



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Basic Energy Sciences: *Past, Present, and Future*

Materials Research Society
2015 Spring Meeting

Harriet Kung
Associate Director of Science
For Basic Energy Sciences



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7 April 2015



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Basic Energy Sciences

The Program:

Materials sciences & engineering—exploring macroscopic and microscopic material behaviors and their connections to various energy technologies

Chemical sciences, geosciences, and energy biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

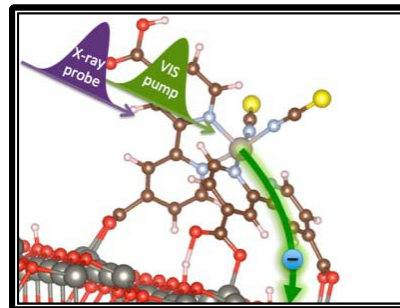
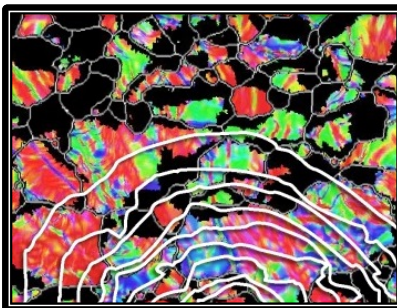
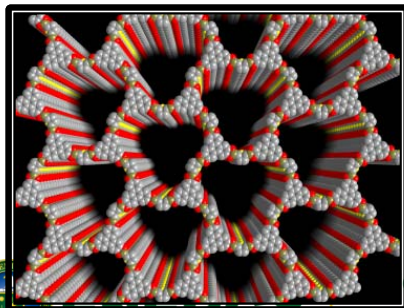
Supporting:

- 32 Energy Frontier Research Centers
- Fuels from Sunlight & Batteries and Energy Storage Hubs
- The largest collection of facilities for electron, x-ray, and neutron scattering in the world

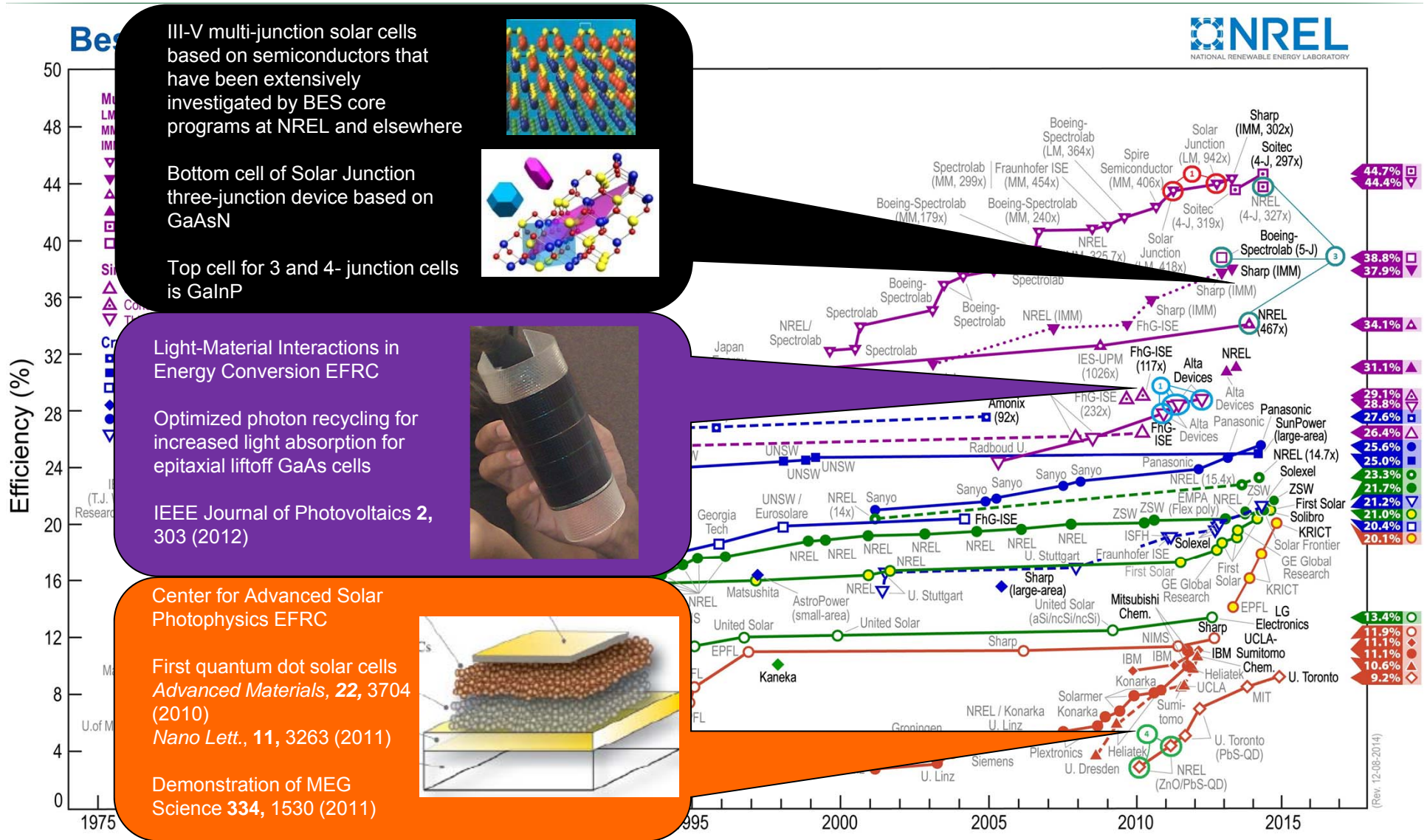
The Scientific Challenges:

