

# ENERGY FRONTIER RESEARCH CENTERS

SCIENCE FOR OUR NATION'S ENERGY FUTURE



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

September 2016

# 36 CURRENT EFRCs

## CALIFORNIA

Light-Material Interactions in Energy Conversion (LMI)  
*California Institute of Technology*

Center for Nanoscale Controls on Geologic CO<sub>2</sub> (NCGC)  
*Lawrence Berkeley National Laboratory*

Center for Gas Separations Relevant to Clean Energy Technologies (CGS)  
*University of California, Berkeley*

Spins and Heat in Nanoscale Electronic Systems (SHINES)  
*University of California, Riverside*

## COLORADO

Center for Next Generation of Materials by Design: Incorporating Metastability (CNGMD)  
*National Renewable Energy Laboratory*

## DELAWARE

Catalysis Center for Energy Innovation (CCEI)  
*University of Delaware*

## DISTRICT OF COLUMBIA

Energy Frontier Research in Extreme Environments (EFree)  
*Carnegie Institution of Washington*

## FLORIDA

Center for Actinide Science & Technology (CAST)  
*Florida State University*

## GEORGIA

Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy (UNCAGE-ME)  
*Georgia Institute of Technology*

## ILLINOIS

Center for Electrochemical Energy Science (CEES)  
*Argonne National Laboratory*

Center for Bio-Inspired Energy Science (CBES)  
*Northwestern University*

Argonne-Northwestern Solar Energy Research Center (ANSER)  
*Northwestern University*

Center for Geologic Storage of CO<sub>2</sub> (GSCO2)  
*University of Illinois at Urbana-Champaign*

## INDIANA

Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio)  
*Purdue University*

Materials Science of Actinides (MSA)  
*University of Notre Dame*

## MARYLAND

Nanostructures for Electrical Energy Storage (NEES)  
*University of Maryland*

## MASSACHUSETTS

Integrated Mesoscale Architectures for Sustainable Catalysis (IMASC)  
*Harvard University*

Center for Excitonics (CE)  
*Massachusetts Institute of Technology*

Solid-State Solar-Thermal Energy Conversion Center (S<sup>3</sup>TEC)  
*Massachusetts Institute of Technology*

## MINNESOTA

Inorganometallic Catalyst Design Center (ICDC)  
*University of Minnesota*

## MISSOURI

Photosynthetic Antenna Research Center (PARC)  
*Washington University in St. Louis*

## MONTANA

Center for Biological Electron Transfer and Catalysis (BETCy)  
*Montana State University*

## NEW MEXICO

Center for Advanced Solar Photophysics (CASP)  
*Los Alamos National Laboratory*

## NEW YORK

NorthEast Center for Chemical Energy Storage (NECCES)  
*Binghamton University*

Center for Emergent Superconductivity (CES)  
*Brookhaven National Laboratory*

Center for Mesoscale Transport Properties (m2M)  
*Stony Brook University*

## NORTH CAROLINA

Center for Solar Fuels (UNC)  
*University of North Carolina*

## OHIO

Center for Performance and Design of Nuclear Waste Forms and Containers (WastePD)  
*The Ohio State University*

## PENNSYLVANIA

Center for Lignocellulose Structure and Formation (CLSF)  
*Pennsylvania State University*

Center for the Computational Design of Functional Layered Materials (CCDM)  
*Temple University*

## SOUTH CAROLINA

Center for Hierarchical Waste Form Materials (CHWM)  
*University of South Carolina*

## TENNESSEE

Fluid Interface Reactions, Structures and Transport Center (FIRST)  
*Oak Ridge National Laboratory*

Energy Dissipation to Defect Evolution (EDDE)  
*Oak Ridge National Laboratory*

## TEXAS

Center for Frontiers of Subsurface Energy Security (CFSES)  
*University of Texas at Austin*

## WASHINGTON

Center for Molecular Electrocatalysis (CME)  
*Pacific Northwest National Laboratory*

Interfacial Dynamics in Radioactive Environments and Materials (IDREAM)  
*Pacific Northwest National Laboratory*

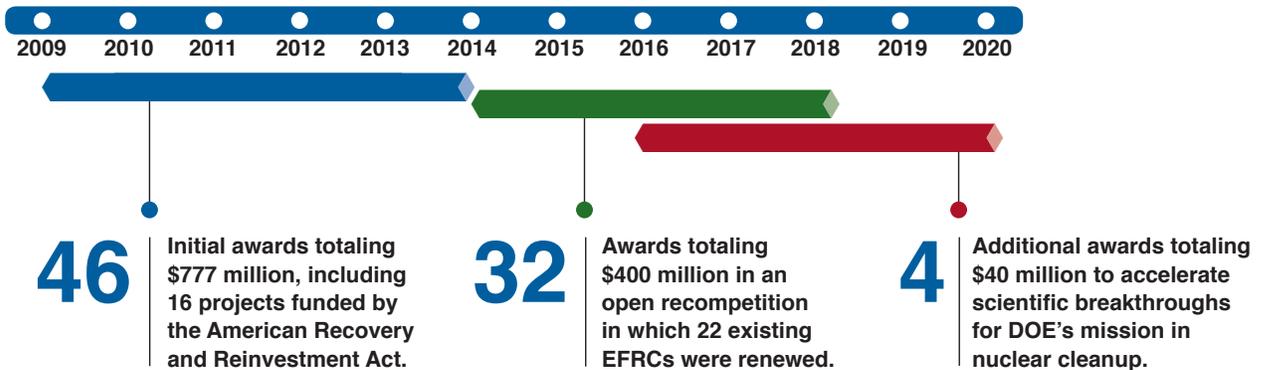
**For more information:**  
[science.energy.gov/bes/efrc](http://science.energy.gov/bes/efrc)

# ENERGY FRONTIER RESEARCH CENTERS SCIENCE FOR OUR NATION'S ENERGY FUTURE

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 Center (EFRC) program in 2009. The EFRCs represent a unique approach, bringing together creative, multidisciplinary scientific teams to perform energy-relevant basic research with a complexity beyond the scope of single-investigator projects. These centers take full advantage of powerful new tools for characterizing, understanding, modeling, and manipulating matter from atomic to macroscopic length scales. They also train the next-generation scientific workforce by attracting talented students and postdoctoral researchers interested in energy science.

