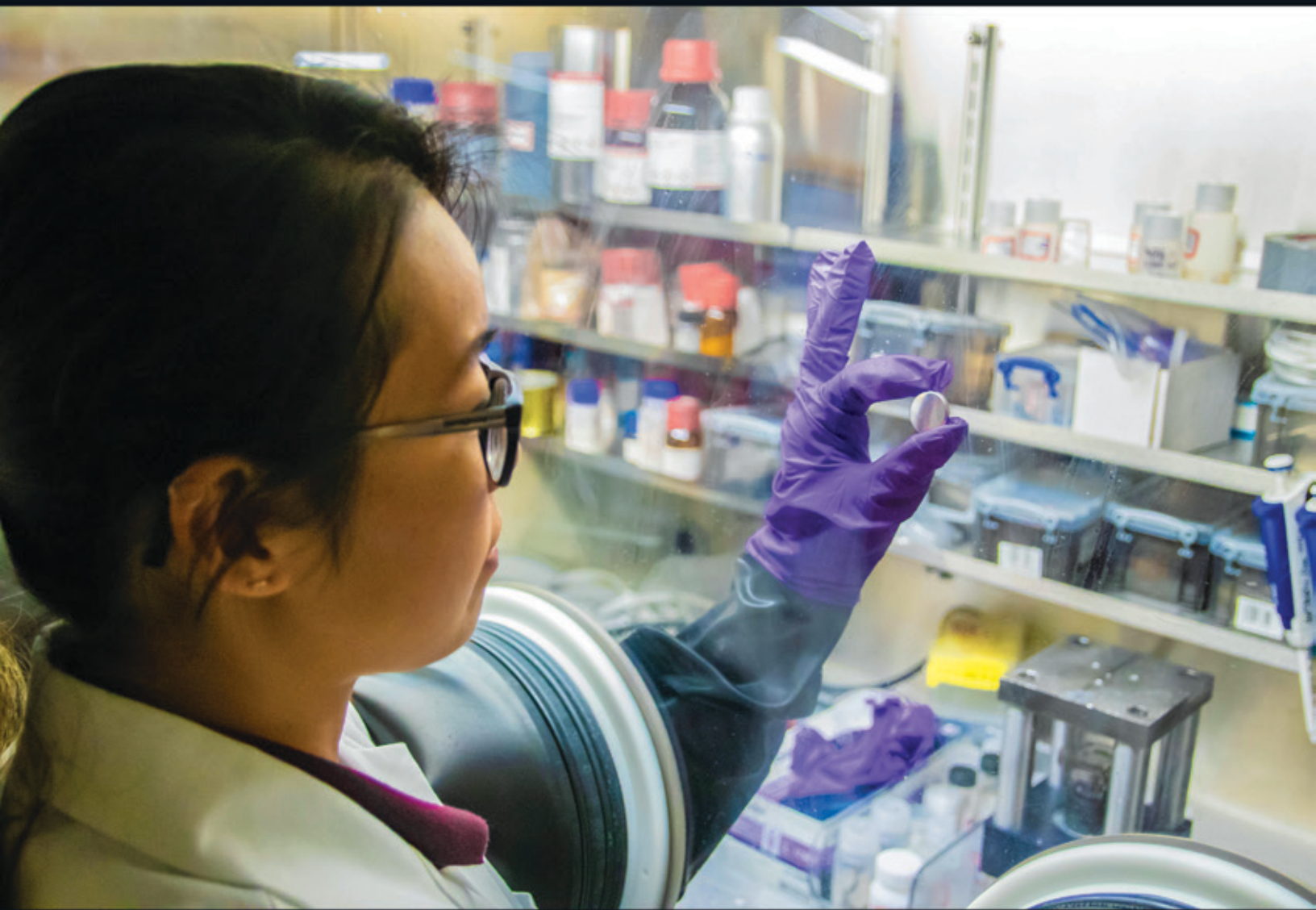


HOW BASIC RESEARCH PAYS OFF

10 Winners *from an*
Extraordinary Competition



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Energy Frontier Research Centers

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About the cover image: Dr. Carrie Siu, a postdoctoral researcher at Binghamton University in New York, works in a glove box to ensure safety and freedom from contaminants and holds a sample cell of a novel cathode material she synthesized that can markedly improve battery performance. *(Marc Francis Hidalgo)*

The ENERGY FRONTIER RESEARCH CENTERS **10@10 Competition**

In celebration of the Energy Frontier Research Centers (EFRC) ten-year anniversary, the U.S. Department of Energy (DOE) sponsored a competition among current and past EFRC awardees. The competition aimed to select ten awardees that best embody the extraordinary impact of EFRC-sponsored basic research. The competition solicited entries in three categories: the training of the next generation of scientific talent; the discovery of novel scientific ideas; and the development of advanced technologies and tools.

The competition was open to all 82 EFRCs, past and present. EFRC directors were invited to submit nominations from their center in up to two of the categories. For the people awards, the EFRC program must have made a profound impact on the individual's career; for scientific ideas, the discovery must have been primarily the result of EFRC-sponsored research; for technologies and tools, EFRC-sponsored research must have made a significant contribution to the resulting technology or tool development, but additional follow-on funding from other sources was allowed.

The competition attracted more than 40 entries across all categories. The winners were selected by a review panel convened by DOE. The selection criteria included:

- ▶ Scientific and technical excellence.
- ▶ How well the nomination exemplifies bringing together creative, multi-disciplinary teams of researchers to tackle the toughest scientific challenges preventing advances in energy technologies.
- ▶ Diversity of research topics.

The winning applications were announced and honored during an annual meeting of EFRC researchers on July 29, 2019.



SUMROENG CHINNAPAN / SHUTTERSTOCK

ENERGY FRONTIER RESEARCH CENTERS: A Summary

As world demand for energy rapidly expands, transforming the way energy is collected, stored, and used has become a defining challenge of the 21st century. At its heart, this challenge is a scientific one, inspiring the U.S. Department of Energy's (DOE) Office of Basic Energy Sciences (BES) to establish the Energy Frontier Research Centers (EFRC) program in 2009.

Mission and Strategy. While BES continues to support individual investigators, small groups at universities, and the National Laboratories, the EFRCs represent a unique approach—supporting and leveraging large-scale collaborations. The Centers bring together creative, multi-disciplinary scientific teams—typically 14–18 principal investigators and many more junior scientists and students. These teams bring a widely diverse set of skills to undertake complex energy-relevant basic research beyond

the scope of single-investigator research projects. They also take full advantage of powerful new tools located at DOE National Laboratories for characterizing, understanding, modeling, and manipulating matter from atomic to macroscopic scales. In addition, the EFRCs attract and train the next-generation scientific workforce by involving talented students and postdoctoral researchers interested in energy science.

Scope. As of July 2019, BES has supported 82 EFRCs, involving more than 1,600 senior investigators and at least 5,400 students and postdoctoral researchers at over 170 institutions. The 46 currently active EFRCs comprise 721 senior investigators, 519 postdocs, 844 graduate students, 142 technical staff, and 61 undergraduate students and involve over 115 universities, National Laboratories, and industrial companies through partnerships in 36 states and 4 foreign countries.

“EFRCs are my favorite way to do research. In the last decade, belonging to EFRCs has given me my most intriguing research questions, my most rewarding collaborations, and my most impactful research achievements.”

Professor Karena Chapman, Stony Brook University, has been involved in three EFRCs as a collaborator, senior investigator, and project leader.

Impact. The EFRCs have collectively demonstrated the potential to substantially advance scientific understanding underpinning and enabling transformational energy technologies, including a number of major breakthroughs and unexpected discoveries. The scientific output from the EFRCs is impressive—11,600 scientific publications, 772 invention disclosures, 624 U.S. patent applications, and 212 patents as of May 2019. Many EFRCs have reported that their results have already led to spin-off company startups, industry partnerships, and commercialization of new energy technologies. In addition, extensive mentoring of students and young scientists, establishment of an early career network, and an EFRC community website have boosted workforce development.

