong interest from the military as a tool to help prolong missions, reduce costs and improve safety by decreasing reliance on supply chains and dangerous convoy missions.



However, the simplicity and mobility of the EBR make it a good fit for other applications as well. On farms, EBRs could help owners reduce their operating costs by turning agricultural and animal waste into energy.

The technology is also viewed as a valuable resource for emergency situations and humanitarian activities around the world, offering a means for people to generate their own fuel or electricity in times of crisis.

Phytol is ready for immediate use with no further refinement necessary

To develop the technology into an operational system, Laible said his team will require a relatively small investment of \$2-3 million over the next few years.

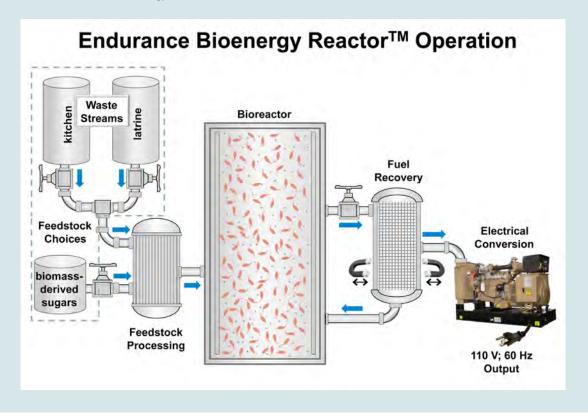
"The difficult phases of development of the primary technologies are behind us; however, integration and scale-up issues lie ahead,"

This work is funded by Argonne's Laboratory-Directed Research and Development Program.

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How It Works

The EBR will comprise a large centralized fermentation vessel with an intake port connected to a supply of sterile, carbon-rich feedstocks (whether from waste streams or sugars and other media components indigenous to the area). Packets of freeze-dried cells can be shipped within the EBR hardware, making initiation of the process a simple step. Just opening a package of bacteria and dropping it into the main tank will begin the conversion of the chosen feedstock to energy.

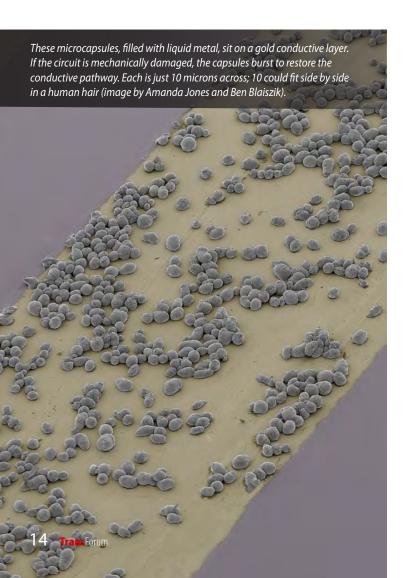


Argonne's Battery R&D Produces Electrifying Results

Even before the Argonne-led JCESR was named the U.S. Department of Energy's new Batteries and Energy Storage Hub, the laboratory has been engaged in a wide variety of research projects aimed at helping the United States win the global race to develop a better battery.

While it may take a number of years for easily affordable all-electric, zero-emissions vehicles to catch on, Argonne's diverse battery research program continues to produce exciting results that could help push things along.

In recent months, Argonne's battery work has involved innovative battery materials that can heal themselves when damaged, and a promising new anode composition that could enhance battery performance and life.



Argonne's innovative battery materials heal themselves

Self-healing batteries

At the Center for Electrical Energy Storage (CEES), a team of researchers from Argonne and the University of Illinois at Urbana-Champaign (UIUC) are exploring ways to design batteries that heal themselves when damaged.

Scientists believe that loss of electrical conductivity is what causes a battery to fade and die, so the research team is investigating a creative approach to addressing this issue.

Their idea is to place tiny microspheres containing liquid metal inside the battery. These capsules lie dormant for most of the battery's lifetime, but when the battery is damaged, the microspheres burst open and release their liquid metal into the battery. The metal fills in the gaps in the electrical circuit, connecting the broken lines, and power is restored.

The team's first step was to test their idea in a simple system, connecting an electrode with a wire. This successful demonstration proved the capsules could indeed "heal" the circuit if cut.

"Our new self-healing materials can completely repair the circuit in less than a millisecond," said Jeff Moore, a UIUC scientist on the

The next step, which the researchers are beginning, is to test the capsules in a prototype battery. Argonne materials scientist and battery expert Khalil Amine is helping the team adapt the capsules for use in lithium-ion batteries.

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



New anode compositions enhance battery performance

Titanium dioxide anode gives batteries a quick charge

A team of researchers led by Argonne nanoscientist Tijana Rajh and battery expert Christopher Johnson recently 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.

By switching out conventional graphite anodes for ones composed of the titanium nanotubes, Rajh and her colleagues witnessed a surprising phenomenon. As the battery cycled through several charges and discharges, its internal structure began to orient itself in a way that dramatically improved the battery's performance.