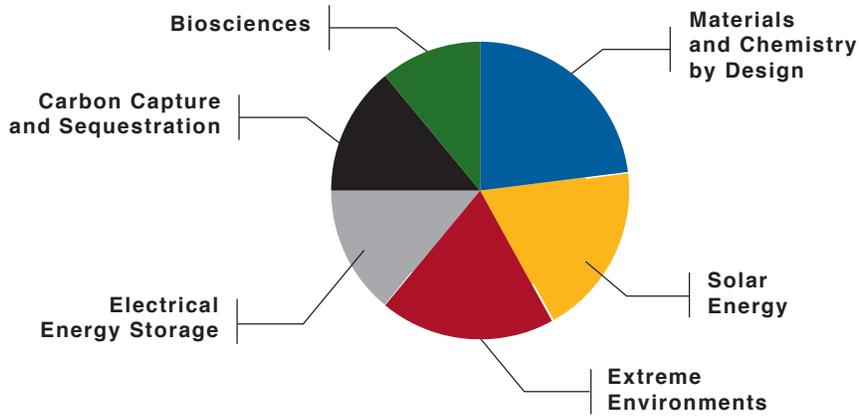
The EFRCs have collectively demonstrated the potential to substantially advance the scientific understanding underpinning transformational energy technologies. Both a BES Committee of Visitors and a Secretary of Energy Advisory Board Task Force have found the EFRC program to be highly successful in meeting its goals. The scientific output from the EFRCs is impressive, and many centers have reported that their results are already impacting both technology research and industry. This report on the EFRC program includes selected highlights from the initial 46 EFRCs and the current 36 EFRCs.

## EFRC AWARDS HISTORY



The EFRCs are large team efforts as shown here from the all hands meeting for the Center for Understanding and Control of Acid Gas Induced Evolution of Materials for Energy. Each EFRC holds an annual meeting with its team of researchers and advisory board members to review and plan research activities. Combined, the current EFRCs have more than 220 scientific advisory board members from 12 countries and 41 companies.

# EFRC TOPICAL AREAS



**DISTRIBUTION OF CURRENT EFRCs**

EFRC awards span the full range of energy research challenges, as depicted in the chart above. The scientific community identified these and other challenges in a series of BES workshop reports that describe basic research for advancing technologies to support Department of Energy missions in energy, environment, and national security. Workshop topics included solar energy utilization, clean and efficient combustion, electrical energy storage, carbon capture and sequestration, advanced nuclear systems, catalysis, materials in extreme environments, hydrogen science, solid state lighting, superconductivity, and environmental management. The EFRCs also address scientific grand challenges described in the reports *Directing Matter and Energy: Five Challenges for Science and the Imagination* and *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science*. In all, 20 community workshops have been held since the early 2000s, with over 2,000 participants identifying “basic research needs” for energy applications and “grand-challenge science.” These workshops form the foundation for the EFRC program.

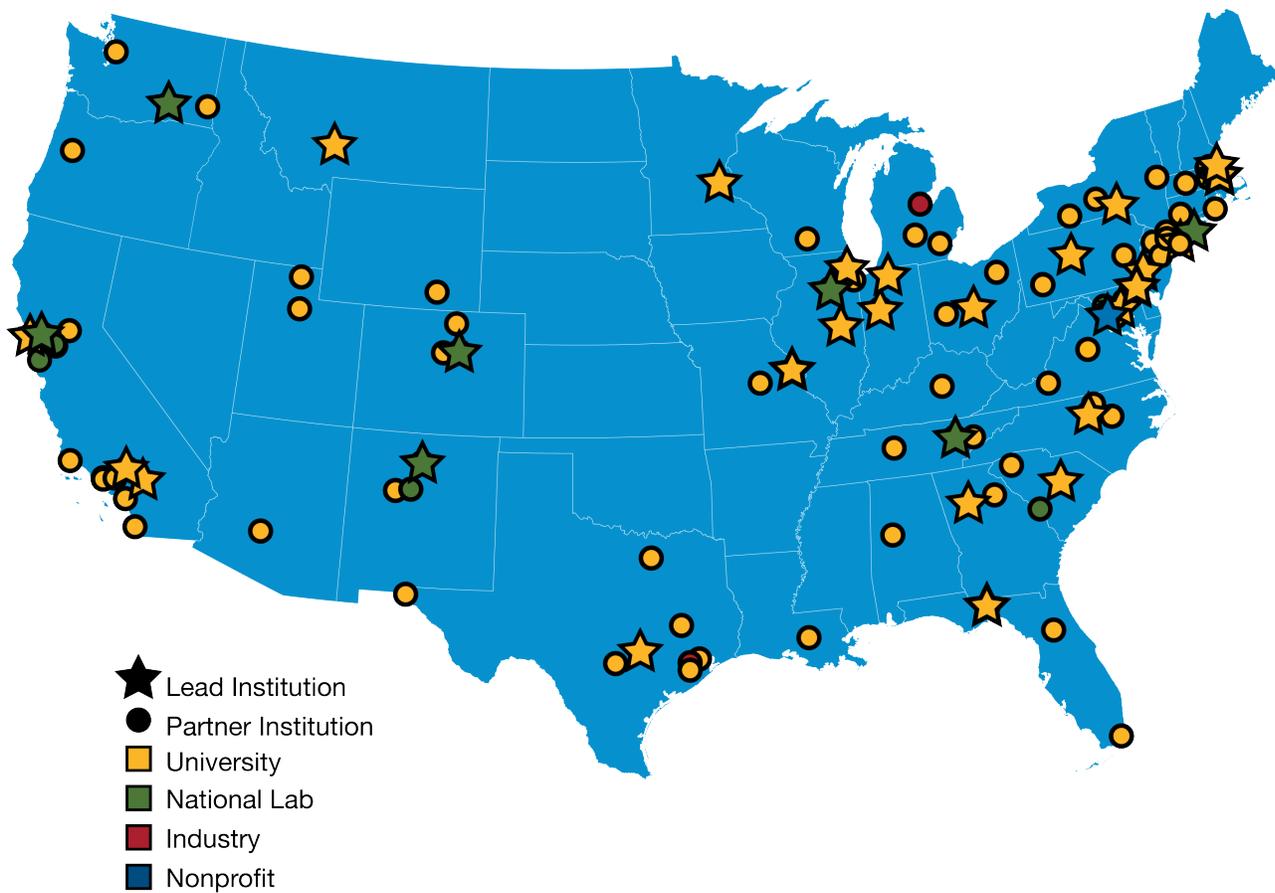
## WORKSHOP REPORTS



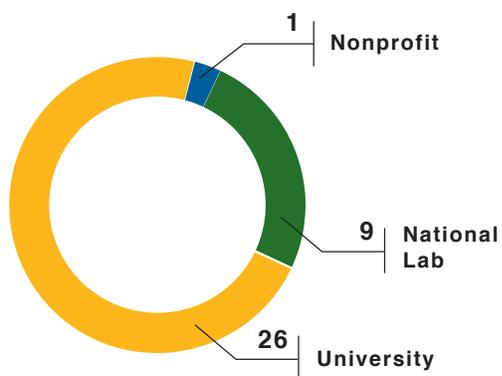
For more information: [science.energy.gov/bes/community-resources/reports/](https://science.energy.gov/bes/community-resources/reports/)