Illustrative Examples. EFRC research has spanned the full spectrum of energy challenges, including advanced materials, more efficient solar energy systems, novel energy storage solutions, improved biofuels, advanced nuclear systems, carbon capture from fossil fuel power plants, solid state lighting improvements, superconductivity, and environmental management.

- ▶ Development by two separate EFRCs of improved anode and cathode materials for lithium ion batteries that show promise for improved safety and longer battery lifetimes, as well as potentially doubling energy storage capacity and cutting re-charging times in half. Two startup companies—Nanograf and Volexion—spun off from one of the EFRCs are helping commercialize these technologies and assist the transition to electric vehicles.
- ▶ Discovery of a unique metal organic framework that can absorb large amounts of carbon dioxide and also readily release it, enabling reuse of the material. The underlying process is attracting broad industrial interest as an inexpensive means of scrubbing carbon dioxide from power plant emissions and removing it from natural gas.

- ▶ Development of advanced materials that convert thermal radiation from a heat source to electricity more efficiently than conventional power generation equipment, which a startup company, Antora Energy, is working to commercialize as a low-cost solution for grid-scale energy storage.
- ▶ Development of novel nanocrystals of a perovskite material that absorb sunlight readily and are more stable than larger crystals, as well as a method of combining the nanocrystals into low-cost, high-efficiency solar cells.
- ▶ Development of a rapid irradiation process that more than doubles the current-carrying capacity of superconducting wires through an EFRC partnership with an industrial partner, American Superconductor. The advanced wires are critical for applications such as lightweight wind turbines and motors.
- ▶ Discovery of the molecular-level structure of cellulose fibers and lignin in living biomass and how they interact with other plant materials, which is expected to enable improved processing of biofuels and other agricultural and industrial applications.

“A great aspect about the EFRCs is that they pull together many young and talented scientists, match them up with experienced scientists in the field, and give them the opportunity to think creatively. In the end, they cultivate an ecosystem that allows researchers to do basic science with applied results.”

Cary Hayner was a graduate student in an EFRC and is now Chief Technology Officer at Nanograf, a startup he co-founded based on his EFRC research.

- ▶ Development of quantum dot solar windows that introduce no distortion or color changes and yet generate electric power. A startup, UbiQD, is using the technology to build self-powered greenhouses that can improve crop yields.
- ▶ Development of a new class of surfactants for use in detergents and cleaners that work much more effectively in hard water, which is found in many U.S. homes. A startup, Sironix Renewables, is commercializing this new class of products made from biomass.



Developing the Next Generation of Scientific Talent:

KATLYN TURNER



Katlyn Turner had other options for undergraduate studies but chose to stay close to home and attend the University of Notre Dame where her mother worked. A talented piano player, she had a strong interest in music but decided to study chemical engineering in order to be sure she could find a good job. During her time at Notre Dame, she worked as a babysitter to help pay her college fees and in the process got to know Notre Dame Professor Peter Burns. Burns had received an Energy Frontier Research Center (EFRC) award, Materials Science of Actinides (MSA), from the U.S. Department of Energy's Office of Science to explore fundamental issues in nuclear energy. Burns asked Katlyn if she would be interested in stopping by his laboratory to learn about his project. She was indeed interested, so he asked if she would like to work on that project in his laboratory. She had never considered a career as a research scientist, but she accepted his offer and became a research assistant during school terms and over the summers. Over the course of her undergraduate career, she blossomed into a promising researcher. Burns notes that she was trusted to undertake procedures normally reserved for graduate students.



Her research focused on uranium peroxide clusters—nano-sized particles that Burns had discovered. These clusters came in a wide variety of shapes and sizes and were thought to be potentially important to the behavior of spent nuclear fuel and nuclear waste. As she neared graduation, Katlyn was asked to give a presentation on her work at a scientific conference, where Professor Rodney Ewing—a co-principal investigator on the MSA EFRC—heard her talk and was impressed with her work, her poise, her scientific maturity, and her communication skills. He invited her to join his research group at the University of Michigan, where he was studying the incorporation of uranium and other actinides into crystal-line materials for waste disposal, as well as the effects of radiation on such materials.

Top: Katlyn Turner as a graduate student at the University of Michigan (R. Ewing)

Middle: Turner giving a seminar on international nuclear energy policy at Harvard University's Belfer Center for Science and International Affairs (Harvard University)

Bottom: Turner receiving her PhD hood at Stanford University commencement in 2017 with assistance from Professor Rodney Ewing

Next page: Turner receiving her EFRC 10@10 award in July 2019 (U.S. Department of Energy Office of Science)



“I was impressed by Katlyn’s poise, her scientific maturity, and her communication skills—especially for an undergraduate—and on the spot invited her to join my research group.”

—Rodney Ewing, Stanford University

Professional Affiliations



University of Notre Dame



University of Michigan



Stanford University



Harvard University
Belfer Center for Science & Int’l Affairs

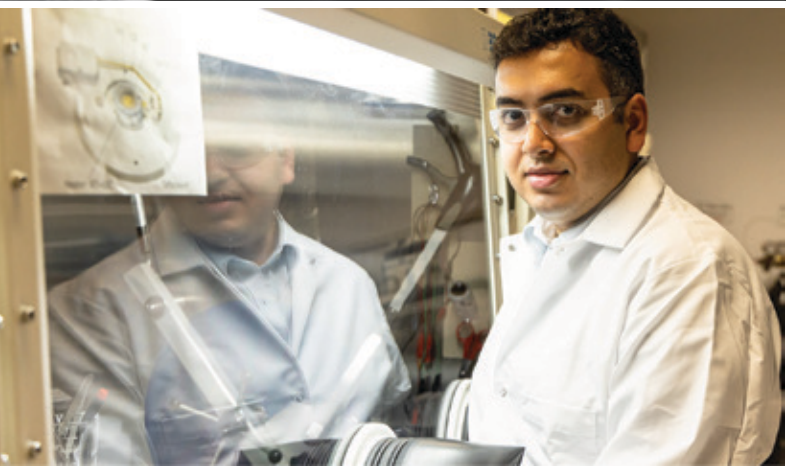
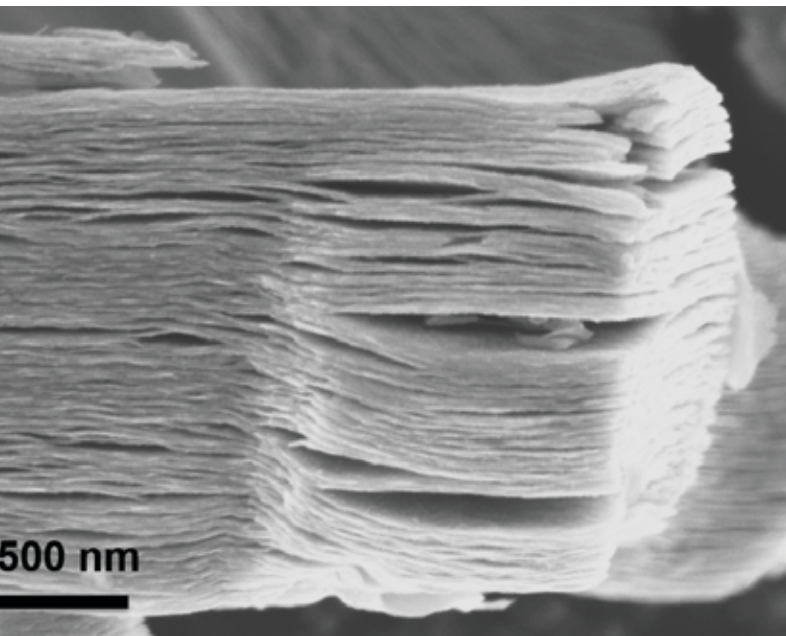
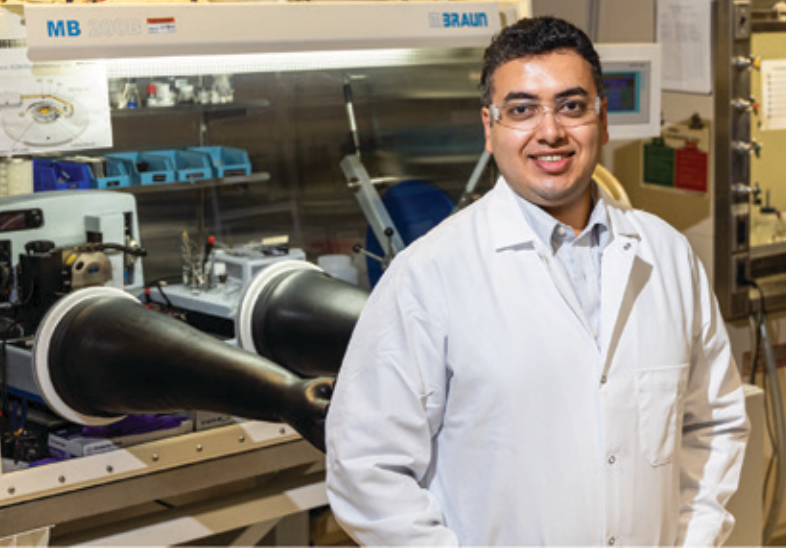
Within a year, Ewing moved to Stanford and took Katlyn and others of his research team with him. Katlyn broadened the team’s research strategy through her knowledge of uranium clusters as well as the study of both the clusters and ceramic materials of interest for nuclear waste storage under very high pressures—a process using diamond anvils. In effect, she used high pressure as a probe to understand both types of materials. In addition to her work at Stanford, she traveled back and forth between Argonne National Laboratory and Notre Dame to use analytic tools available there. She completed her doctorate, publishing her research in major journals.