"We did not expect this to happen when we first started working with the material, but the anode spontaneously adopted the best structure," Rajh said. "There's an internal kind of plasticity to the system that allows it to change as the battery gets cycled."

Having anodes composed of titanium dioxide instead of graphite would also improve the reliability and safety of lithium-ion batteries.

Funding for titanium dioxide anode work is provided by Argonne's Laboratory-Directed Research and Development Program and the U.S. Department of Energy, Office of Basic Energy Sciences, User Facilities Program.

Self-healing batteries

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Titanium dioxide anodes

Tijana Rajh, rajh@anl.gov and Christopher Johnson, cjohnson@anl.gov







A Natural Solution for Transportation

As the United States transitions away from a primarily petroleumbased transportation industry, a number of different alternative fuel sources—ethanol, biodiesel, electricity and hydrogen—have each shown their own promise. Hoping to expand the pool even further, researchers at the U.S. Department of Energy's Argonne National Laboratory have begun to investigate the addition of one more contender to the list of possible energy sources for light-duty cars and trucks: compressed natural gas (CNG).

Natural gas is composed primarily of methane, which when compressed occupies less than one percent of the volume it occupies at standard pressure. CNG is typically stored in cylindrical tanks that would be carried onboard the vehicles it fuels.

Because the domestic production of natural gas has increased dramatically over the past ten years, making a large number of the cars and light trucks currently on the road CNG-compatible would help to improve U.S. energy security. "As a country, we don't lack for natural gas deposits," said Argonne mechanical engineer Thomas Wallner. "There are fewer obvious challenges with direct supply than with most other fuels."

Like gasoline, both the production and combustion of CNG release greenhouse gases into the atmosphere. "To be able to make an accurate comparison to gasoline, scientists and engineers will need to look at each stage of the fuel's production and use," said Argonne environmental scientist Andrew Burnham.

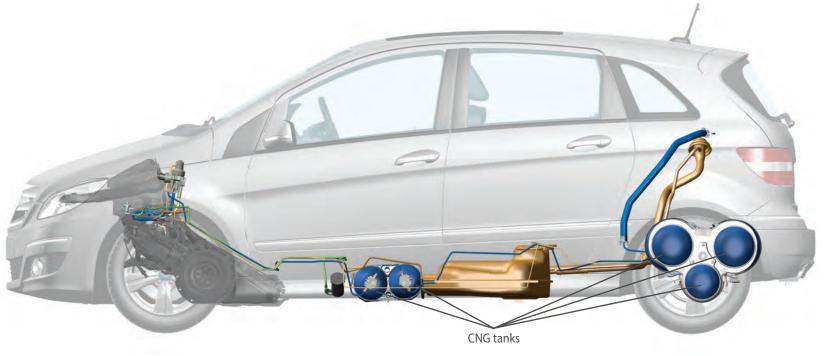
Argonne has years of expertise working with industry to develop alternative-fuel vehicles, as well as the tools necessary for the public to understand the impact of these vehicles on the environment

Unlike gasoline, however, CNG markets in the United States are relatively insulated from geopolitical shocks, said Wallner. "The price of CNG has been and will probably continue to be both cheaper and more stable over the long term than gasoline," he said.

CNG currently costs the equivalent of about \$2 per gallon, roughly half that of current gasoline prices, according to Wallner.



Natural gas is proving to be a valuable option for city buses, delivery trucks and other high-mileage, centrally fueled fleets (image courtesy of Natural Gas Vehicles for America).



Compressed natural gas is another potential energy source for light-duty cars and trucks (image courtesy of Daimler).

In order for CNG to take hold, many more stations will need to offer it as an option, and the infrastructure for delivering and distributing the fuel around the country will have to be increased. There are roughly 500 publicly available CNG refueling stations in the United States, compared to around 150,000 gas stations.

Argonne already has the capability to help automotive industry leaders test and analyze CNG vehicles. In particular, Argonne's Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model gives experts the ability to examine the greenhouse gas emissions of various fuels from "well-towheels," involving each stage of production, distribution and combustion.

"We have years of expertise working with industry to develop alternative-fuel vehicles, as well as the tools necessary for the public to understand the impact of these vehicles on the environment," said Argonne mechanical engineer Michael Duoba.

Although CNG vehicles emit fewer greenhouse gases than conventional automobiles as fuel is combusted, "upstream" challenges in production and distribution of CNG—particularly methane leakage—make it somewhat less attractive when it comes to preventing climate change. "There are a lot of points in the life cycle of the fuel where we still need better data," Burnham said. "There are technological opportunities for us to capture the leaked natural gas and reduce greenhouse gas impacts."

For heavy-duty applications, like city buses, CNG can help cut down emissions of particulate matter and nitrogen oxides, giving municipalities another option to meet more stringent

U.S. Environmental Protection Agency (EPA) standards enacted in the past few years, according to Burnham.