# CURRENT EFRCs

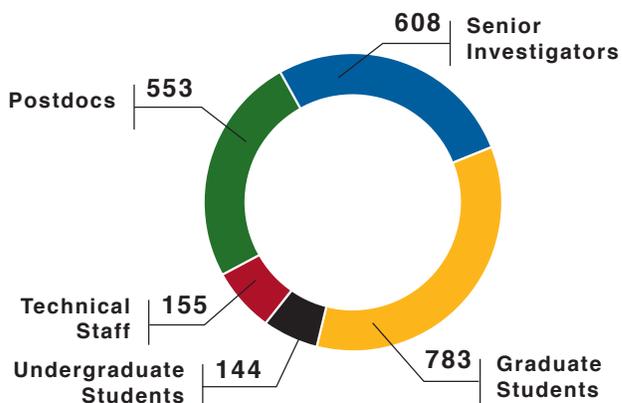
The EFRCs are integrated, multi investigator partnerships among universities, national laboratories, nonprofit organizations, and for profit firms to conduct fundamental research focusing on one or more “grand challenges” and use inspired “basic research needs” identified by the scientific community in a series of BES workshop reports. The 36 EFRCs involve over 110 unique institutions through 250 partnerships in 34 states, the District of Columbia, and 4 foreign countries.



## LEAD INSTITUTIONS

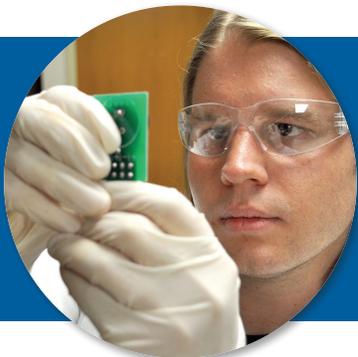
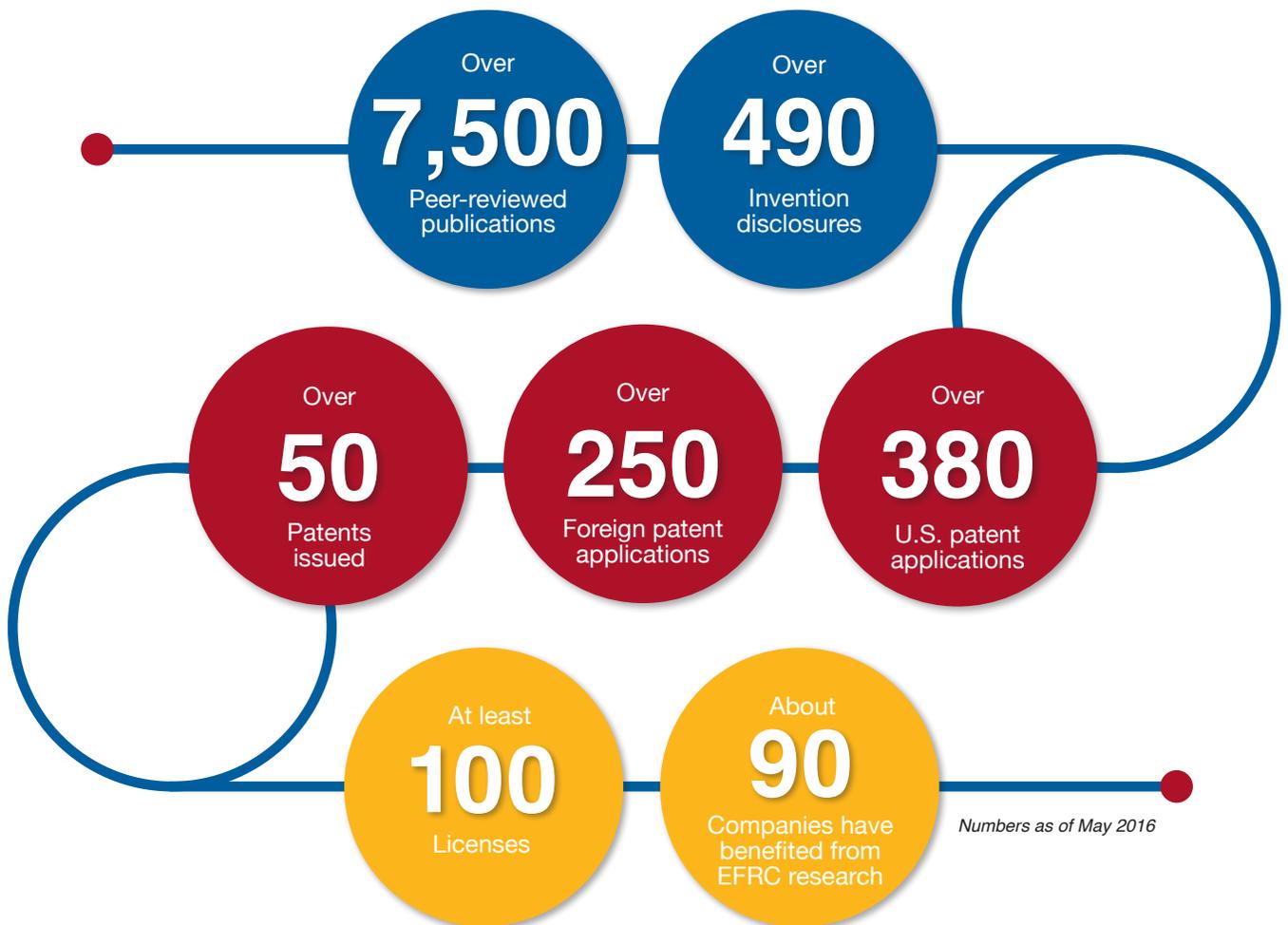


## EFRC MEMBERS



# EFRC IMPACT BY THE NUMBERS

The EFRCs focus on grand challenge and use inspired science. Consequently, dissemination of scientific results through peer reviewed publications is the primary measure of success. However, the EFRCs also impact energy technology research and industry through licensing of patented inventions, transfer of scientific results to technology development projects, and collaborations with industry.



“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 the Center for Electrochemical Energy Science (CEES) and is now the Chief Technology Officer at SiNode Systems, a company he co founded based on his EFRC research.



## TECHNOLOGY TRANSITION

Activated Research Company (ARC) is commercializing the Polyarc® reactor system, a technology developed by the Catalysis Center for Energy Innovation (CCEI). This detector can be added to existing gas chromatographs (GCs) to reduce operating costs and improve accuracy without the need for calibration standards. GCs are widely used in the petroleum, chemical, and other analytical industries. In June 2016, Wasson-ECE Instrumentation, a leading provider of GCs, partnered with ARC to distribute the Polyarc® reactor system worldwide and incorporate the technology into its products.