Along the way, Katlyn also became interested in international science policy issues. While she was serving as a teaching assistant to Ewing, she helped with a high-profile course on the Fukushima nuclear disaster in Japan and related issues in international nuclear waste management. Her participation in this course turned out to be substan-

tial, which enhanced her interest in policy and led to a post-doctoral appointment at Harvard’s Belfer Center for Science and International Affairs. She has subsequently written several publications on science policy.

Katlyn credits the MSA EFRC with providing both support and a unique opportunity to conduct important basic research related to nuclear energy, both as an undergraduate and a graduate student. In addition, it showed her what is possible in the larger-scale collaborative research that EFRCs make possible. She also credits support from Stanford fellowships. The result is still something of a rarity—a young minority woman who is both a first-class research scientist and an exceptionally knowledgeable science policy analyst.

Materials Science of Actinides (MSA)
Winner — Workforce Development Award
www.science.osti.gov/bes/efrc/Centers/MSA



Top: Michael Naguib in a laboratory at DOE's Oak Ridge National Laboratory, where he participated in the research that led to improved understanding of the new class of MXene materials—materials he had previously discovered as a graduate student.

Middle: Multiple layers of the remarkable two-dimensional material known as a MXene, shown here under powerful magnification (each layer is less than 1 nanometer in thickness).

Bottom: Naguib is now a faculty member at Tulane University in New Orleans, where he is continuing his research on novel energy materials and helping to build that university's first doctoral program in materials physics and engineering.

(All photos from Carlos Jones at Oak Ridge National Laboratory)

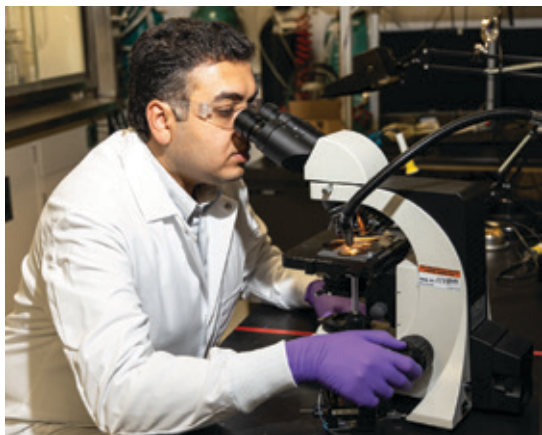
Developing the Next Generation of Scientific Talent:

MICHAEL NAGUIB

Michael Naguib was born in Egypt and completed his undergraduate and master's degrees at Cairo University. He wanted to study advanced materials, but there was no place to do so in Egypt. Instead he enrolled in a PhD program at Drexel University in Philadelphia. There he was assigned to explore whether certain materials that have a layered structure (with three layers, each having a different chemical composition) could be used to make better electrodes for lithium ion batteries. Michael found that the materials were not useful as electrodes because lithium ions (the charge carriers in modern batteries) could not penetrate the material. To address this, he tried to modify the material by removing the middle layer with acid. The unexpected result was the discovery of a completely new nano-material: a titanium-carbon compound in the form of a two-dimensional sheet less than a nanometer thick. He and his advisors at Drexel immediately recognized the new material's potential for energy storage.

Publication of that discovery—of what soon became clear was a whole family of two-dimensional materials now called MXenes—triggered a world-wide surge of research. To explore MXenes and related phenomena in more detail, the U.S. Department of Energy's Office of Science funded an Energy Frontier Research Center (EFRC) on Fluid Interface Reactions, Structures and Transport. The research team included computational modelers, university experts in materials synthesis and thermodynamic analysis, and scientists at DOE's Oak Ridge National Laboratory (ORNL) who could probe the material's structure with neutrons and powerful microscopes.

After completing his PhD, Michael moved to ORNL with a prestigious fellowship. There he played a major role in the research on MXenes as one of the team's principal investigators—unusual for a young scientist. What has already emerged from the research is a much clearer understanding of the structure, chemistry, and the electronic behavior of these new materials—including how they behave in the presence of battery electrolytes, water, or other fluids.



Because their properties can be fine-tuned by adjusting their composition, MXenes may find a wide range of industrial uses:

- > They can be used to shield mobile phones and other devices from electromagnetic interference.
- > They have major potential in energy storage devices. Lithium ions can diffuse very readily into MXene and thus may enable batteries with increased energy storage and more rapid re-charging.
- > They can store large amounts of electric energy on their surface, acting as a supercapacitor (which stores energy as electric charges as opposed to storing energy in a chemical reaction as in a battery). Small supercapacitors already play an important role in micro-electronic circuits, and those made from MXenes could store even more energy. Larger-scale supercapacitors, because of their rapid reaction time, could help stabilize the electrical grid by smoothing out surges.

There are now some 20 different MXenes known. They can be easily synthesized and are stable in water and in a variety of organic solvents, making them relatively easy to process—even in large-scale production. A big Japanese company has licensed the MXene technology for a wide range of applications and is said to be nearing commercial production.

For Michael, the EFRC experience proved invaluable. He developed leadership skills and learned how to work as part of an interdisciplinary team. Perhaps most important, he became literate in the many areas of science

“Michael’s achievements—some 60 publications and more than 12,000 citations in the scientific literature—in such a short time are simply unique.”