- Synthesize, atom by atom, new forms of matter with tailored properties, including nano-scale objects with capabilities rivaling those of living things
- Direct and control matter and energy flow in materials and chemical assemblies over multiple length and time scales
- Explore materials & chemical functionalities and their connections to atomic, molecular, and electronic structures
- Explore basic research to achieve transformational discoveries for energy technologies

Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels



Recent BES Impacts on PV Technologies

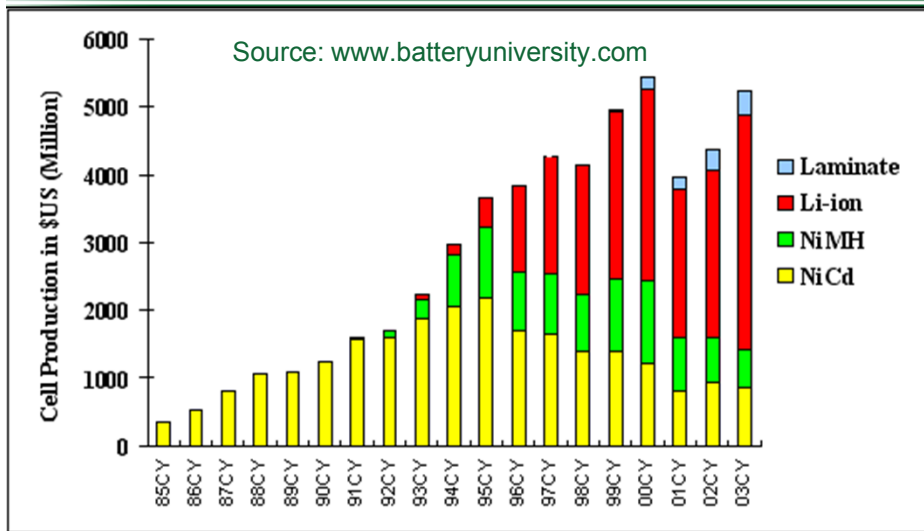


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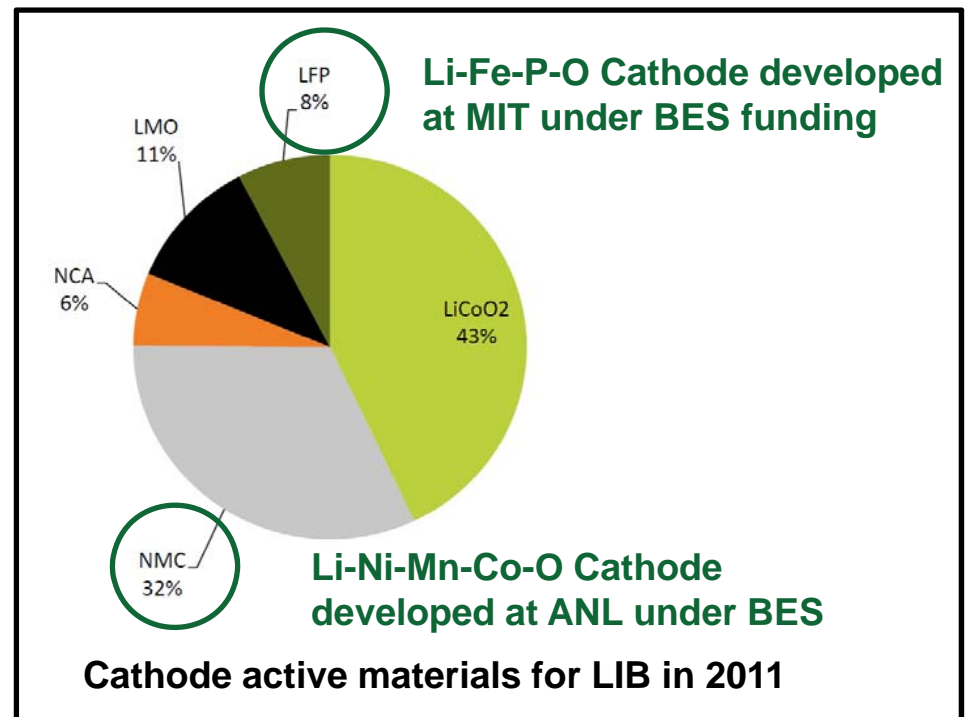
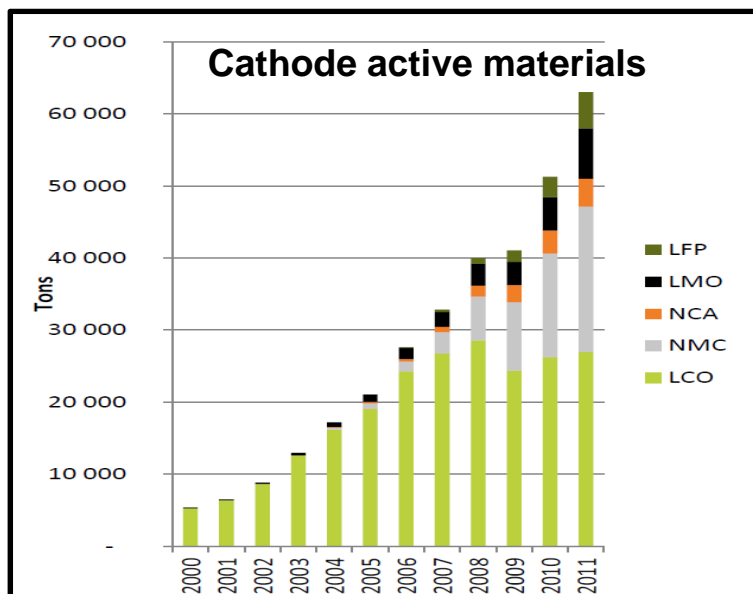
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Plot courtesy of the National Renewable Energy Laboratory, Golden, CO