## COMPANY SPIN-OFF

EFRC research is being commercialized by new companies, one of which is Spero Energy, a 2014 start-up that has licensed a technology developed by the Center for Direct Catalytic Conversion of Biomass to Biofuels (C3Bio). C3Bio discovered a catalytic process that converts lignin in plant biomass and waste into high-value chemicals in one step. This process also leaves behind a cellulosic residue that could be readily converted to biofuels. Spero Energy is working on development and scale-up of a commercially viable process to produce renewable chemicals.



start-up that has licensed a technology developed by the Center for Direct Catalytic Conversion of Biomass to

## HIGHLY CITED PAPERS

- 1 **Atomically Thin MoS<sub>2</sub>: A New Direct-Gap Semiconductor**  
Mak, K.F., et al. 2010. *Physical Review Letters* **105**, 136805. DOI:10.1103/PhysRevLett.105.136805
- 2 **Carbon Dioxide Capture in Metal-Organic Frameworks**  
Sumida, K., et al. 2012. *Chemical Reviews* **112**, 724–81. DOI:10.1021/cr2003272
- 3 **Solution-Processed Small-Molecule Solar Cells with 6.7% Efficiency**  
Sun, Y.M., et al. 2012. *Nature Materials* **11**, 44–48. DOI:10.1038/nmat3160
- 4 **Ultrahigh-Power Micrometre-Sized Supercapacitors Based on Onion-Like Carbon**  
Pech, D., et al. 2010. *Nature Nanotechnology* **5**, 651–54. DOI:10.1038/nnano.2010.162
- 5 **Enhanced Absorption and Carrier Collection in Si Wire Arrays for Photovoltaic Applications**  
Kelzenberg, M.D., et al. 2010. *Nature Materials* **9**, 239–44. DOI:10.1038/nmat2635
- 6 **High-Performance Bulk Thermoelectrics with All-Scale Hierarchical Architectures**  
Biswas, K., et al. 2012. *Nature* **489**, 414–18. DOI:10.1038/nature11439
- 7 **Semiconducting Tin and Lead Iodide Perovskites with Organic Cations: Phase Transitions, High Mobilities, and Near-Infrared Photoluminescent Properties**  
Stoumpos, C.C., et al. 2013. *Inorganic Chemistry* **52**, 9019–38. DOI:10.1021/ic401215x
- 8 **A Universal Method to Produce Low-Work Function Electrodes for Organic Electronics**  
Zhou, Y.H., et al. 2012. *Science* **336**, 327–32. DOI:10.1126/science.1218829
- 9 **Peak External Photocurrent Quantum Efficiency Exceeding 100% via MEG in a Quantum Dot Solar Cell**  
Semonin, O.E., et al. 2011. *Science* **334**, 1530–533. DOI:10.1126/science.1209845
- 10 **Porous Hollow Carbon@Sulfur Composites for High-Power Lithium-Sulfur Batteries**  
Jayaprakash, N., et al. 2011. *Angewandte Chemie-International Edition* **50**, 5904–908. DOI:10.1002/anie.201100637

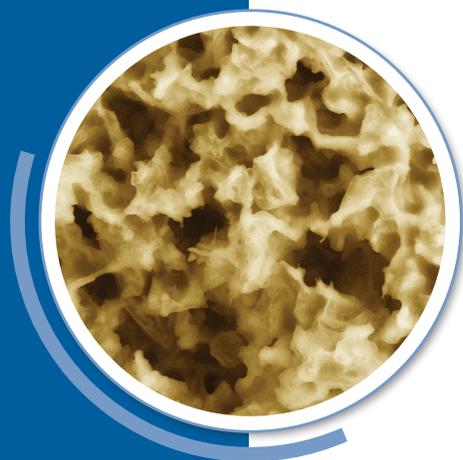
# SCIENCE HIGHLIGHTS



## Solar concentrators based on quantum dots

*Core-shell quantum dots were rationally designed for efficient light collection and transmission*

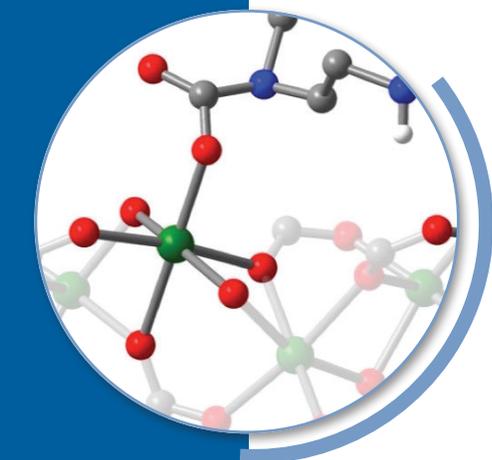
Luminescent solar concentrators are cost-effective complements to photovoltaic systems that can boost the power output of standalone solar cells by increasing the amount of light collected using architectural elements like semi-transparent windows. Researchers at the Center for Advanced Solar Photophysics developed a luminescent solar concentrator using rationally designed core-shell quantum dots to funnel light over tens of centimeters. The new concentrator's power output is 100 times more efficient than those that use standard core-only quantum dots.



## Magnetic resonance imaging of brains, knees, and now batteries

*MRI method can non-destructively image chemical and structural changes in a lithium-ion battery*

Scientists at the NorthEast Center for Chemical Energy Storage have developed non-destructive, quantitative MRI methods to image lithium (Li) metal microstructures in electrodes and electrolytes in Li-ion batteries. The technique can be used to understand and characterize the electrochemical conditions under which unwanted Li microstructures form as well as the effects of different electrolytes and additives. Designs, materials, and operating conditions can be explored to minimize, for example, dangerous Li dendrite formation, leading to safer, higher-capacity, and higher-power Li-ion batteries.



## Energy-efficient carbon capture by a material that mimics a plant enzyme

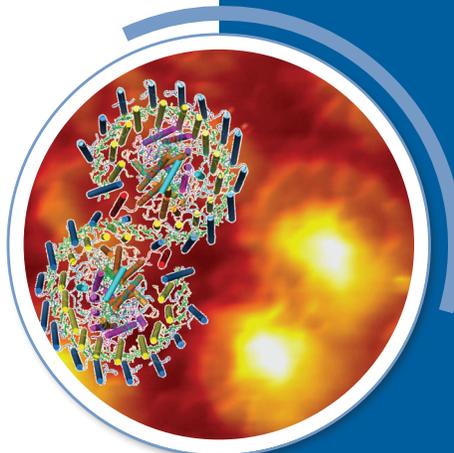
*Innovative material adsorbs carbon dioxide via a new cooperative insertion mechanism*

Researchers at the Center for Gas Separations Relevant to Clean Energy Technologies discovered a novel metal-organic framework (MOF) material that exhibits an unprecedented cooperative insertion mechanism for capturing and releasing carbon dioxide ( $\text{CO}_2$ ) with only small shifts in temperature. The MOF structure, with  $\text{CO}_2$  adsorbed, closely resembles the RuBisCO enzyme found in plants, which captures atmospheric  $\text{CO}_2$  for conversion into nutrients. Such adsorbent materials could significantly reduce the energy required for  $\text{CO}_2$  capture from power plants.