Argonne's GREET model already helps automotive industry leaders test and analyze CNG vehicles

In Wallner's view, CNG vehicles—like plug-ins and diesel-powered automobiles—will serve the transportation needs of some, not all. "It's important to see each of these technologies as a part of the solution but not the entire solution," he said. "The more we invest in their development, the closer we'll come to a portfolio that makes sense both economically and environmentally."

Natural gas has also attracted the attention of the railroad industry. Because of the laboratory's long standing research on locomotive engines and natural gas stationary engines, Argonne was asked by the Federal Railroad Administration to host a workshop last November for industry stakeholders to discuss the potential of natural gas locomotives. A follow-up article will appear in the next issue of TransForum.

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Bridges: To Paint or Not to Paint

Over the lifetime of a bridge, painting and repainting the steel to protect it from the elements can equal a large fraction of the original construction cost.

In addition to monetary costs, maintenance workers face health risks if strict procedures are not in place to avoid exposure to hazardous dust when old paint is removed and the fumes of hazardous chemicals when new paint is applied.

However, weathering steel offers a low-maintenance alternative. The use of weathering steel in bridges avoids the large cost of periodic painting and the hazards of paint removal and repainting because this type of steel never requires painting. When exposed to weather, the initial corrosion of weathering steel forms a natural rust-resistant layer that prevents further corrosion under a wide variety of conditions.

Given the advantages of using weathering steel, the choice might appear to be obvious. However, the large potential savings in bridge maintenance costs from using weathering steel are not always realized; corrosion can continue under its protective patina layer when the steel is exposed to excessively salt- and moistureladen environments, such as the use of de-icing salt following snow and ice events.

Very little information is available on the corrosion risk for weathering steel resulting from the use of de-icing salt. Existing federal guidelines contain a limited number of potential causes of

increased corrosion risk. For instance, the "tunnel effect" causes salt to be blocked from spreading out to below-grade roadways with steep berms and vertical or near-vertical abutments, potentially increasing salt concentration and deposition on bridge beams.

TRACC modeling provides new insights into the COrrosion of weathering steel

To increase the understanding of corrosion risk, analysts at Argonne's Transportation Research and Analysis Computing Center (TRACC) are supporting the Federal Highway Administration (FHWA) in a multiyear study to better quantify the conditions that lead to excessive corrosion in weathering steel bridges.

Researchers are using advanced computational fluid dynamics (CFD) techniques and high-performance cluster computing to study the conditions and mechanisms that lead from the salt spray thrown from truck tires to salt water droplets reaching bridge beams. Computer simulations use an advanced motion modeling capability called a "sliding mesh" in the CFD software to move one or more large trucks under bridges at 60 mph. The computations also include multiphase spray droplet tracking.

Velocity: Magnitude (m/s) 14.4 Parcel 0000 1000 2 3 4 Droplet Parcel Vertical Position (m)

Simulation of spray distribution from a truck moving at 60 mph using sliding mesh model with histogram showing count of droplets reaching the bridge beam level with 45-degree tailwind.

In a recent study, Argonne scientists found that

- ▶ Spray droplet size matters. Large droplets greater than 200 microns in diameter settle back onto the road in seconds, whereas smaller droplets take minutes to days, depending on size, to settle back onto the road.
- ▶ With no wind or following traffic, the tire spray in a truck wake does not rise higher than half the trailer height.
- ▶ The combination of depressed approach roadway and wind increases salt deposition on bridge beams, but without wind there is no tunnel effect.
- ▶ Traffic causes a significant cumulative effect: droplets in a truck wake can be carried up to bridge beam level as the air and droplets in the wake are diverted up and over a following truck.
- ▶ Wind can play a very significant role in carrying small droplets from truck spray wakes up to bridge beam level.

Results of the FHWA study included animated visualizations that were presented to bridge engineers at the American Iron and Steel Institute's (AISI) Bridge Task Force meeting in Chicago in August 2012. AISI, together with the American Association of State and Highway Transportation Officials, assure the highest quality of products and optimal and safe bridge design practices in the United States.

The study provides new insights into the mechanisms that increase corrosion risk for weathering steel bridges and guidance for ongoing field studies. The CFD results and data collected from the



Argonne researchers Steven Lottes and Cezary Bojanowski in front of TRACC's Phoenix high-performance computing cluster.

field studies will be used to produce new federal guidelines for the use of weathering steel in bridges.

This work was funded by the FHWA through the Turner-Fairbank Highway Research Center under an interagency agreement between the U.S. Department of Transportation and the U.S. Department of Energy.

Excessive corrosion on weathering steel beam and bearing plate.



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New Wind Turbine on Argonne's Campus

Argonne has installed a 10-kilowatt wind turbine on the east side of its campus. The turbine is being used by Argonne scientists and engineers to study the interaction of wind energy, electric vehicle charging and grid technology. Energy generated by wind is fed back into the electric grid. An electric vehicle charging station is located near the turbine. It is estimated that wind energy will save the lab \$1,000 on electricity and reduce greenhouse gas emissions by more than 10 metric tons annually. The wind turbine has a 23-foot diameter rotor which weighs more than 1,200 pounds; the immense, 120-foot tower alone weighs 14,000 pounds.