Trends in Lithium-Ion Batteries: Increased Energy Density, Decreased Cost



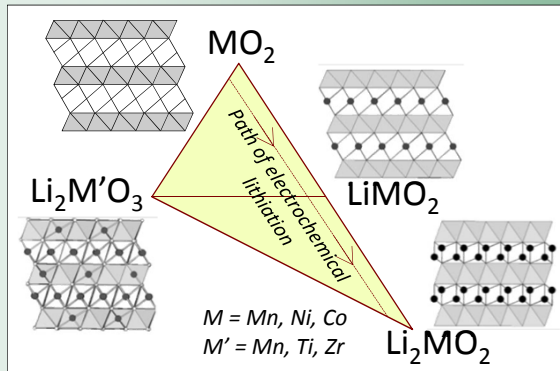
- Significant growth in the production of Li-ion batteries starting in the mid-90s (red); trends have continued. In that same timeframe, energy density increased by a factor of ~2.5 and cost decreased by a factor of 10.



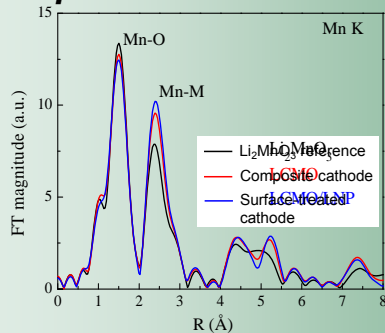
High-Energy Lithium Batteries: From Fundamental Research to Cars on the Road

BES Basic Science

Discovered new nanostructured composite cathode materials and interfaces



Used the Advanced Photon Source to characterize and understand composite cathode structures

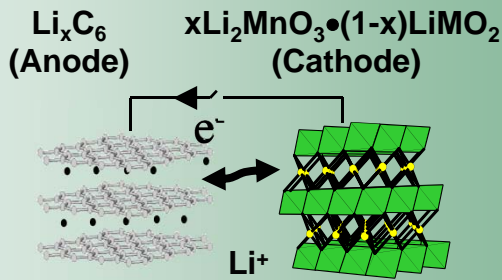


Fourier-transformed X-ray absorption data of a composite cathode structure



EERE Applied R&D

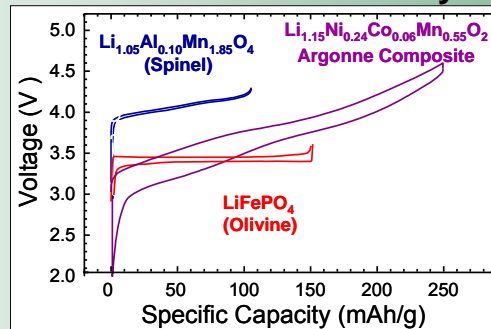
Used advanced composite cathode materials to create high energy lithium ion cells with improved performance



High energy Li-ion cells...