—David Wesolowski, Oak Ridge National Laboratory

Professional Affiliations



Cairo University



Drexel University



Oak Ridge National Laboratory



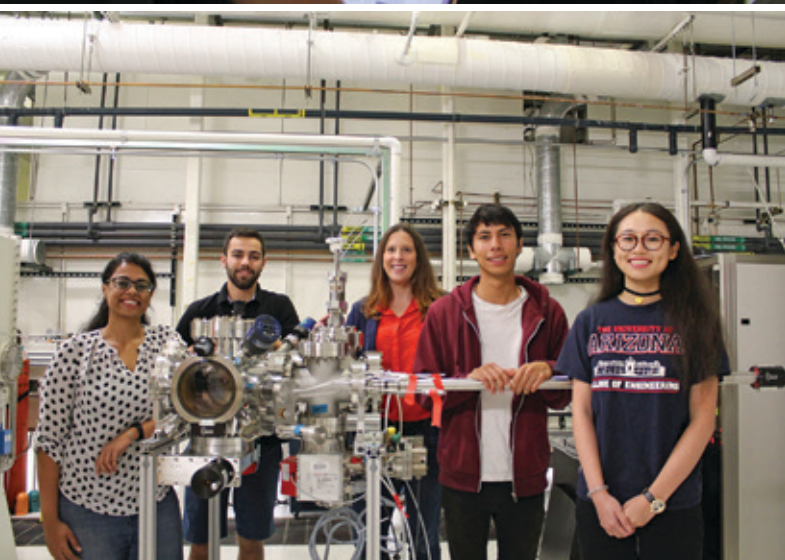
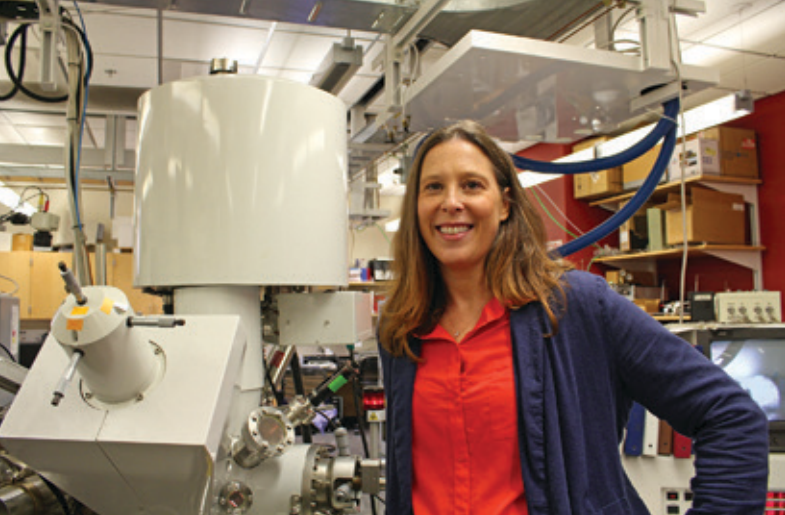
Tulane University

required to undertake the investigation—“learning to speak the language” of computational modeling; of neutron, x-ray, and scanning probes; and of potential energy storage materials. He also established himself as far more than a junior scientist, with some 60 publications and more than 12,000 citations in the scientific literature—more than most scientists achieve in a lifetime.

David Wesolowski of Oak Ridge National Laboratory and former director of the EFRC Center says, “Michael’s achievements in such a short time are simply unique.” At the end of his stay at Oak Ridge, Michael accepted an assistant professorship at Tulane University in New Orleans, where he is helping to build that institution’s (and Louisiana’s) first doctoral program in materials physics and engineering. As an immigrant on his way to becoming a U.S. citizen, Michael is a significant addition to the scientific talent pool in this country.

Fluid Interface Reactions, Structures and Transport Center (FIRST) Winner — Workforce Development Award

www.science.osti.gov/bes/efrc/Centers/FIRST



Top: Erin Ratcliff at work in her laboratory at the University of Arizona, where she is a faculty member in the Department of Materials Science and Engineering.

Middle: Ratcliff teaching a class on the basic principles of a solar cell, part of a course on solid state chemistry at the University of Arizona, where she has also become a mentor for women engineering students.

Bottom: Ratcliff and her research team are conducting investigations aimed at developing advanced thin-film solar cells, building on the knowledge she helped to develop under the EFRC grant.

(All photos from University of Arizona College of Engineering)

Developing the Next Generation of Scientific Talent:

ERIN RATCLIFF

Erin Ratcliff studied chemistry, mathematics, and statistics as an undergraduate at St. Olaf College in Minnesota and then completed a doctorate in physical chemistry at Iowa State University. That breadth of knowledge combined with her enthusiasm, drive, and ability to communicate were what convinced Regents Professor Neal Armstrong to offer her a postdoctoral position in his laboratory at the University of Arizona. One of her first tasks there was to help with the application for what became an Energy Frontier Research Center (EFRC), the Center for Interface Science: Solar Electric Materials, focused on thin-film solar cell materials. When the grant came through, Armstrong created a position for Erin as a research scientist for the Center.

Thin-film solar cells have a number of potential advantages:

- > They are thin, so even multi-layer cells don't require a lot of raw material.
- > They lend themselves to manufacture by depositing or "printing" onto glass or other inexpensive structural materials, lowering costs.
- > If made of transparent materials, they can both transmit light and generate electricity, potentially enabling "smart" windows and self-powered greenhouses.

A key challenge has been to increase the efficiency with which thin-film cells convert sunlight to electricity, a challenge that depends on understanding the electron transfer mechanisms between the active layers that absorb sunlight (and generate electrons) and the conductors that carry away those charges as electric current. That interaction was the focus of the Center's research.

The Center was a large and geographically diverse team—15 principal investigators at four universities and the National Renewable Energy Laboratory (NREL). Erin quickly became the glue that held the entire effort together. She



“Erin became a poster child for cross-disciplinary research, as well as the most prolific scholar of the Center.”

—Neal Armstrong, University of Arizona

Professional Affiliations



St. Olaf College



Iowa State University



University of Arizona
Dept. of Materials Science and Engineering

worked with university scientists to explore potential new materials and interfaces and with NREL staff to create and test prototype devices in the lab. She developed new measurement techniques to characterize the structure and properties of the materials and measure their interactions. She published joint research with all 15 of the principal investigators, spending a lot of time in their labs.

The diverse team worked productively together. They created both a greater understanding of the interface issues—between two types of materials “that don’t want to be together,” as Armstrong describes it—and especially of the mysterious sites that formed to recombine opposite charges and thus lower the effective current generated. Creating ways to remove such recombination sites was a key outcome of the research.

The five-year effort led to significant improvements in the efficiency of organic semiconductor thin-film cells, which have now reached 17%. The knowledge and measurement techniques developed have since carried over to inorganic thin-film cells. Companies such as a California startup, Next Energy Technologies, are commercializing thin-film solar cells for smart windows that can harvest light from both inside and outside and convert it to electricity, significantly lowering energy consumption in buildings. And Ratcliff’s

own research is now exploring how such cells might be used for self-powered greenhouses.

The other significant impact of this EFRC was on Erin herself, as she is the first to acknowledge. “The experience was ideal; it gave me a chance to see many different management styles in the different labs and gain a real understanding of what organized, large-scale science can accomplish,” Erin says. And following the EFRC, she accepted a tenure-track position in the Department of Materials Science and Engineering at the University of Arizona, where she has already built her own research lab and team and emerged as a mentor of women engineering students. “I had experience I could put to immediate use and 15 senior mentors.” Armstrong concurs: “Erin already had strong networking skills when she came to me. But during the EFRC she really matured in her ability to collaborate with and manage both young and established scientists, and in her own capacity as a scientist: she became a poster child for cross-disciplinary work—a key EFRC workforce development goal—as well as the most prolific scholar of the Center.”

Center for Interface Science: Solar Electric Materials (CISSEM) Winner — Workforce Award

www.science.osti.gov/bes/efrc/Centers/CISSEM



As the costs of solar cells drop and their efficiency improves, solar power is set to play an ever-larger role in generating electricity and moving the U.S. toward a climate-friendly energy system. *(Matteo Fes / Shutterstock)*

MORE EFFICIENT, LOW-COST SOLAR CELLS

Silicon solar cells have dominated industrial solar energy facilities, but they convert only about a quarter of the sunlight that reaches them to electric power. To explore alternative approaches, the U.S. Department of Energy's Office of Science funded an Energy Frontier Research Center (EFRC) that is now called Light Energy Activated Redox Processes.