## 3D structure of a light-harvesting reaction center complex

*Insight into such complexes allows the design of better “bio-inspired” materials for light harvesting*

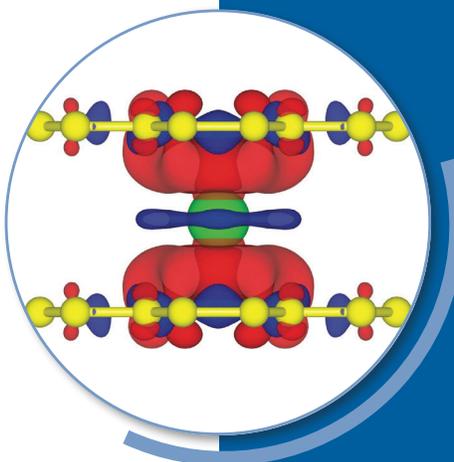
The photosynthetic apparatus used by green plants and some bacterial species can convert light energy into chemical energy at high efficiencies. Using a combination of several biophysical techniques, researchers at the Photosynthetic Antenna Research Center determined the three-dimensional structure of the reaction center light-harvesting complex of the purple photosynthetic bacterium *Rhodobacter sphaeroides*. Understanding the structure of such complexes can provide insights into how to design “bio-inspired” mimics with enhanced capabilities and functionalities.



## Accurately modeling materials for energy applications

*Optimal method identified for multiscale simulations of carbon nanostructures*

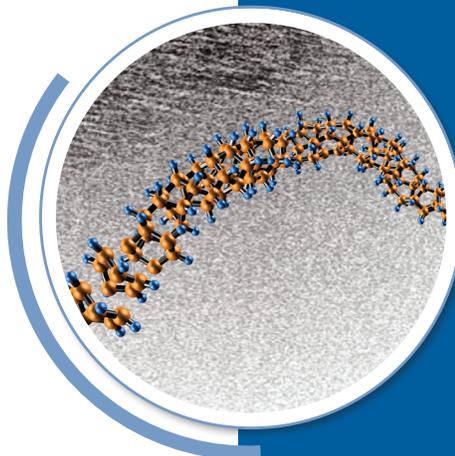
The energy associated with lithium diffusion and binding in the carbon layers of graphite, the most widely used lithium-ion battery anode, was predicted using highly accurate calculations that were not empirically adjusted to match experimental measurements. Researchers at the Fluid Interface Reactions, Structures and Transport Center correctly predicted the graphite primary layering structure, agreeing with experimental measurements. The modeling identified faster methods that can be used to design carbon nanostructures and other layered nanomaterials for energy applications.



## Synthesizing carbon nanothreads from compressed benzene

*One-dimensional material has a diamond-like building block*

A new carbon nanomaterial—the thinnest possible one-dimensional thread that still retains a diamond-like structure—was created by the controlled, slow compression and decompression of benzene at the Energy Frontier Research in Extreme Environments Center. Computational modeling suggests that these nanothreads could be stronger than carbon nanotubes. The synthesis method opens up possible variations, such as cross-linking or chemical functionalization. A family of diamondoid nanothread materials could be created from this versatile synthetic approach.

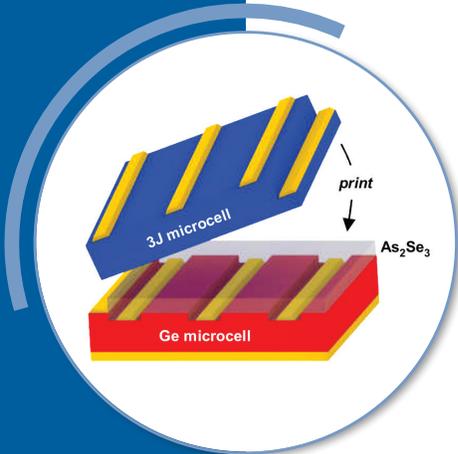


# SCIENCE HIGHLIGHTS

## Quadruple-junction solar cells for high-efficiency modules

*Improved power conversion holds promise for reducing the cost of utility-scale solar power*

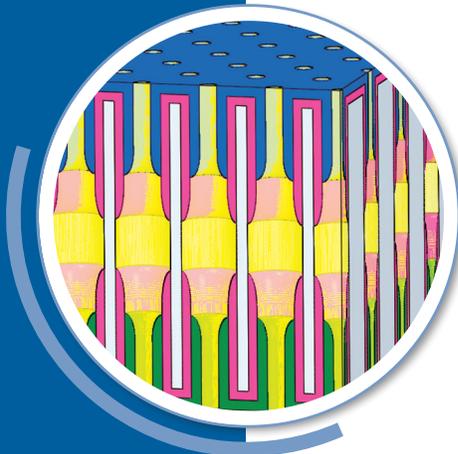
A new printing-based technique was developed at the Light-Material Interactions in Energy Conversion Center. The technique stacks microscale solar cells followed by sol-gel processing of interlayers with advanced optical, electrical, and thermal properties. The resulting mechanically assembled quadruple-junction, four-terminal solar cells had a measured power-conversion efficiency of 43.9%, nearly matching the record value for similar devices fabricated using more arduous processes.



## Building precision nanobatteries by the billions

*Batteries constructed in nanopores promise to deliver energy at much higher power and longer life*

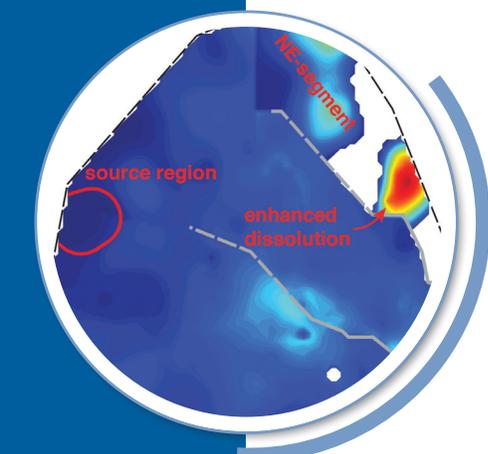
Tiny batteries formed inside nanopores demonstrate that properly scaled nanostructures can use the full theoretical capacity of the charge storage material. These nanobatteries delivered their stored energy efficiently at high power (fast charge and discharge) and for extended cycling. This research from the Nanostructures for Electrical Energy Storage Center shows that precise structures can be constructed to assess the fundamentals of ion and electron transport in nanostructures and to test the limits of three-dimensional nanobattery technologies.