...with increased cathode capacity, enhanced stability



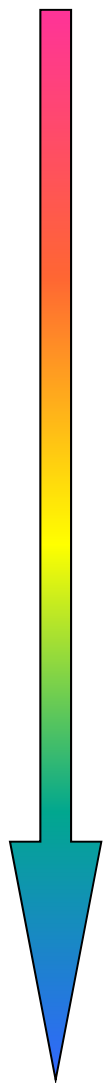
Manufacturing/ Commercialization

Patents for new cathodes from the basic and applied research are licensed to materials and cell manufacturers and automobile companies



BES Research Activities

Increasing scope and size



- **Core Research (>1,300 projects)**
Single investigators (\$150K/year) and small groups (\$500K-\$2M/year) engage in fundamental research related to any of the BES core research activities. Investigators propose topics of their choosing.
- **Energy Frontier Research Centers (32)**
\$2-4 million/year research centers for 4 year award terms; focus on fundamental research described in the Basic Research Needs Workshop reports.
- **Energy Innovation Hubs (2)**
Research centers, established in 2010 (\$15-25 million/year), engage in basic and applied research, including technology development, on a high-priority topic in energy that is specified in detail in an FOA. Project goals, milestones, and management structure are a significant part of the proposed Hub plan.



Energy Storage within Individual Nanopores

Scientific Achievement

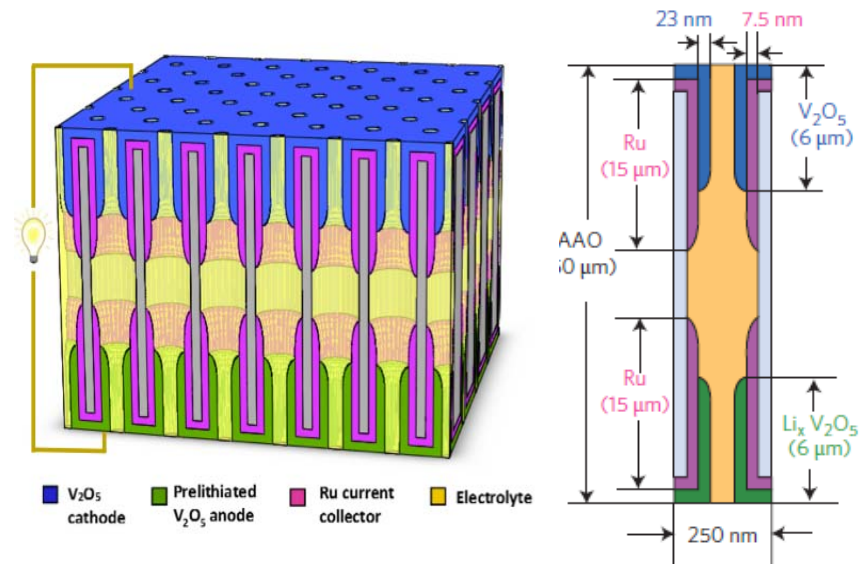
Fully functioning nanobatteries that can quickly charge and discharge over many cycles have been produced in arrays of nanopores.

Significance and Impact

Results demonstrate that precise nanostructures can be constructed to test the limits of 3-D nanobatteries and study the fundamentals of ion and electron transport in confined nanostructures.

Research Details

- Up to a billion nanopore batteries could fit in a grain of sand
- The nanobatteries were fabricated by atomic layer deposition to make oxide nanotubes (for ion storage) inside metal nanotubes for electron transport, all inside each end of the nanopores.
- Tiny nanobatteries can transfer half their energy in just a 30 second charge or discharge time, and they lose only a few % of this after 1000 cycles



Complete nanobatteries are formed in each nanopore of a dense nanopore array (2 billion per cm²). Electrodes at each end are created using atomic layer deposition to carefully control the thickness and length of the multilayer concentric nanotubes.

C. Liu, E.I. Gillette, X. Chen, A.J. Pearse, A.C. Kozen, M.A. Schroeder, K.E. Gregorczyk, S.B. Lee, G.W. Rubloff, "An all-in-one nanopore battery array", *Nature Nanotechnology* Advance Online Publication 10 November 2014, doi: 10.1038/nnano.2014.247

Work was performed at the University of Maryland



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NANOSTRUCTURES for ELECTRICAL ENERGY STORAGE



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Unleaded Perovskite Photovoltaics