Two of the Center's principal investigators, Mercuri Kanatzidis and Robert Chang, both at Northwestern University, collaborated on the project. Many research groups were investigating a type of thin-film solar cell that combines a photo-sensitized material that could efficiently absorb light and generate electrons with a liquid that could capture and conduct the electrons. When Chang investigated these solar cells more carefully, however, he concluded they were not a promising solution because the liquid was corrosive



The perovskite material in solar cells is manufactured in high-tech facilities, but perovskite crystals also occur in nature, such as the shiny pieces found in this sample collected in Arkansas.

(Rob Lavinsky, iRocks.com – CC-BY-SA-3.0, CC BY-SA 3.0
<https://commons.wikimedia.org/w/index.php?curid=10146594>)

and would eventually lead to cell failure. He suggested finding a different material to pair with the photo-sensitized thin-film layer. As it happened, Kanatzidis knew of a class of materials called perovskites that might work and proposed that Chang try it as the substitute material. Perovskites combine several different elements, have a unique structure, and are easy to make. A prototype cell combining a thin layer of perovskite and a photo-sensitized material not only worked, but the thin layer of perovskite also absorbed additional sunlight, boosting efficiency. Additional research improved performance to 10 percent efficiency.

Publication of that research generated enormous interest and a flurry of worldwide research that transformed the perovskite material into a full-fledged semiconductor and improved its ability to absorb sunlight, so that a separate photo-sensitized layer was no longer needed. Development of layered perovskite cells that used organic material to separate the layers helped to improve stability and cell lifetimes. Moreover, perovskite solar cells turned out to be easy and inexpensive to manufacture. Reported efficiencies for perovskite solar cells marched steadily higher, reaching 25 percent in less than a decade from their discovery.

Kanatzidis and Chang also discovered perovskites that could be combined with other solar cell materials, such as a thin layer of perovskite material on top of a standard silicon



Commercial-sized perovskite-silicon solar cells that are nearing commercial production.

(Oxford PV)

cell. This tandem structure allows each material to absorb a different part of the solar spectrum. These cells have reached 28 percent efficiency—above what standalone silicon cells can achieve—with the prospect of even higher efficiencies to come. Rapid advances in perovskite technology have led to strong interest in commercialization, with multiple startup companies leading the way.

In addition to solar cells, perovskites now have other uses: the material makes better light-emitting diode (LED) lights, and commercialization of that application is taking off. Large single crystals of a perovskite material that includes bromine also turned out to be breakthrough detectors for gamma rays and are of great interest to astronomers, particle physicists, and—because nuclear weapons tests emit gamma rays—national security officials.

Reflecting on the bounty of applications and the EFRC process that triggered them, Kanatzidis says that the EFRC process and the collaboration among a dozen or so investigators enabled by the EFRC is “the best R&D system yet” because it fosters faster progress and unexpected breakthroughs.

Center for Light Energy Activated Redox Processes (LEAP)

(formerly the Argonne Northwestern Solar Energy Research Center [ANSER])

Winner — Scientific Ideas Award

www.science.osti.gov/bes/efrc/Centers/LEAP



Giant trees of Sequoia National Park (*mkldesigns / Shutterstock*)

UNLOCKING THE SECRETS OF PLANT SKELETONS

In humans and other mammals, it is our bones that give form to our bodies and enable our muscles to exert force. Insects have a hard exoskeleton for the same reason. But plants—from flowers to trees—are different. Their structure comes from bundles of cellulose biomolecules that form microfibrils, which combined with other materials including lignin make up the walls of plant cells. These walls are so strong that they essentially act as a skeleton. Indeed, cellulose-rich cell walls enable a slender stalk of corn to grow 6 or 8 feet tall and a giant Sequoia to tower more than 300 feet, dwarfing any other life form. Cellulose is the most abundant (and arguably the most important) long-chain biomolecule on earth.

Until recently, however, cellulose—both its structure and how plants make it—was a mystery. That’s why the U.S. Department of Energy’s Office of Science funded an Energy Frontier Research Center (EFRC) to explore the topic and its implications for advanced plant-based materials and biofuels. The Center for Lignocellulose Structure and Formation included a dozen principal investigators spread across a number of universities, including physicists and engineers as well as plant biologists.

The cross-disciplinary research effort pursued several related problems. Plants take carbon dioxide from the air and transform it into sugar, but how do they convert sugar into a long-chain molecule called a polymer? A computer model of plant enzymes involved in cellulose synthesis showed a strong similarity with the structure of a previously identified cellulose-forming protein in a bacterium. Further laboratory and computational testing led to insights into both the structure of cellulose-forming enzymes and how they catalyze microfiber-formation in living plants.

A second mystery was the actual structure of cellulose in plant walls. Plant biologists knew that the fibers they could see under a microscope were made of many individual polymer strands, but the individual strands were too small (less than a nanometer in width) to count accurately. A full-scale effort with different forms of imaging, computational analysis, and biochemical experiments finally established that each cellulose microfiber has 18 polymer chains, tightly bonded to each other to give added rigidity, enabling a crystalline-like character and behavior. The research also provided insights into how the fibers grow within a plant, including understanding the behavior of a group of enzymes that act as a microfiber-spinning machine, directing the clustering of the 18 polymer chains (see image).

With the secrets of plant skeletons in hand, the scientists then tried to replicate the process in the laboratory. In a remarkable breakthrough, they were able to synthesize cellulose polymer chains and see microfiber formation in a test tube. This research opens the door to engineering modified fibers—either in plants or as an industrial process—for specific applications. For example, it now seems possible to grow plants with thicker cell walls, creating a richer source of fiber for biofuels. It may also be possible to make cellulose that is easier to degrade and digest for biofuels or

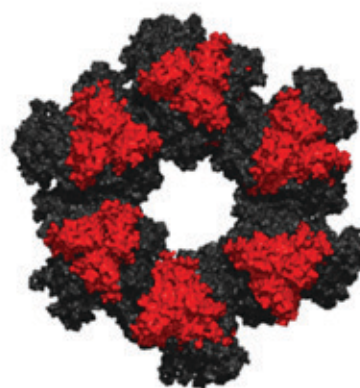


A successful thick crop of sweet corn stands in a tall, straight, dense row and will soon be harvested for market. (Eric Buermeye / Shutterstock)

animal feed, or to develop novel nano-cellulosic materials with new physical properties.

Research is also continuing into lignocellulose, the plant cell wall material that makes wood so strong. New types of cell walls in wood and other plant fiber cells may one day support innovations in structural materials and renewable resources for the pulp, paper, and textile industries.

Mankind has bred plants to improve food supplies for millennia. Only now, however—thanks in part to the EFRC program—have we understood critical parts of their biology sufficiently to imagine using plants in dramatically new ways.



This rosette-like formation of plant proteins—grouped as six units, each with three enzymes—is what catalyzes the formation of 18 cellulose polymer strands that together create the microfibrils that give plant cell walls the strength to serve as the skeleton for every plant. Understanding how this fiber-spinning mechanism works within plants is not only an important advance in basic science, but also opens the door to an array of practical applications. (Under the Creative Commons License, this image is an excerpt of Figure 5 in www.nature.com/articles/srep28696.)

**Center for Lignocellulose Structure and Formation (CLSF)
Winner — Scientific Ideas Award**

www.science.osti.gov/bes/efrc/Centers/CLSF



Dr. Carrie Siu, a postdoctoral researcher at Binghamton University in New York, prepares to test a sample of a novel cathode material she synthesized that holds promise of markedly improving battery performance. *(Marc Francis Hidalgo)*

IMPROVING BATTERY PERFORMANCE FOR ELECTRIC VEHICLES

The impending production of many new electric vehicles means that recharging batteries will become a more common—and for many drivers, a daily—activity. Consequently, advances in battery technology that could enable faster charging and enhanced mileage between charges would be very important. That's why the U.S. Department of Energy's Office of Science funded an Energy Frontier Research Center (EFRC)—the NorthEast Center for Chemical Energy Storage.