Argonne to Study Safer Handling of EV Batteries after Accidents

Argonne has received a \$1.5 million award from the National Highway Traffic Safety Administration to develop a procedure for dealing with the stranded energy left in high-voltage electric vehicle (EV) battery packs after an accident. Crash impact can result in internal battery pack damage or the breaking of contacts in the system, making access to battery condition information difficult. These situations can present a danger to responders tasked with towing away the wreckage, and the storage and eventual scrapping of the wrecked vehicle. This is because the stored energy, if not addressed immediately, can pose a serious danger to workers or lead to a battery fire even weeks after the accident. Argonne's task is to develop a universal tool to enable a quick analysis of the internal condition and charged state of the damaged battery, as well as a procedure for the safe discharge of the stranded energy.

Argonne Co-Chairs SAE Committee to Revise Electric Vehicle Test Procedures

The Society of Automotive Engineers (SAE International) recently published its revised recommended practice for testing electric vehicles, SAE J1634: Electric Vehicle Energy Consumption and Range Test Procedure, based in part upon data, analysis and ideas from Argonne. The practice represents the completion of a substantial multiyear effort to find more efficient and precise ways to measure the energy efficiency and range of electric vehicles (EVs). Since battery technology has changed dramatically since the 1990s, testing methods must be revised to accommodate the increased range that EVs now offer. After many development and validation tests of original equipment manufacturer (OEM) and prototype vehicles at Argonne, a new testing approach was developed and approved by the committee. The U.S. Environmental Protection Agency (EPA) and U.S. Department of Transportation National Highway Traffic Safety Administration (NHTSA) use SAE-recommended practices such as J1634 in their official testing for energy efficiency, wording on EPA vehicle labels and NHTSA corporate average fuel economy requirements. Since 2008, Argonne engineers, including Mike Duoba who worked on J1634, have co-chaired and made significant contributions to the task forces that have revised these test procedures.



Argonne Partners with Aviation on Biofuel Business

Argonne researcher Seth Snyder is one of the leaders of a new advisory panel, the Midwest Aviation Sustainable Biofuels Initiative. The group aims to accelerate research, development and investment in technologies in the Midwest that target renewable energy for commercial airplanes.

One goal of the panel is to develop commercialized products that can be used as a sustainable replacement for traditional imported fuel sources or fashioned



into a fuel blend similar to the way ethanol is used in cars. Joining Argonne in the initiative are the Clean Energy Trust, the Chicago Department of Aviation, United Airlines, Boeing and UOP, a sustainable energy division of Honeywell. The initiative is currently preparing a report on current renewable energy efforts and will develop an action plan to attract more funding and advance biofuel research projects into commercialized products. Listen to Snyder talk about biofuels on YouTube at http://youtu.be/6l6q2_Oi4KM.

Bodycote Licenses Ultra-Fast Boriding Processes

Bodycote, one of the world's largest thermal processing companies, has obtained an exclusive license to use Argonne's breakthrough ultra-fast boriding process for full-scale commercialization. The heat treatment process uses boron compounds to convert metallic surfaces into hard, durable boride layers, enhancing the strength and performance of metal or alloy mechanical parts. Not only does the technology provide a faster and more efficient way to improve and strengthen metallic surfaces, it is also less expensive and more environmentally friendly than traditional thermal treatment processes.



With ultra-fast boriding, metal or alloy mechanical parts are dipped into a molten borax-based solution that rapidly converts the metallic surfaces into hard, durable boride layers.

Autonomie Used to Support CAFE 2017– 2025 Rule

The U.S. Department of Transportation National Highway Traffic Safety Administration (DOT/NHTSA) recently established the Corporate Average Fuel Economy (CAFE) standards for Model Year 2017–2025 passenger cars and light trucks. The standards were developed with the help of Argonne's vehicle simulation software, Autonomie. Using Autonomie, researchers provided DOT with fuel-efficiency improvement results for both transmission and electric drive technologies. The technology effectiveness results were input into the Volpe Model (the CAFE Compliance and Effects Modeling System) used to establish the standards. The standards can be viewed at http://www.nhtsa.gov/fuel-economy and Autonomie's work can be viewed at http://tinyurl.com/cuqt6fn.

Co-Simulation Buses Available in Autonomie Using CosiMate

Autonomie now links to CosiMate (developed and licensed by ChiasTek), giving users the ability to launch a heterogeneous model analysis through co-simulation buses to improve simulation performance. The process is transparent to users since CosiMateready models are automatically recognized by Autonomie. Prior to the integration of CosiMate, Autonomie allowed the usage of heterogeneous models only through the Simulink environment (i.e., using Sfunctions). The link with CosiMate will help users accelerate the product development process.



The University of Tennessee, Knoxville EcoCAR 2 Team at their 2013 Chevy Malibu Arrival Event.