Scientific Achievement

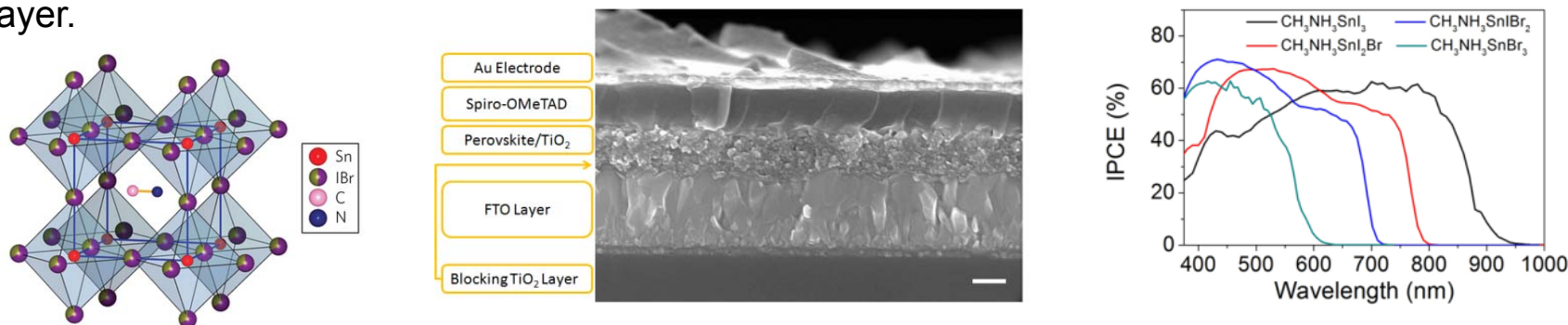
Discovered a method to make solution-processed, perovskite-based photovoltaics (PVs) that use tin instead of lead and exhibit a 5.8% power conversion efficiency.

Significance and Impact

PVs based on organo-lead halide perovskites exhibit high power conversion efficiencies, but lead compounds are highly toxic and harmful to the environment. The discovery of efficient lead-free perovskite PVs may enable low-cost, environmentally benign solar cells.

Research Details

- The PVs are based on methylammonium tin halide ($\text{CH}_3\text{NH}_3\text{SnI}_{3-x}\text{Br}_x$) perovskite semiconductors as the light absorber; band gap can be tuned over the visible spectrum by chemical substitution ($x = 0, 1, 2, 3$).
- Solar cells were fabricated by spin coating the perovskite on mesoporous TiO_2 films, followed by deposition of an organic hole transport layer (spiro-OMeTAD) and thermal evaporation of a gold layer.



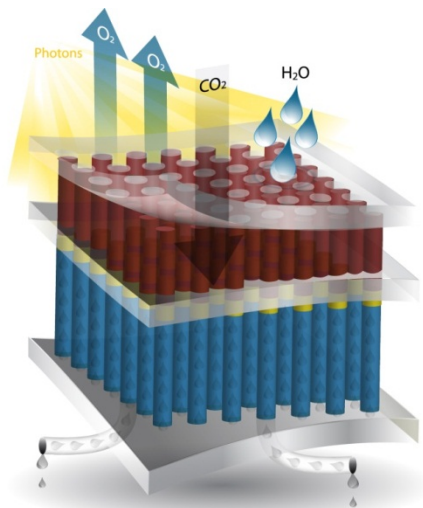
Crystal structure of the $\text{CH}_3\text{NH}_3\text{SnI}_{3-x}\text{Br}_x$ perovskites (left), cross-sectional SEM of a PV prototype (center), and incident-photon-conversion-efficiency (IPCE) spectra of the prototypes (right).

Nature Photonics, 2014, 8, 489-494

Work was performed at Northwestern University.

Fuels from Sunlight Hub

Joint Center for Artificial Photosynthesis (JCAP)



Photoelectrochemical Solar-Fuel Generator

Overview:

- Mission: Develop a solar-fuels generator to produce fuel from the sun 10x more efficiently than crops
- Launched in Sept. 2010; 5-yr award ends in Sept. 2015
- Led by Caltech with LBNL as primary partner; additional partners are SLAC, Stanford, UC Berkeley, UC San Diego, UC Irvine
- 2010 - 2015: Development of prototypes capable of efficiently producing hydrogen via photocatalytic water splitting
- 2015: Renewal to focus on CO₂ reduction discovery science

Goals and Legacies:

- Library of fundamental knowledge
- Prototype solar-fuels generator
- Science and critical expertise for a solar fuels industry

Renewal Planning:

- Renewal project would restructure R&D to focus primarily on discovery science related to CO₂ reduction for efficient solar-driven production of carbon-based fuels
- Annual funding of up to \$15M for a maximum of 5 years reflects reduced project scope
 - De-emphasis of discovery efforts targeted solely towards hydrogen production
 - Development of integrated prototypes mainly to test the capability of new materials, concepts, and/or components
- Renewal decision is expected by end of March 2015

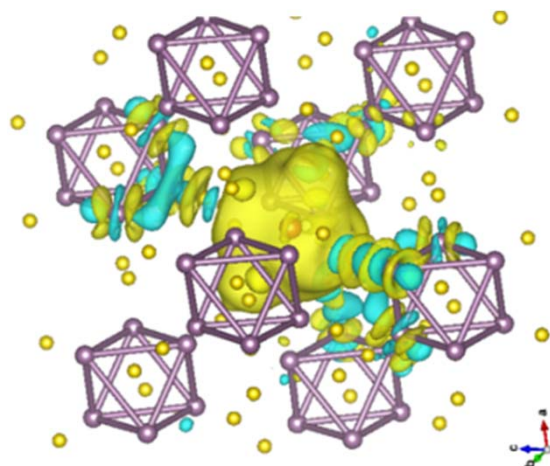
Research Accomplishments:

- Discovered method to protect light-absorbing semiconductors (e.g. Si, GaAs) from corrosion in basic aqueous solutions while still maintaining excellent electrical charge conduction
- Developed novel high throughput capabilities to prepare and screen light absorbers and electrocatalysts
- Established benchmarking capabilities to compare large quantities of catalysts and light absorbers
- Fabricated and tested integrated artificial photosynthetic prototypes with optimized properties
- Developed new multi-physics modeling tools for analysis of solar-fuels prototypes and processes



Batteries and Energy Storage Hub

Joint Center for Energy Storage Research (JCESR)



Overview:

- Mission: Discovery Science to enable next generation batteries—beyond lithium ion—and energy storage for transportation and the grid
- Launched in December 2012; Led by George Crabtree (ANL) with national laboratory, university and industrial partners: LBNL, SNL, SLAC, PNNL, UI-UC, NWU, UCh, UI-C, UMich, Dow, AMAT, JCI, CET.

Goals and Legacies:

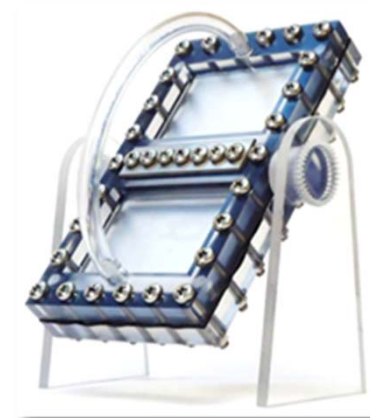
- 5x Energy Density, 1/5 Cost, Within 5 years
- Library of fundamental knowledge
- Research prototype batteries for grid and transportation
- New paradigm for battery development

FY 2015 - 2016 Milestones:

- For the “electrolyte genome,” calculate data for >10,000 molecular systems.
- Complete techno-economic modeling for electrolyte systems identified by the electrolyte genome, that have the potential to meet the “5-5-5” goals

Research Accomplishments:

- Rational design of high-performance Li_2S cathodes;
- Discovery that incorporation of percolating networks of nanoscale conductors improves charge transfer kinetics in liquid electrodes;
- Techno-economic modeling of alternate designs for lithium-air batteries; Fabrication/testing of the first research prototype Mg-ion battery to establish baseline capability.



Bench-top prototype flow battery



DOE Office of Basic Energy Sciences: Scientific User Facilities



- ★ Available to all researchers *at no cost* for non-proprietary research, regardless of affiliation, nationality, or source of research support
- ★ Access based on external peer merit review of brief proposals
- ★ Coordinated access to co-located facilities to accelerate research cycles
- ★ Collaboration with facility scientists an optional potential benefit
- ★ Instrument and technique workshops offered periodically
- ★ A variety of on-line, on-site, and hands-on training available
- ★ Proprietary research may be performed at full-cost recovery

Light Sources

- Advanced Light Source (LBNL)
- Advanced Photon Source (ANL)
- Linac Coherent Light Source (SLAC)
- National Synchrotron Light Source-II (BNL)
- Stanford Synchrotron Radiation Laboratory (SLAC)