The Center focused its research on understanding how chemical reactions involving battery cathodes occur, so that the battery's performance could be improved. In today's lithium ion batteries, for example, a lithium ion interacting with an active site in the cathode transfers a single electron. But what if the cathode was made of a material that could accept the transfer of two electrons—in effect, interacting with two

lithium ions—at each active site? Could that also double the rate at which the battery can be recharged and substantially improve the amount of energy stored? The scientists knew that the element vanadium had that kind of electronic character, and they set out to find a structure for the cathode and test whether such a battery would be stable.

The multi-disciplinary team included theoretical chemists, experts skilled in synthesizing new materials, and others skilled at analyzing them. The theorists suggested a particular vanadium phosphate compound to explore; the synthesizers made trial materials; and the analysts studied their properties with a variety of methods, including X-ray analysis at Argonne and Brookhaven National Laboratories. After multiple cycles of research, the team understood why existing battery materials don't achieve their theoretical capacity. Dr. Carrie Siu of Binghamton University then used that understanding to create a synthesis method that optimized the properties of the vanadium material. The result was a nano-sized material that could interact with nearly twice as many lithium ions, pound for pound, as the cathodes in current batteries.

In tests of its electrochemical behavior, this type of cathode proved able to charge and discharge two lithium ions per site, potentially halving re-charging time and doubling the energy storage capacity of a battery. Moreover, the material appeared to be stable after many charge and discharge cycles, suggesting that battery lifetimes might also be improved. Tests showed that such cathodes work best at low voltage, but this should not be a limitation for vehicle batteries.

The Center Director, M. Stanley Whittingham—who was awarded the 2019 Nobel Prize in chemistry for his earlier development of the first lithium ion battery—believes that the new cathode should be easy to manufacture because of broad industry experience with similar materials. The university has patented the new cathode material, and the research team is talking to potential commercial partners.

More broadly, EFRC-supported research has yielded at least two additional approaches to improved batteries—wrapping anode and cathode materials in a nanoscale layer of carbon, and making them from a newly discovered MXene material. With so many novel approaches, it seems clear that the next generation of vehicle batteries is likely



Top: Dr. Siu conducts electrochemical tests on potential battery materials.

Bottom: The lefthand stack of battery cells made of a novel cathode material has the same energy storage capacity as the righthand stack of cells used in the current generation of batteries.

(Marc Francis Hidalgo)

to have significantly better performance—enabling faster recharging, greater driving range, and likely improved battery lifetime. This in turn will help enable a transition to electric vehicles.

**NorthEast Center for Chemical Energy Storage (NECCES)
Winner — Scientific Ideas Award**

www.science.osti.gov/bes/efrc/Centers/NECCES



NASA Flight Engineer Reid Wiseman and two other astronauts spent five months onboard the International Space Station, which would not be possible without removing excess carbon dioxide from the air they breathe. (NASA / Bill Ingalls)

TRANSFORMING INDUSTRIAL SEPARATION OF GASES

Separating one gas from another—removing carbon dioxide from power plant emissions, for example—is not easy. To do so would prevent carbon dioxide, a greenhouse gas, from entering the atmosphere, but present methods are very expensive. Carbon dioxide is also a contaminant found in the methane from natural gas wells. And in submarines or space capsules, carbon dioxide from human respiration must be removed from the air the crew breathes before it reaches toxic levels.

That challenge, to find new and more efficient ways of separating gases, prompted the U.S. Department of Energy's Office of Science to fund an Energy Frontier Research Center (EFRC) based at the University of California at Berkeley. The Center for Gas Separations research team decided to explore the potential of metal organic frameworks—metal atoms bound together by organic molecules to form a porous, sponge-like material. In this case, the researchers intended to also coat the metal atoms with another organic chemical that bonds readily with carbon dioxide.

Tom McDonald, a new graduate student, was assigned to test a wide variety of organic chemicals called amines as part of the metal organic framework to see how well the material could bond with, or capture, carbon dioxide gas. One particular amine showed promise. But the metal organic framework had small pores that became easily blocked, inhibiting the carbon dioxide molecules from entering. McDonald spent time learning how to make different metal organic frameworks with larger pores and more potential binding sites for carbon dioxide. In addition, instead of adding the amine molecules to the material used to make the metal organic framework, he added amines after the metal organic framework was already formed. When he tested the resulting material, it was able to absorb and release large amounts of carbon dioxide and to do so with a very small change in conditions, almost like an on-and-off switch—an unexpected and dramatically different behavior.

At this point, the collaborative nature of an EFRC became important. The materials were studied theoretically with computational chemistry models and analyzed in the laboratory with several different techniques. These were repeated in materials with slightly altered compositions. But the data didn't seem to make any sense—the material's ability to absorb carbon dioxide defied understanding—at least under the long-standing assumption that each potential binding site operated independently of the others.

McDonald finally asked himself: suppose that the behavior of one site (binding to a carbon dioxide molecule) influenced the next site? There were no known examples of such behavior in physical chemistry systems, but there is a well-known biological example: the hemoglobin system in human blood that carries iron to cells. When the metal organic framework data were analyzed as “cooperative adsorption” (in which the binding of a carbon dioxide molecule to one site activated a neighboring site), the data suddenly made sense. And once that cooperative or self-catalytic model was understood, it became possible to design materials and industrial separation processes that were more efficient, much less energy intensive, and potentially far less costly. In particular, McDonald's material absorbed large amounts of carbon dioxide even at relatively low temperatures and, equally important, could be regenerated (to release the carbon dioxide) with a small drop in pressure or a small increase in temperature, thus enabling efficient reuse of the material.



Top: Coal-fired power plants are a major source of carbon dioxide entering the atmosphere; “cooperative adsorption” may enable a low-cost way of removing it from exhaust gases. (Heidi Besen / Shutterstock)