EcoCAR Vehicles Arrive

Colleges participating in the EcoCAR 2 student vehicle design competition received their 2013 Chevrolet Malibu vehicles this summer as a kick-off to the second year of the contest. EcoCAR teams will install one of five plug-in hybrid vehicle architectures into their vehicles: split-parallel, series-parallel, parallel through the road, series or hydrogen fuel cell.

In Year Two, students will build the vehicle designed through their modeling efforts in Year One, and continue to refine their simulation, testing and hardware control efforts while improving vehicle efficiency and functionality. By May 2013, teams must deliver a working vehicle to a competition at General Motors' Desert Proving Grounds in Yuma, Arizona. In Year Three, the teams will focus on improving, refining and validating their vehicles to near-showroom quality and performance.

EcoCAR 2, sponsored by the U.S. Department of Energy and General Motors, and managed by Argonne, also goes beyond automotive engineering with a major emphasis on business and communication to help educate and raise awareness about the benefits of advanced vehicle technology and how it reduces the overall impact of transportation on the environment. Teams create business and communication plans, build local sponsorship materials, implement media and youth campaigns, increase team recruitment activities and utilize program management tactics.

To learn about EcoCAR, visit www.ecocar2.org or visit the Green Garage Blog at www.greengarageblog.org.



Fastrax

Larry Johnson Named Argonne Distinguished Fellow

The U.S. Department of Energy's (DOE) Argonne National Laboratory has named **Larry Johnson**, Director of the Argonne Transportation Technology R&D Center, a Distinguished Fellow, the laboratory's highest scientific and engineering rank.

Johnson joined Argonne in 1979 when the transportation research program consisted of five people; now the program exceeds \$80 million per year. Among his accomplishments are adding major facilities including the Advanced Powertrain Research Facility; the transportation beamline in the Advanced Photon Source; and the Transportation Research and Analysis Computing Center, a supercomputer program supporting the U.S. Department of Transportation. His other accomplishments include increasing Argonne's international collaboration and overseeing Memorandums of Understanding (MOUs) between Argonne and transportation research organizations in China, India and South Korea.



Johnson has testified before Congress on transportation energy and planning issues and is the author or co-author of more than 100 publications or presentations in journals, books, technical reports and activities, and conference proceedings. He also holds a patent for a suspension and propulsion system for magnetically levitated vehicles.

Don Hillebrand Elected President of SAE

Don Hillebrand, Director of Argonne National Laboratory's Energy Systems Division, has been elected 2013 President of the Board of Directors of SAE International, the organization formerly known as the Society of Automotive Engineers (SAE).

At Argonne, Hillebrand previously served as director of the Center for Transportation Research. He came to Argonne from DaimlerChrysler A.G. in



Stuttgart, Germany, where he worked as the manager of Research and Technology Policy in the DaimlerChrysler research labs. He also worked two years in the White House Office of Science and Technology Policy as a Senior Policy Advisor for Transportation to the Executive Office of the President. Before the White House, he spent 20 years as a product engineer with Chrysler Motors working on a range of advanced technology programs that resulted in patents, publications and the launch of commercial products on the road.

SAE International is a global association of more than 133,000 engineers and related technical experts in the aerospace, automotive and commercial-vehicle industries. SAE International's core competencies are life-long learning and voluntary consensus standards development. SAE International's charitable arm is the SAE Foundation, which supports many programs, including *A World In Motion*® and the Collegiate Design Series.



New Cathode Material Wins 2012 R&D 100 Award

Argonne and several partners recently received a 2012 R&D 100 Award for the development of a novel high-energy and high-power cathode material for use in lithium-ion batteries especially suited for plug-in hybrids and electric vehicles. Led by Argonne Distinguished Fellow **Khalil Amine**, the research team invented a material that provides much higher energy and longer life than any other lithium-ion cathode material, making it ideal for batteries in hybrid vehicles and a wide range of consumer electronics applications.

All other things being equal, the energy density of a lithium-ion battery depends on the capacity of the cathode material in each cell and the number of cells in the battery. To meet the extremely high energy-density requirement of the Chevy Volt or Nissan Leaf, for example, a battery manufacturer must either develop a high-capacity cathode or compensate for a low cathode capacity by greatly increasing the number of cells, even though doing so makes the overall battery larger and heavier.

Argonne's new cathode material allows battery pack size to shrink significantly both at the individual cell level and through a reduction in the number of cells needed in the battery pack, thus achieving a significant reduction in overall battery cost.

The R&D 100 Awards, sponsored by *R&D Magazine*, have been given out annually since 1962 for the top technologies of the year and are widely considered to be the "Oscars of Innovation."

Michael Wang Named One of Top 100 People in Biofuels

Argonne senior scientist **Michael Wang** is among the Top 100 People in Bioenergy for 2012–13, as voted by the readers of *Biofuels Digest* and the magazine's editorial board.