Neutron Sources

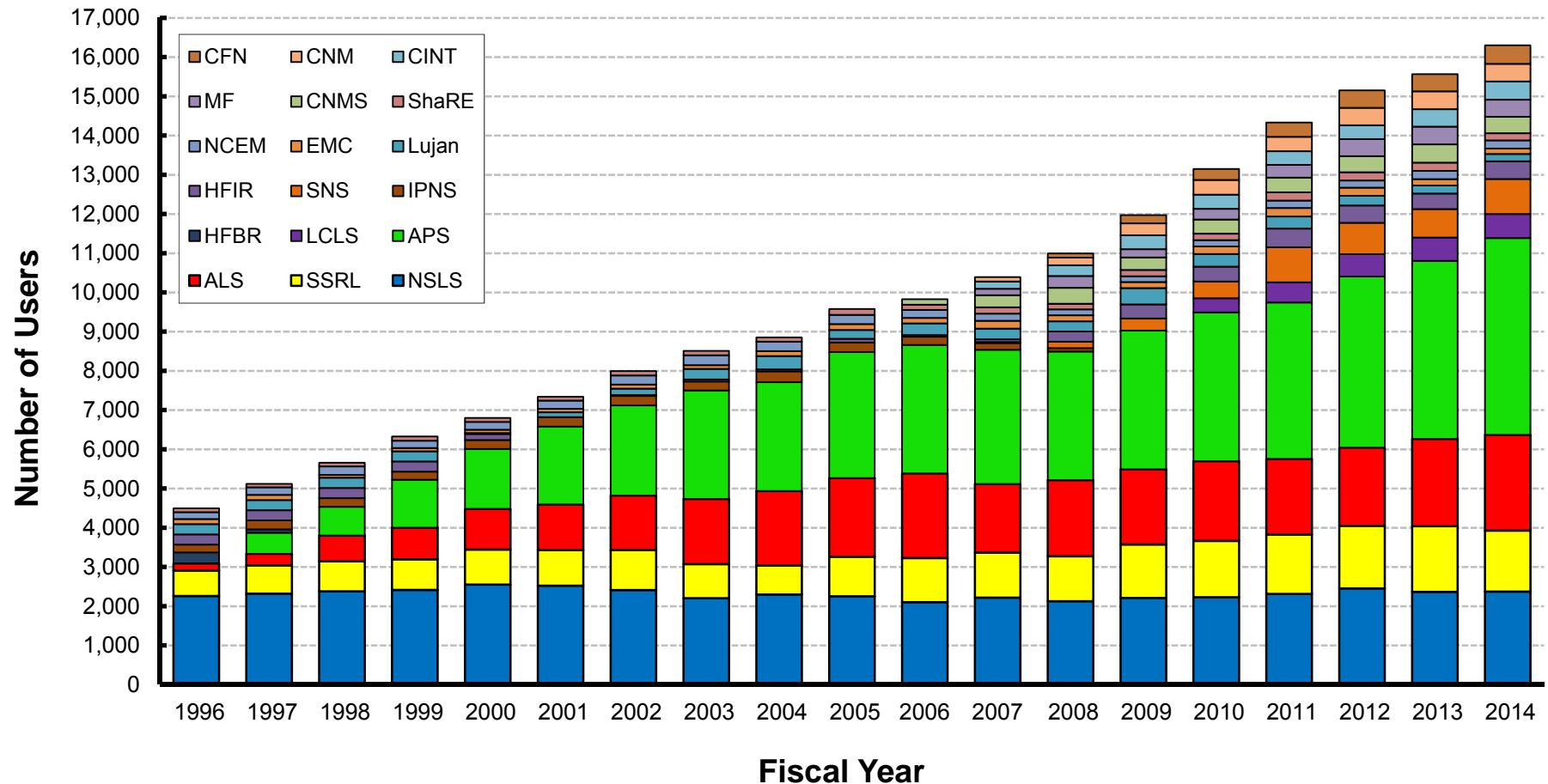
- High Flux Isotope Reactor (ORNL)
- Spallation Neutron Source (ORNL)

Nanoscale Science Research Centers

- Center for Functional Nanomaterials (BNL)
- Center for Integrated Nanotechnologies (SNL & LANL)
- Center for Nanophase Materials Sciences (ORNL)
- Center for Nanoscale Materials (ANL)
- Molecular Foundry (LBNL)



BES User Facilities Hosted Over 16,000 Users in FY 2014



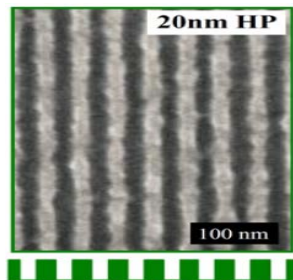
More than 300 companies from various sectors of the manufacturing, chemical, and pharmaceutical industries conducted research at BES scientific user facilities. Over 30 companies were Fortune 500 companies.

Industrial R&D at BES Scientific User Facilities



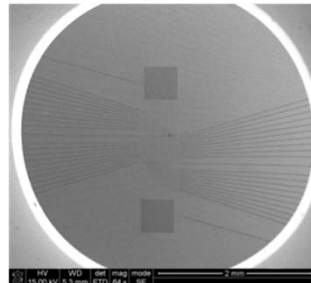
Next Generation Integrated Circuits

Novel Extreme Ultraviolet (EUV) photoresist was developed at NSRCs that has both high resolution and high sensitivity. This approach may be the key to achieving the industrial goals for sub14 nm nodes.



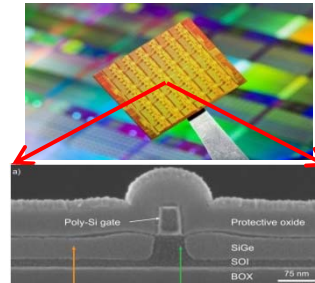
Improving NanoBioSensing Chips

NSRC User Vista Therapeutics, Inc. launched the first commercial NanoBioSensor™ System which uses nanowire transistors to instantly detect target biomarkers via their electrical charge.