## Viability of long-term carbon sequestration in the subsurface

*The Bravo Dome gas field was used to estimate  $CO_2$  dissolution rates over millennia*

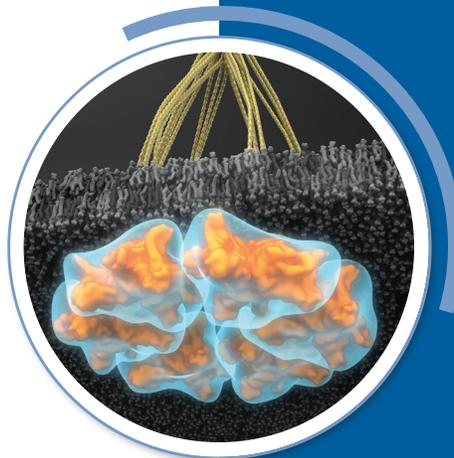
Understanding the viability of long-term subsurface storage of  $CO_2$  is critical for carbon capture and sequestration implementation. Researchers from the Center for Frontiers of Subsurface Energy Security used the Bravo Dome gas field in New Mexico as a natural laboratory to examine  $CO_2$  behavior in the subsurface. Their research showed that, averaged across the reservoir, only 20% of the  $CO_2$  had dissolved into the field's saline brine over 1.2 million years, while the rest remained as a free gas trapped by the cap-rock. This study documents the first field evidence for the safe long-term storage of very large amounts of  $CO_2$  in saline aquifers.



## Examining the enzyme complex that makes cellulose microfibrils

*Imaging and computational modeling revealed new structural insights*

Researchers at the Center for Lignocellulose Structure and Formation discovered that the cellulose synthase complex (CSC) that makes cellulose microfibrils consists of three types of cellulose synthases (CESAs) organized into trimers. Additional experiments and modeling indicate that these trimers form hexameric assemblies containing 18 CESAs, contrary to the long-held assumption that CSC contains 36 CESAs. These results are an important step in developing a detailed nano- to mesoscale understanding of plant cell wall formation.



## Perovskite-inspired search identified new photovoltaic materials

*Experiments confirmed new non-toxic solar materials predicted by theory*

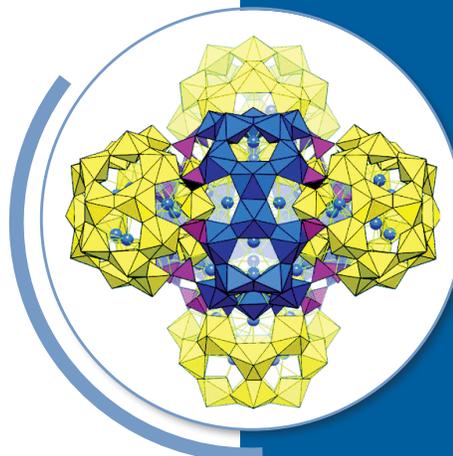
Lead-based perovskite photovoltaic solar cells have achieved efficiencies of more than 20% in only a few years, but lead is toxic. Researchers at the Center for Next Generation of Materials by Design identified defect tolerance and long carrier lifetime as the key properties of the lead-based materials. Using these criteria and theoretical calculations, they evaluated 27,000 compounds in the Materials Project database to identify nine additional classes of non-toxic materials likely to exhibit these properties. The team then experimentally showed that five new materials have the desired properties.



## Nanoscale control of uranium for solvent-free recovery

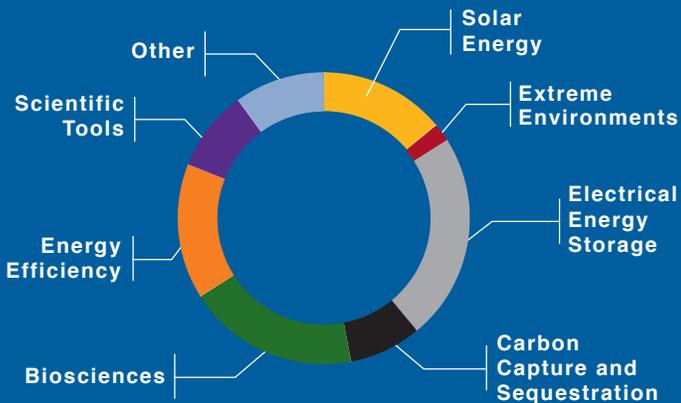
*Water-soluble uranium-oxygen clusters are large enough to be filtered using commercial membranes*

Processing of uranium, including spent fuel, uses organic solvents that become radioactive waste. A simple treatment of uranium-bearing water creates nanoscale uranium-oxygen clusters recoverable by ultrafiltration, without organic solvents, reducing the cost and environmental impact of processing. Researchers at the Materials Science of Actinides Center used ultrafiltration to recover more than 85% of the uranium in treated solutions without fouling the membrane surface.



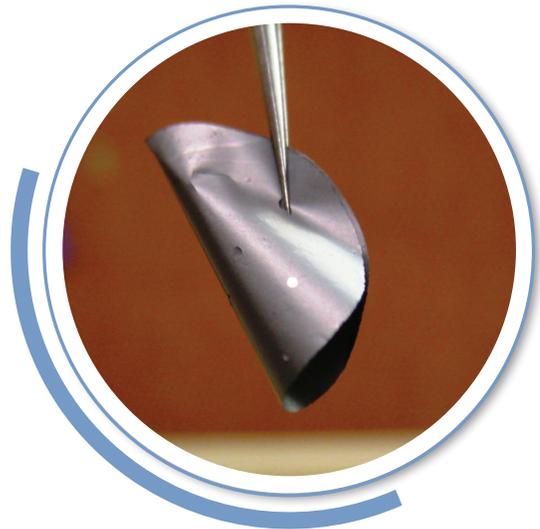
# SCIENCE COMMERCIALIZATION

The EFRCs provide an important bridge between basic research and energy technologies and complement other research activities funded by the U.S. Department of Energy. Some EFRC researchers are developing their basic research results into commercial products with funding from other federal and private sources. They are also forming new companies based on their EFRC research.



## DISTRIBUTION OF COMPANIES THAT HAVE BENEFITTED FROM EFRC RESEARCH

EFRC interactions with companies span a wide range of energy research, as depicted in the chart above. Companies are involved with the EFRCs through licensing of EFRC intellectual property, establishing cooperative research and development agreements, using EFRC ideas in their business, providing follow-on funding, or substantial interactions involving personnel or sample exchange. The companies range in size as well: approximately 33% are start-ups, 23% are mid-size companies, and 44% are large companies.