Ranked at No. 76, Wang joins other dignitaries on the list such as U.S. Secretary of Energy Steven Chu, U.S. Senator Al Franken and Jim Collins, President of DuPont Industrial Biosciences.

Wang is the lead developer of Argonne's GREET (Greenhouse gases, Regulated Emissions, and Energy use in Transportation) software model for life cycle analysis of advanced vehicle technologies and transportation fuels. There are currently more than 20,000 users of GREET worldwide, including government agencies, the auto and energy industries, research institutions, universities and public interest groups.

His research areas include the evaluation of the energy and environmental impacts of vehicle technologies and new

transportation fuels, the assessment of market potentials of new vehicle and fuel technologies, and the projection of transportation development in emerging economies such as China.

See the full list of honorees at http://tinyurl.com/cgybkvu.



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Research Results

Recent Patents

"Nano-sized Structured Layered Positive Electrode Materials to Enable High Energy Density and High Rate Capability Lithium Batteries"; **Haixia Deng**, **Ilias Belharouak** and **Khalil Amine**; United States Patent 8,277,683, issued October 2, 2012.

"Electrolyte Salts for Nonaqueous Electrolytes"; **Khalil Amine, Zhengcheng Zhang** and **Zonghai Chen**; United States Patent 8,283,074, issued October 9, 2012.

"Surface Modification Agents for Lithium Batteries"; **Zonghai Chen, Khalil Amine** and **Ilias Belharouak**; United States Patent 8,292,974, issued October 23, 2012.

"Lithium-oxygen (AIR) Electrochemical Cells and Batteries"; **Michael Thackeray**, **Christopher Johnson**, **Sun-Ho Kang**, **Lynn Trahey** and **John Vaughey**; United States Patent 8,313,721, issued November 20, 2012.

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

Recent Presentations

"Thermoelectric Measurements of Sliding Asperity Contact Flash Temperatures," **R.A. Erck**, **O. O. Ajayi** and **G.R. Fenske**, 2012 STLE Annual Meeting & Exhibition, May 6–10, 2012, St. Louis, MO.

"Which Is Greener: Idle, or Stop and Restart? Comparing Fuel Use and Emissions for Short Passenger-Car Stops," **Linda Gaines**, **Eric Rask** and **Glenn Keller**, 2012 DEER Conference, October 12, 2012, Washington, D.C.

"Synthesis, Mechanical and Chemical Characterization, and Tribological Testing of Iron-Doped Hydrogenated Amorphous Carbon Coatings," **P. Gupta**, **M.E. Graham** and **R.A. Erck**, presented at the 2012 STLE Annual Meeting, May 6–10, 2012, St. Louis, MO.

"Influence of Surface Texture on Micro EHL in Boundary Regime Sliding," **R.A. Erck**, **0.0. Ajayi**, **C. Lorenzo-Martin** and **G.R. Fenske**, presented at the ASME/STLE 2012 International Joint Tribology Conference, October 7–10, 2012, Denver, CO.

"Tribological Effects of BN and MOS₂ Nanoparticles Added to Polyalphaolefin Oil in Piston Skirt/Cylinder Liner Tests," **Nicholaos G. Demas, Elena V. Timofeeva**, **Jules L. Routbort** and **George R. Fenske**, presented at the ASME/STLE 2012 International Joint Tribology Conference, October 7–10, 2012, Denver, CO.

"Thermoelectric Measurements of Sliding Asperity Contact Flash Temperatures," **R.A. Erck**, **0.0. Ajayi** and **G.R. Fenske**, presented at the 2012 STLE Annual Meeting & Exhibition, May 6–10, 2012, St. Louis, MO.

"Effect of Carbon-based Thin-film Coatings on Frictional Behavior under Boundary Lubrication Regime," **C. Lorenzo-Martin**, **0.0. Ajayi**, **R.A. Erck** and **G.R. Fenske**, presented at the 2012 STLE Annual Meeting & Exhibition, May 6–10, 2012, St. Louis, MO.

Recent Publications

"Model for the Part Manufacturing and Vehicle Assembly Component of the Vehicle Life Cycle Inventory," J.L. Sullivan, A. Burnham and M. Wang, JIE, in press.

"Friction-reducing Properties of Onion-like Carbon under High Contact Pressure in Liquid Lubricant," Naohiro Matsumoto, Kuldeep K. Mistry, Jong-Hyoung Kim, Osman L. Eryilmaz, Ali Erdemir, Hiroshi Kinoshita and Nobuo Ohmae, Materials Letters, 2012.

"Tribological Properties of Nanodiamond-epoxy Composites," I. Neitzel, V. Mochalin, J. Bares, R. Carpick, A. Erdemir and Y. Gogotsi, Tribology Letters, 2012.

"Experimental Investigation of Transition in Lubrication Regime for Thin-film Coated Surfaces," **C. Lorenzo-Martin**, **0.0. Ajayi**, **S. Torrel**, **G.R. Fenske** and **R.A. Erck**, Proceedings of ASME/SSTLE 2012 International — Joint Tribology Conference (IJTC-2012), October 7–10, 2012, Denver, CO.