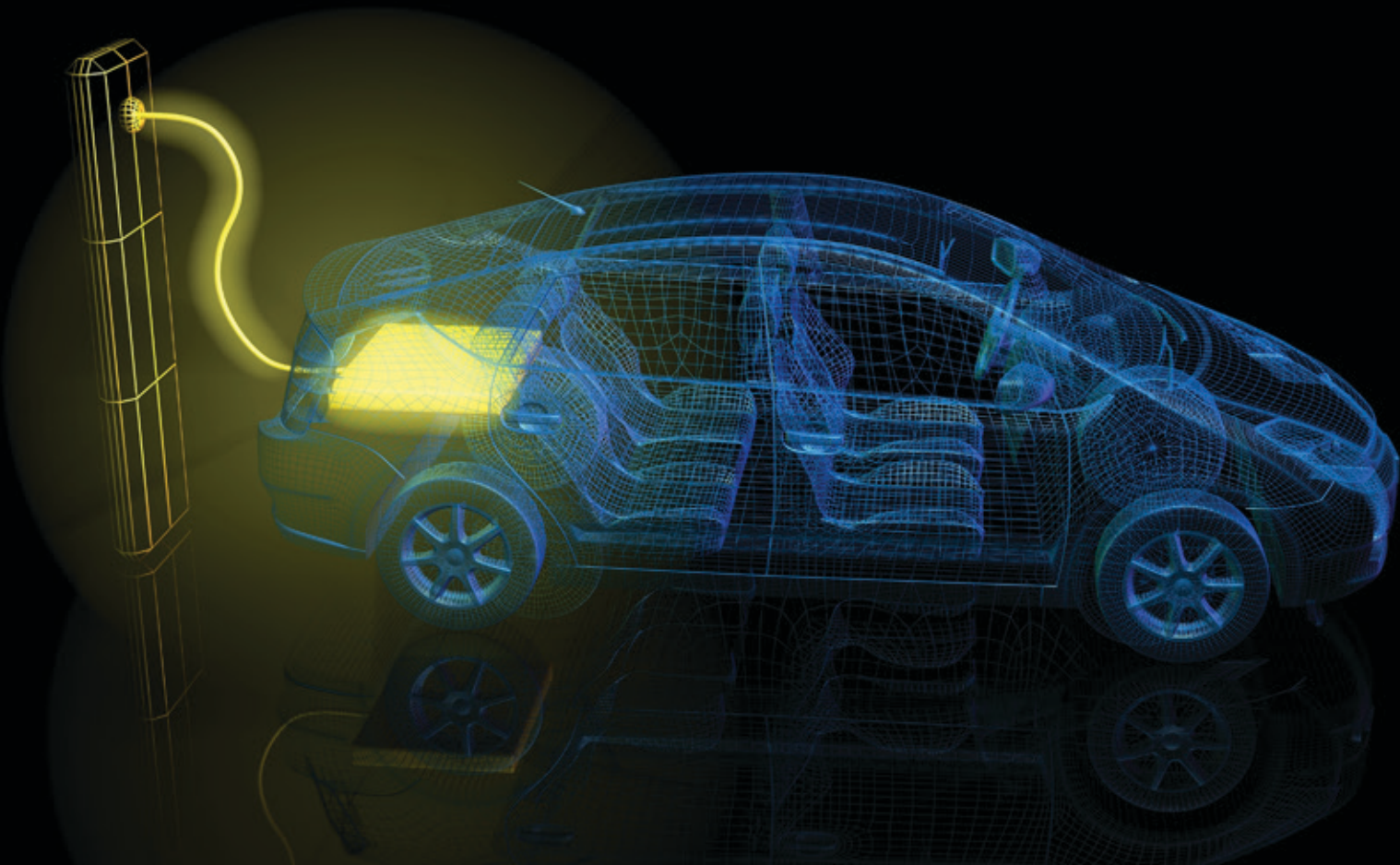
Bottom: Drilling in the Texas Permian Basin is now a major source of U.S. natural gas. (GB Hart / Shutterstock)

This fundamental discovery led to formation of a U.S.-based startup company—Mosaic Materials—which will focus initially on commercializing cooperative adsorption for human life-support systems that remove carbon dioxide from air—targeting the naval and space markets. A number of companies are now exploring the potential of cooperative adsorption for scrubbing carbon dioxide from electric power plant exhausts. Perhaps the largest existing market is in removing carbon dioxide from methane, given the rapidly growing U.S. production of natural gas. Moreover, it is already clear that metal organic frameworks can potentially be used to separate carbon monoxide and other commonly used gases, so this EFRC research provides a pathway to develop new materials and separation processes that could lower costs and save energy use for a broad cross-section of industry.

Center for Gas Separations (CGS)

Winner — Scientific Ideas Award

www.science.osti.gov/bes/efrc/Centers/CGS



Wire frame rendering of an electric car charging its battery (highlighted in yellow) (vrx / Shutterstock)

MAKING MORE POWERFUL, LONGER-LIVED BATTERIES

Lithium ion batteries power your phone, your laptop, and the growing number of electric vehicles on the road. Such batteries are also critical to the rapidly expanding market for airborne drones. However, current versions of these batteries don't hold as much power as their users would like, need frequent recharging (a lengthy process, especially for vehicles), and wear out in a few years when the materials in the battery degrade. To understand why and to find better materials, the U.S. Department of Energy's Office of Science funded an Energy Frontier Research Center (EFRC), the Center for Electrochemical Energy Science, led by Argonne National Laboratory with Northwestern University and other university partners.

The initial research phase focused on the battery's negative terminal or anode. The team of researchers studied how lithium ions flowed into and interacted with anodes made of materials ranging from traditional graphite (carbon) to silicon and silicon/carbon composites. The structure and performance of these materials were studied using a coordinated series of computational calculations and laboratory studies with advanced analytical tools. The key breakthrough was the creation of an anode composed of nanoparticles of silicon, each coated with a protective layer of a material called graphene—a sheet of carbon just one atom in thickness. These materials are now under commercial development for use in next-generation lithium ion batteries by Nanograf, a U.S. startup spun out of Northwestern. They consist of anodes with many layers of such coated particles, each layer sandwiched between thin sheets of copper foil.

This structure significantly enhances battery performance in two ways. Micropores in the graphene allow lithium ions to penetrate readily, enabling faster charging. Graphene is also flexible and expands readily, enabling the silicon to swell as it absorbs more lithium ions, thus increasing the battery's energy storage capacity (and an electric vehicle's driving range) by as much as 30 to 50 percent. The batteries are also expected to be lighter and safer (because of greater chemical stability) than existing lithium ion batteries.

The second phase of research built on the earlier work but focused on the battery's positive terminal, the cathode. A key problem with current batteries is that the organic solvent that transports lithium ions between the terminals also reacts chemically with the cathode. These reactions create a barrier around the cathode and also eventually cause the cathode to dissolve, both of which limit a battery's useful lifetime. Here again, coordinated studies allowed the process to be thoroughly understood and a solution developed: coating each particle of cathode material with a few sheets of graphene. The coating stabilized the chemistry, further boosted the amount of energy the battery could store, enabled still faster charging and, importantly, looks likely to significantly extend battery lifetimes. Commercialization of such cathodes is now underway by a second U.S.-based startup company—Volexion—also spun out of Northwestern. The graphene-encapsulated anode and cathode materials also enable lithium ion batteries to function at tempera-



Top: Farmers are using battery-powered drones for terrain scanning, monitoring soil hydration, checking on crop conditions, and much else—including sending data to the cloud for analysis. (MONOPOLY919 / Shutterstock)

Middle: Consumers would welcome batteries for their devices that held more power. (Georgejmclittle / Shutterstock)

Below: Silicon nanoparticles protected by a graphene coating enable better lithium ion batteries. (Nanograf)

tures well below freezing—critical if you want an electric car but live in a cold region.

The lithium ion battery industry is now primarily based in Asia, but the EFRC research and subsequent commercial developments that license those discoveries have given the U.S. a potentially key advantage: intellectual property critical to the emerging electric vehicles revolution.



Center for Electrochemical Energy Science (CEES)
Winner — Technologies and Tools Award
www.science.osti.gov/bes/efrc/Centers/CEES



Solar power capacity is growing rapidly, and so are installations of solar photovoltaic panels such as the industrial-scale system shown here. Without some means of energy storage, however, solar cannot replace all of the fossil fueled power stations. *(Jenson / Shutterstock)*

TACKLING THE ENERGY STORAGE PROBLEM FOR GRID-SCALE SOLAR POWER

Power from the electric grid that is generated by solar panels is already less expensive in many areas than that generated by fossil fuels. But as solar power facilities expand, the clean energy movement faces a difficult problem: while such facilities can generate more power than is needed in the middle of the day when the sun is shining, they can't power the electrical grid in the evening or overnight. Storing grid-scale power in batteries would be extremely expensive. But what if solar energy could be stored cheaply as heat, and the heat converted to electricity when needed? That potential was among the reasons why the U.S. Department of Energy's Office of Science funded an Energy Frontier Research Center (EFRC), the Solid-State Solar-Thermal Energy Conversion Center.

The Center focused its research on improving novel thermo-photovoltaic cells that can convert heat radiation into electricity—much as a conventional solar cell converts solar radiation into electricity. Thermo-photovoltaic cells are similar to thin-film photovoltaic cells used to power satellites and drones, and in principle their efficiency can be higher than that of conventional power generation equipment such as coal- or gas-fired power plants. The researchers also developed a prototype device that could absorb and store the sun’s heat and re-emit it as photons in a narrow band of wavelengths appropriate for thermo-photovoltaic cells—in effect, a thermo-photovoltaic converter that turns heat into electricity. That required precisely etching the surface of materials such as tungsten, working at extremely high temperatures. The resulting prototype converter attracted a lot of attention. Additional research focused on mating it with thermo-photovoltaic cells.