## Novel anode materials for lithium-ion batteries

### BASIC SCIENCE

The Center for Electrochemical Energy Science (CEES) used highly characterized model systems to establish a robust mechanistic-level understanding of the electrochemical reactions in lithium-ion energy storage systems with an emphasis on the reactivity of anode materials, mostly silicon/carbon materials and composites. This research included the creation of novel nanostructured materials and interfaces and the observation of lithiation reactions through advanced characterization tools and computation.

### APPLIED R&D

Researchers created highly flexible graphene composites (“graphene papers”) for use as lithium-ion anodes. The encapsulation of silicon nanoparticles by these graphene papers led to enhanced electrochemical properties, including improved cyclability and a capacity greater than 1000 mAh/g, far exceeding graphite’s capacity of 372 mAh/g.

### COMMERCIALIZATION

SiNode Systems, a start-up co-founded in 2012 by an EFRC graduate student, is based on intellectual property developed within CEES. The company has raised \$6.5 million in capital through a 2015 DOE Clean Energy Prize, DOE Small Business Innovation Research (SBIR) award (2013–2014), the U.S. Advanced Battery Consortium (2016), and venture capital. SiNode focuses on commercializing silicon/carbon materials for electric vehicle applications.



## Metal-organic frameworks for low-energy carbon capture

### BASIC SCIENCE

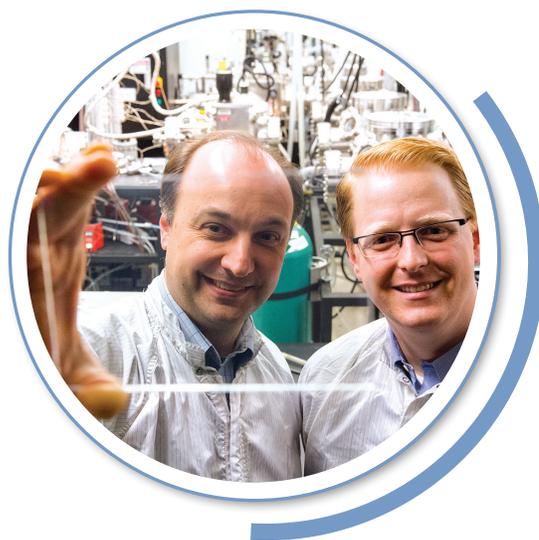
Researchers at the Center for Gas Separations Relevant to Clean Energy Technologies (CGS) discovered a new metal-organic framework material, with large working capacity, that can adsorb and desorb CO<sub>2</sub> with only moderate temperature swings. This function arises from an unprecedented cooperative CO<sub>2</sub> adsorption mechanism that enables energy-efficient carbon capture.

### APPLIED R&D

With funding from the Advanced Research Projects Agency-Energy (ARPA-E), CGS researchers used high-throughput screening to identify materials for the low-energy capture of CO<sub>2</sub> from the flue gas of a coal-fired power plant. A material was discovered that can adsorb more than 10% by weight of CO<sub>2</sub> at 25°C and release it with heating to just 80°C, lowering the energy penalty for carbon capture from 30% for existing technology to an estimated 15% or less.

### COMMERCIALIZATION

Mosaic Materials, a start-up founded in 2014, is focused on the low-cost scale-up synthesis and commercialization of these novel materials for CO<sub>2</sub> capture from coal-fired power plants. Initial funding through Cyclotron Road, an incubator at Lawrence Berkeley National Laboratory, is supporting the development of an inexpensive means of producing the metal-organic framework materials in a pelletized form on the ton scale.



## World's first transparent organic solar technology

### BASIC SCIENCE

The Center for Excitonics demonstrated the first transparent solar cell using near-infrared absorbing organic photovoltaics that are highly transparent to visible light. Researchers showed that a series-integrated array of these transparent cells can power electronic devices under near-ambient lighting. This architecture suggests strategies for high-efficiency power-generating windows.

### APPLIED R&D

Ubiquitous Energy was established in 2011 to improve the efficiency and transparency of these solar cells through follow-on funding from the National Science Foundation SBIR and Small Business Technology Transfer (STTR) programs.

### COMMERCIALIZATION

Ubiquitous Energy is producing highly transparent, efficient solar cells in its Silicon Valley pilot plant. They have raised over \$10 million to date and won numerous awards, including the 2015 Display Week Innovation Award. Their technology is a thin film that covers the display area of electronic products—including wearables, tablets, internet-of-things devices, and digital signage—generating electricity to power these devices.

# EFRC COMMUNICATIONS

## BES OVERSIGHT

Basic Energy Sciences provides effective oversight and management through frequent interactions with the EFRCs, including annual progress reports, monthly phone calls, site visits, directors' meetings, management reviews, and mid-term progress reviews. To facilitate communication of research advances and technology needs and ensure that research activities are not duplicated, the EFRC management team coordinates EFRC research within BES and with the DOE technology offices.



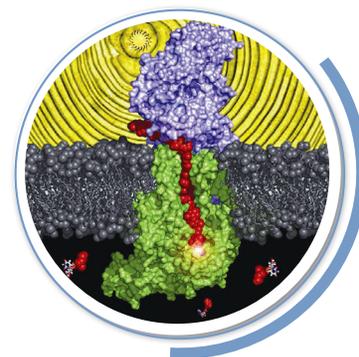
## EFRC MEETINGS

EFRC Principal Investigators' (PI) meetings are held biennially in Washington, D.C., to strengthen connections within the EFRC community. Starting in 2011, between 500 and 1,000 of America's top energy researchers and policymakers have attended each meeting (see Meetings at [www.energyfrontier.us](http://www.energyfrontier.us)). These events included plenary talks, scientific oral and poster presentations from all the EFRCs, and a student and postdoc competition. The meetings have also included a Women in Energy Science Breakfast, panel discussions, and other contests and networking events.



## FACILITATING OUTREACH

The EFRCs have established effective collaborations and communication strategies, particularly through the EFRC Community Website ([www.energyfrontier.us](http://www.energyfrontier.us)). EFRC early-career scientists started the Frontiers in Energy Research newsletter, which contains quarterly research highlights selected and written by early-career scientists invested in the public communication of science. The EFRC Early Career Network plans informal gatherings at national scientific meetings and "virtual events" on topics of broad interest to students and postdocs across the EFRCs.



"I feel so fortunate to have been part of the S<sup>3</sup>TEC community because it is rich in experience, knowledge, and people with different backgrounds. ... I may be in the Department of Mechanical Engineering, but I feel like what I really am is an engineer who works on energy problems." Maria Luckyanova was a graduate student in the Solid State Solar Thermal Energy Conversion Center (S<sup>3</sup>TEC). She served on the editorial board for the EFRC newsletter and won a graduate student award at the 2013 EFRC PI meeting.