"Effect of Coating Thickness on Tribological Performance of CrN in Dry Sliding Contact," **C. Lorenzo-Martin**, **O. Ajayi**, **S. Torrel**, **N. Demas**, **A. Erdemir** and **R. Wei**, Proceedings of ASME/SSTLE 2012 International — Joint Tribology Conference (IJTC-2012), October 7–10, 2012, Denver, CO.

"Tribological Studies of Coated Pistons Sliding against Cylinder Liners under Laboratory Test Conditions," **Nicholaos G. Demas, Robert A. Erck, Oyelayo O. Ajayi** and **George R. Fenske**, *Lubrication Science*, v. 24, iss. 5, Aug. 2012, pp. 216–227.

"Protective Coatings for Enhanced Performance in Biomedical Applications," R.L. Leonard, S.A. Hasan, A.Y. Terekhov, C. Thompson, R.A. Erck, J.H. Dickerson and J.A. Johnson, Surface Engineering, v.28, No. 7, Aug. 2012, pp. 473—479.

"Antifog Coating for Bronchoscope Lens," R.L. Leonard, A.Y. Terekhov, C. Thompson, R.A. Erck and J.A. Johnson, Surface Engineering 28 (6), pp. 468–472.

"White Light Interferometry for Quantitative Surface Characterization in Ion Sputtering Experiments," **S.V. Baryshev**, **A.V. Zinovev**, **C.E. Tripa**, **R.A. Erck** and **I.V. Veryovkin**, *Applied Surface Science*, 258 (18), July 2012, pp. 6963–6968.

"Vehicle Technologies Program Government Performance and Results Act (GPRA) Report for Fiscal Year 2012," **J. Ward, T.S. Stephens** and **A.K. Birky**, *Argonne Report* ANL-12/25.

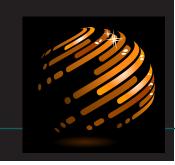
"Fuel Quality Issues with Biogas Energy — An Economic Analysis for a Stationary Fuel," **Dionissios D. Papadias**, **Shabbir Ahmed** and **Romesh Kumar**, *Energy*, 44 (2012), pp. 257–277.

"Facilitating Analysis of Trace Impurities in Hydrogen: Enrichment Using Pressure Swing Adsorption Facilitating Analysis of Trace Impurities in Hydrogen: Enrichment Based on the Principles of Pressure Swing Adsorption," **Dionissios D. Papadias**, **Sheldon H.D. Lee** and **Shabbir Ahmed**, *International Journal of Hydrogen Energy* 37 (2012), pp. 14413-14426.

"How Efficient are Hydrogen-fueled Internal Combustion Engines?," **S. Verhelst**, **R. Sierens** and **T. Wallner**, *Green Energy and Technology*, edited by H. Machrafi, Bentham Science Publishers. 2012.

Visit our website to download copies of these papers and presentations:

http://www.transportation.anl.gov/ publications/papers_presentations.html



Media Highlights

ABC News: Taking the Future Out for a Spin. Argonne transportation project engineer Glenn Keller was interviewed on the myriad of choices available to drivers who are considering going green. He says that while electric vehicle technology has grown tremendously, it's not "one size fits all" for consumers. "One should not go out and buy a battery-powered vehicle if the goal is



to take the family to Disney World—the distance and all that makes it very impractical because those batteries have to be charged at intervals. There are other technologies that step in like the plug-in hybrids. They'll retain an internal combustion engine working on gasoline that allows you to visit grandma and come back, but while you're in the city commuting to and from work you can go all on electric power," said Keller. Read the complete article at http://tinyurl.com/ a9darz6.

Equities.com: Kentucky Gov. Beshear Announces Opening of \$20.7 Million Facility for Research on Renewable **Energy, Advanced Batteries.** Argonne and the University of Kentucky (UK) have announced the opening of a new \$20.7 million facility dedicated to the research and development of renewable energy and energy storage technologies. A portion of UK's new 43,000-squarefoot building houses the **Kentucky-Argonne Battery** Manufacturing Research and Development Center, an advanced "open access" battery manufacturing R&D facility. "It's not enough to invent a better battery. We need to continue to revitalize our domestic battery industry by building tomorrow's batteries here in America. This Center in Kentucky is specifically designed to focus on developing and deploying advanced manufacturing processes for batteries and other types of energy storage devices to build America's battery industry," said Argonne Director Eric Isaacs. Read the complete article at http://tinyurl.com/crgtpa6.

SmartPlanet: Electric Car? So 2011! DOE Eyes Compressed

Natural Gas. Argonne mechanical engineer Mike Duoba was interviewed on the advantages of natural gas vehicles. As Duoba

sees it, the availability of natural gas could make CNG a more compelling fuel replacement than any other alternative to conventional petroleum. Although natural gas-powered vehicles emit more carbon dioxide than EVs do, they would help the United States cut its reliance on imported oil and still reduce greenhouse gas emissions when compared to gasoline engines, Duoba said. Read the complete article at http://tinyurl. com/ae8n28s.