David Bierman was one of the graduate students working on the EFRC project at the Massachusetts Institute of Technology. He was inspired by the research, but he also wanted to do something more hands-on that could help mitigate climate change—such as develop a practical energy storage system. So he linked up with other like-minded young engineers, founded a company now called Antora Energy, and gained the support of Cyclotron Road, an incubator for technology-based enterprises. The company is now working with DOE’s National Renewable Energy Laboratory (NREL) to commercialize a low-cost thermal energy storage system for grid-scale solar power.

In the years since the EFRC Center work began, however, the cost of solar cells has declined precipitously and their efficiency has improved. So capturing the sun’s energy as heat turned out not to be as important as anticipated. The Antora team believes that it’s more practical to just convert excess electricity from the grid into heat, then turn it back into electric power at night or as needed. In the storage system the company envisions, that excess electric power would be directed through blocks of carbon, heating them up to extremely high temperatures. Effective insulation traps the heat until it’s needed. Then the radiation from the hot carbon blocks is directed to advanced thermo-photovoltaic cells that generate power for the grid. Antora’s prototype systems are already as efficient as most conventional power generation processes (such as gas turbines), and the company believes it can reach 50 percent



Top: The Tarraleah Power Station is a pumped-storage hydroelectric power station in Tasmania, Australia. Pumped-hydro is one of the few current grid-scale means of storing electric power. (Ikonya / Shutterstock)

Bottom: Solar-powered charging station for electric cars that also shades the cars from the sun’s heat. (Jenson / Shutterstock)

efficiency. Such an energy storage system could, in principle, operate at far lower costs—perhaps 30 times lower—than storing electrical power in conventional batteries.

As renewable energy production—such as that from solar panels and wind turbines—expands, finding an effective grid-scale energy storage system becomes increasingly critical. Pumped-hydro storage—in which water is pumped uphill during the day and then flowed downhill through turbines to generate power at night—can’t be built everywhere that solar power will be deployed. The storage system Antora hopes to create could be. And even though that system will differ from what the EFRC effort envisioned, Bierman credits the Center for the inspiration that led him to form the company.

Solid-State Solar-Thermal Energy Conversion Center (S³TEC)
Winner — Technologies and Tools Award
www.science.osti.gov/bes/efrc/Centers/S3TEC



Algae being decomposed in a bioreactor in preparation for transformation into a biofuel. The decomposition leads to many different types of molecules, which a new analytical tool can help quantify. (Chokniti Khongchum / Shutterstock)

TRANSFORMING CHEMICAL ANALYSIS FOR SCIENCE AND FOR INDUSTRY

Biofuels and industrial chemicals made from renewable resources could help reduce use of the fossil fuels that contribute to climate change. That's one reason why the U.S. Department of Energy's Office of Science funded the Catalysis Center for Energy Innovation, an Energy Frontier Research Center (EFRC). The Center's research focused on new ways to process biofuels and to catalyze chemical reactions that could more efficiently make bio-oils or other products from crops such as corn, sugar cane, or algae.

Sometimes, though, fundamental research generates unexpected and important ideas that lead to valuable technologies, and that's what happened to one of the Center's principal investigators, Paul Dauenhauer of the University of Minnesota. He and his team were studying the products of biofuel processing reactions so they could fine-tune the process to produce more of the desired biofuel products. To do that, however, the

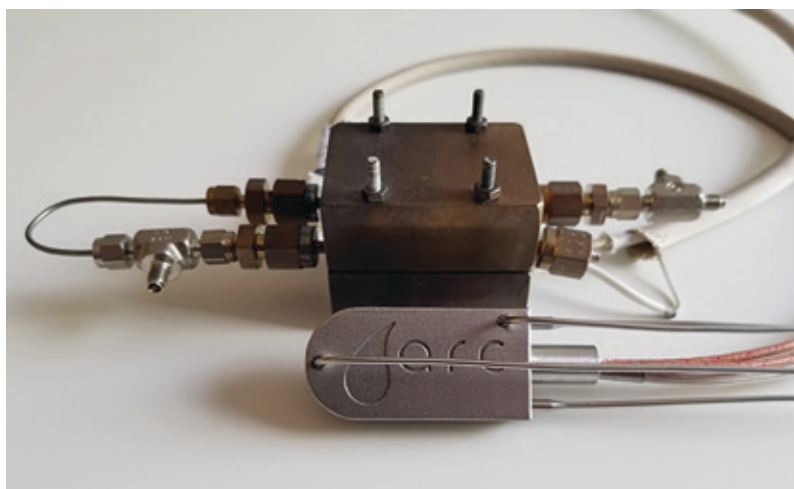
scientists had to repeatedly analyze mixtures of thousands of different molecules to sort out how much of each molecule was present in the reaction products. With then-available techniques, it was a tedious process, to say the least.

One day Dauenhauer and his team were discussing this challenge over coffee, and it occurred to them that if they could first separate the reaction products by type of molecule and then measure the amount of each type separately in some standardized way, then their work would flow much more easily. So they built a micro-reactor that could first separate the molecules, guiding each type down a separate tiny channel. (Ultimately, 3-D printing was used to construct the micro-channels precisely.) Then each stream of molecules was converted to a standardized form that could be automatically analyzed to measure the amount of carbon present. The result was a reliable, quantitative way to compare the relative amounts of all of the molecular types present in a mixture. The device and the overall analytical process required some fine-tuning, but it worked well.

Realizing that every analytical chemistry lab in the world—in universities and in industry—often faced similar problems, the team launched a startup company, Activated Research, to refine and commercialize the device. The resulting Polyarc micro-reactor is a lab-on-a-chip, about the size of a human thumb (see image). A mixture to be analyzed is fed to a mass spectrometer or a gas chromatograph (standard analytical tools that identify each molecular type present by comparing its signature to a library standard) and simultaneously to the micro-reactor. In the micro-reactor, each separate stream of molecules is first combusted to carbon dioxide, then converted to methane, then measured for the amount of carbon present—all in a few seconds. Comparison of the two data streams gives the amount of each unique molecular type present in a mixture.

The award-winning micro-reactor removes a huge burden for any laboratory responsible for analyzing fuels or industrial chemicals, testing ingredients in foods for purity, or even checking standard chemical mixtures received from suppliers. In effect, it automates a critical part of analytical chemistry, making research and testing more productive and improving the accuracy of routine tests required by health and safety regulations.

More recently, the micro-reactor has been integrated with another standard device, a liquid chromatograph, which can separate and identify the components of liquid



Top: Analytical chemistry labs test fuels, industrial chemicals, and ingredients in food or pharmaceuticals to ensure quality, or help to decipher the constituents of an unknown substance. This analysis requires testing multiple samples—such as those shown here—in an automated and standardized manner. (Cergios / Shutterstock)

Bottom: The Polyarc micro-reactor—shown here in its current form (foreground) along with an earlier prototype (background)—gives laboratories a novel tool to complement mass spectrometers, gas and liquid chromatographs, and other analytical devices because it can quickly determine the amount of each type of molecule present in a mixture. (Activated Research Company)

mixtures while the micro-reactor measures the amount of each component present. This combination provides a powerful new toolset for molecular biology and the pharmaceutical industry.

None of this was contemplated in the EFRC proposal. But this technology development illustrates the potential of collaborative thinking over coffee—very much what the EFRC program intends to foster.

Catalysis Center for Energy Innovation (CCEI)
Winner — Technologies and Tools Award
www.science.osti.gov/bes/efrc/Centers/CCEI

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