# IMAGE CREDITS

## FRONT COVER



**Poly(ethylene) microspheres prepared by a solvent evaporation technique to demonstrate automatic shutdown of an unsafely operating lithium-ion battery.** Reprinted with permission from Baginska, M., et al. 2012. "Autonomic Shutdown of Lithium-Ion Batteries Using Thermoresponsive Microspheres," *Advanced Energy Materials* 2(5), 583–90. DOI:10.1002/aenm.201100683. Copyright 2012 John Wiley and Sons.

## PAGE 1



**All-hands meeting for the Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy.** Courtesy UNCAGE-ME.

## PAGE 4



**Cary Hayner.** Courtesy Bethany Hubbard.

## PAGE 5



**Polyarc® reactor system.** Courtesy Activated Research Company (ARC).

## PAGE 6



**Solar concentrators based on quantum dots.** Center for Advanced Solar Photophysics. Meinardi, F., et al. 2014. "Large-Area Luminescent Solar Concentrators Based on 'Stokes-Shift-Engineered' Nanocrystals in a Mass-Polymerized PMMA Matrix," *Nature Photonics* 8, 392–99. DOI:10.1038/nphoton.2014.54.



**Magnetic resonance imaging of brains, knees, and now batteries.** NorthEast Center for Chemical Energy Storage. Chandrashekar, S., et al. 2012. "Li MRI of Li Batteries Reveals Location of Microstructural Lithium," *Nature Materials* 11, 311–15. DOI:10.1038/nmat3246.



**Energy-efficient carbon capture by a material that mimics a plant enzyme.** Center for Gas Separations Relevant to Clean Energy Technologies. McDonald, T. M., et al. 2015. "Cooperative Insertion of CO<sub>2</sub> in Diamine-Appended Metal-Organic Frameworks," *Nature* 519, 303–08. DOI:10.1038/nature14327.

## PAGE 7



**3D structure of a light-harvesting reaction center complex.** Photosynthetic Antenna Research Center. Reprinted with permission from Qian, P., et al. 2013. "Three-Dimensional Structure of the *Rhodospirillum rubrum* RC-LH1-PufX Complex: Dimerization and Quinone Channels Promoted by PufX," *Biochemistry* 52(43), 7575–85. DOI:10.1021/bi4011946. Copyright 2013 American Chemical Society.



**Accurately modeling materials for energy applications.** Fluid Interface Reactions, Structures and Transport Center. Reprinted with permission from Ganesh, P., et al. 2014. "Binding and Diffusion of Lithium in Graphite: Quantum Monte Carlo Benchmarks and Validation of van der Waals Density Functional Methods," *Journal of Chemical Theory and Computation* 10(12), 5318–23. DOI:10.1021/ct500617z. Copyright 2014 American Chemical Society.



**Synthesizing carbon nanofibers from compressed benzene.** Energy Frontier Research in Extreme Environments, courtesy Enshi Xu, Vincent Crespi Laboratory, Pennsylvania State University. Fitzgibbons, T. C., et al. 2014. "Benzene-Derived Carbon Nanofibers," *Nature Materials*, 14, 43–47. DOI:10.1038/nmat4088.

## PAGE 8



**Quadruple-junction solar cells for high-efficiency modules.** Light-Material Interactions in Energy Conversion. Sheng, X., et al. 2014. "Printing-Based Assembly of Quadruple-Junction Four-Terminal Microscale Solar Cells for the Realization of High-Efficiency Modules," *Nature Materials*, 13, 593–98. DOI:10.1038/nmat3946.



**Building precision nanobatteries by the billions.** Nanostructures for Electrical Energy Storage. Liu, C., et al. 2014. "An All-in-One Nanopore Battery Array," *Nature Nanotechnology* 9, 1031–39. DOI:10.1038/nnano.2014.247.



**Viability of long-term carbon sequestration in the subsurface.** Center for Frontiers of Subsurface Energy Security. Sathaye, K. J., et al. 2014. "Constraints on the Magnitude and Rate of CO<sub>2</sub> Dissolution at Bravo Dome Natural Gas Field," *Proceedings of the National Academy of Sciences* 111(43), 15332–37. DOI:10.1073/pnas.1406076111.

## PAGE 9



**Examining the enzyme complex that makes cellulose microfibrils.** Center for Lignocellulose Structure and Formation. Nixon, B. T., et al. 2016. "Comparative Structural and Computational Analysis Supports Eighteen Cellulose Synthases in the Plant Cellulose Synthesis Complex," *Scientific Reports* 6, 28696. DOI:10.1038/srep28696.



**Perovskite-inspired search identified new photovoltaic materials.** Center for Next Generation of Materials by Design. Hoye, R. L. Z., et al. 2016. "Methylammonium Bismuth Iodide as a Lead-Free, Stable Hybrid Organic-Inorganic Solar Absorber," *Chemistry—A European Journal* 22(8), 2605–10. DOI:10.1002/chem.201505055.



**Nanoscale control of uranium for solvent-free recovery.** Materials Science of Actinides. Reproduced with permission from The Royal Society of Chemistry from Qiu, J., et al. 2014. "Water-Soluble Multi-Cage Super Tetrahedral Uranyl Peroxide Phosphate Clusters," *Chemical Science* 5(1), 303–10. DOI:10.1039/C3SC52357H.

## PAGE 10



**Novel anode materials for lithium-ion batteries.** Center for Electrochemical Energy Science. Zhao, X., et al. 2011. "In-Plane Vacancy-Enabled High-Power Si-Graphene Composite Electrode for Lithium-Ion Batteries," *Advanced Energy Materials*, 1(6), 1079–84. DOI:10.1002/aenm.201100426.

## PAGE 11



**Metal-organic frameworks for low-energy carbon capture.** Center for Gas Separations Relevant to Clean Energy Technologies, courtesy Thomas McDonald.



**World's first transparent organic solar technology.** Center for Excitronics. Justin Knight, courtesy Massachusetts Institute of Technology Energy Initiative.

## PAGE 12



**BES EFRC management team.** Courtesy Natalia Melcer.



**2013 EFRC PI Meeting.** Courtesy Pacific Northwest National Laboratory.



**First place in the Poetry of Science Contest at the 2015 EFRC PI Meeting.** Read the poem at [www.energyfrontier.us/content/afterlife-photon](http://www.energyfrontier.us/content/afterlife-photon). Courtesy Jochen Zimmer, Sarah Kiemle, and Daniel Cosgrove.



**Maria Luckyanova.** Courtesy Maria Luckyanova.

**DISCLAIMER:** This report was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government.

**Contact**

Basic Energy Sciences  
U.S. Department of Energy  
SC-22/Germantown Building  
1000 Independence Ave., SW  
Washington, D.C. 20585  
[sc.bes@science.doe.gov](mailto:sc.bes@science.doe.gov)  
Phone: 301.903.3081  
Fax: 301.903.6594  
[science.energy.gov/bes/efrc](http://science.energy.gov/bes/efrc)