Christian Science Monitor: U.S. Train Companies Eye Shift from Diesel to Natural Gas. Argonne engineer Doug Longman

commented on the train industry's potential interest in a new fuel



source. "The railroads would really like to be able to use natural gas in their locomotives. It's a cost issue," Longman said. According to the article, some proponents in the industry say natural gas would be a "huge transition in locomotive technology, similar to the move from coal engines to diesel." Read the complete article at http://tinyurl.com/ avmo5bm.

SAE Vehicle Electrification: Argonne Heats Up Lithium-ion **Battery Research.** The SAE Vehicle Electrification magazine visited

Argonne in May 2012 to meet with Daniel Abraham, a materials scientist who has been at the lab for 19 years and has focused on lithium battery technology for the past 12. He highlighted some of the work Argonne is doing and offered a Li-ion battery primer. Read the complete article at http://tinyurl.com/ czwp222.



Consumer Reports: Stop-Start Systems Have Great Promise for Saving Fuel. Argonne transportation system analyst Linda Gaines' poster, To Idle or Not to Idle—that is the Question, was featured in

Argonne News Room: Alternative Battery Systems for Transportation Uses. Explore Argonne's innovative work in advanced batteries in this video narrated by battery researcher and Argonne Distinguished Fellow Michael Thackeray. Argonne is uniquely positioned to make a difference to future generations of vehicle drivers. Watch the complete video at http://tinyurl.com/ blxfkj7.



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



OEM Off-Highway: Battery Recycling.

article at http://tinyurl.com/6m9ahdh

and view the poster at http://tinyurl.

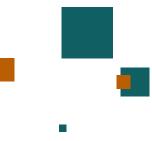
com/alfts2k.

an article about stop-start vehicle systems. According to Argonne,

if each car in the United States idles just six minutes per day, about 3 billion gallons of fuel are wasted annually. Read the complete

Argonne's **Linda Gaines** was also featured in the July/August issue of OEM Off-Highway. In the article, Linda discusses the future of lithium-ion battery recycling, which is being investigated as a possible solution to the "if and when" time when lithium might become scarce. Working with the DOE, Gaines is looking at recycling processes that produce highvalue end products. To read the article, go to http://tinyurl.com/bmftwzu.





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Parting Shots

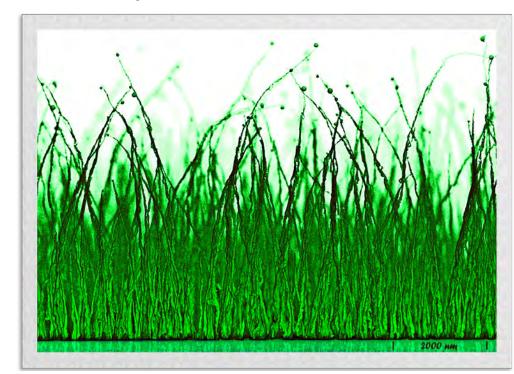
On September 15, Argonne hosted an "Energy Showcase" to give the public an opportunity to learn more about the laboratory's exciting energy research. The Transportation Technology R&D Center (TTRDC) exhibit highlighted Argonne's work in advanced technology vehicles, biofuels, batteries, the smart grid and much more. More than 12,000 people visited and were exposed to the future of energy.



Left: A plug-in Chevy Volt was on display to show visitors how electric vehicles will interact with the grid. (The Volt's battery is partially made up of materials developed at Argonne.)

Below: Biophysicist Philip Laible explains the Endurance Bioenergy Reactor, a simple, easyto-use portable system that uses bacteria to produce fuel that can go directly into engines and generators.

Below: These silica nanowires, shown in a scanning electron microscope photograph, form tree-like structures when they are bombarded with energetic ions. Supported by a silicon wafer and sporting small indium droplets at their tips, these nanowires emerge and grow several microns tall. Free-standing silicon nanowire arrays could lead to the development of new energy storage devices, such as batteries. (Image courtesy of researchers Martin Bettge and Daniel Abraham.)





Above: Electrical engineer Brian Benoy explains the EcoCar project to visitors. EcoCar2 is a three-year, collegiatelevel advanced vehicle technology engineering competition established by the U.S. Department of Energy and General Motors, and managed by Argonne.





Above: These colorful "lanterns" are really tiny carbon spheres, each just a few microns across—smaller than the diameter of a single strand of spider silk. They could be useful when added to engines to reduce wear and tear or as parts in lithium-ion batteries. (Image courtesy of researchers Vilas G. Pol and Michael Thackeray.)



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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 TransForum 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 costs 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.

Technology Development and Commercialization Argonne National Laboratory, Bldg. 201 9700 South Cass Avenue, Argonne, IL 60439 800.627.2596 partners@anl.gov www.anl.gov/techtransfer

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