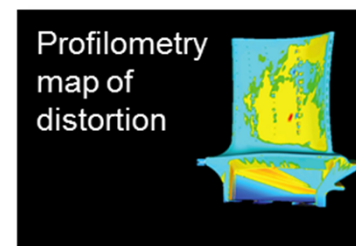
Advanced Microprocessors

Unique NSRC hard x-ray Nanoprobe enables nondestructive measure of in-situ stress distributions in silicon-on-insulator (SOI)-based CMOS for sub 75nm microprocessor technology.



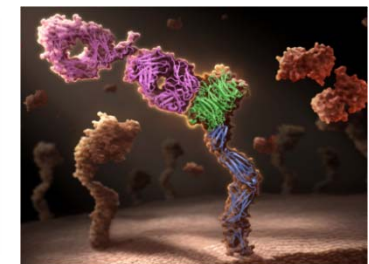
Laser Additive Manufacturing of Turbine Blades

Neutron imaging and scattering have been used to understand the link between residual stress distortions and laser additive manufacturing of turbine blades with optimized internal cooling structures.



From Protein Structures to Drugs

Developing a unique therapeutic antibody, onartuzumab, for treating multiple cancer types based on the structure information obtained from BES light source facilities



FY 2016 BES Budget Request

Research programs

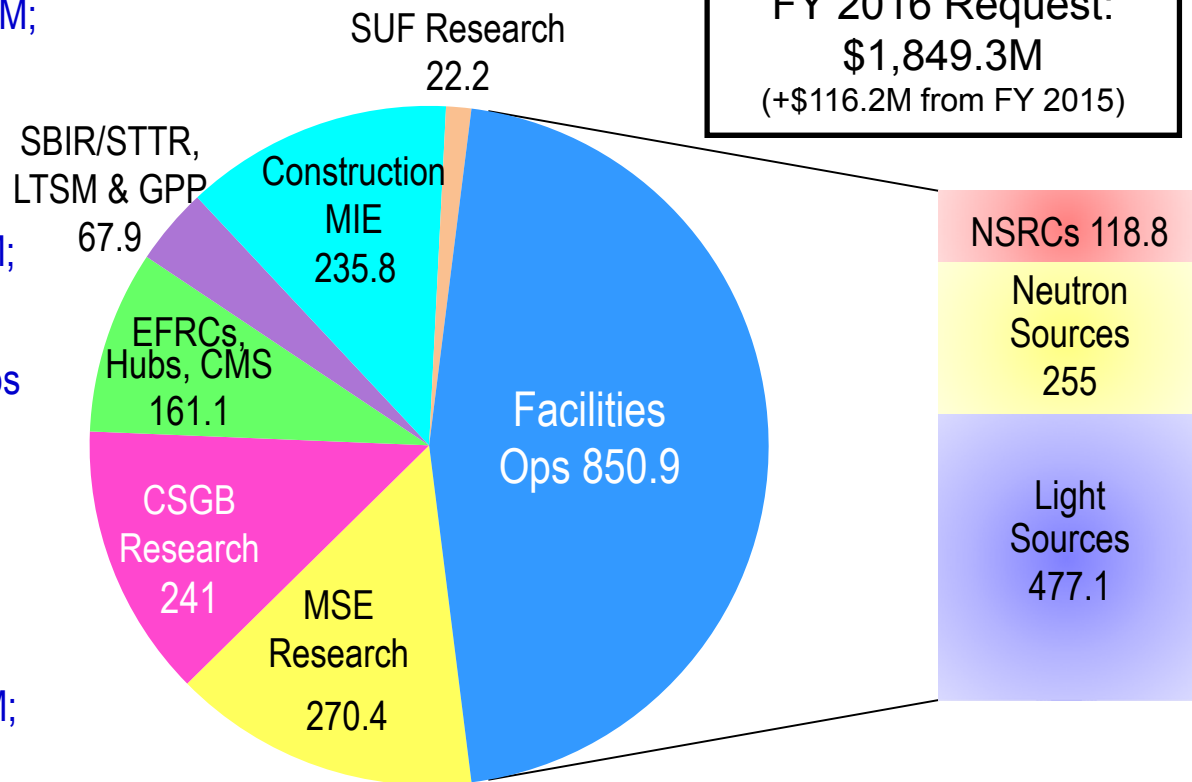
- Energy Frontier Research Centers (\$110M; $\Delta = \$10M$)
- Mid-scale Instrumentation for ultrafast electron scattering (\$5M)
- Computational Materials Sciences (\$12M; $\Delta = \$4M$)
- Core Research & Energy Innovation Hubs at ~FY 2015 level (\$550.5M)

Scientific user facilities

- All full operating facilities at near optimal (~99%) operations (\$850.9M)
- NSLS-II 1st year of full operations (\$110M; $\Delta = \$19.6M$)

Construction and instrumentation

- NSLS-II instrumentation (NEXT) (\$15.5M)
- Advanced Photon Source upgrade (\$20M)
- Linac Coherent Light Source-II (\$200.3M; $\Delta = \$52.3M$)



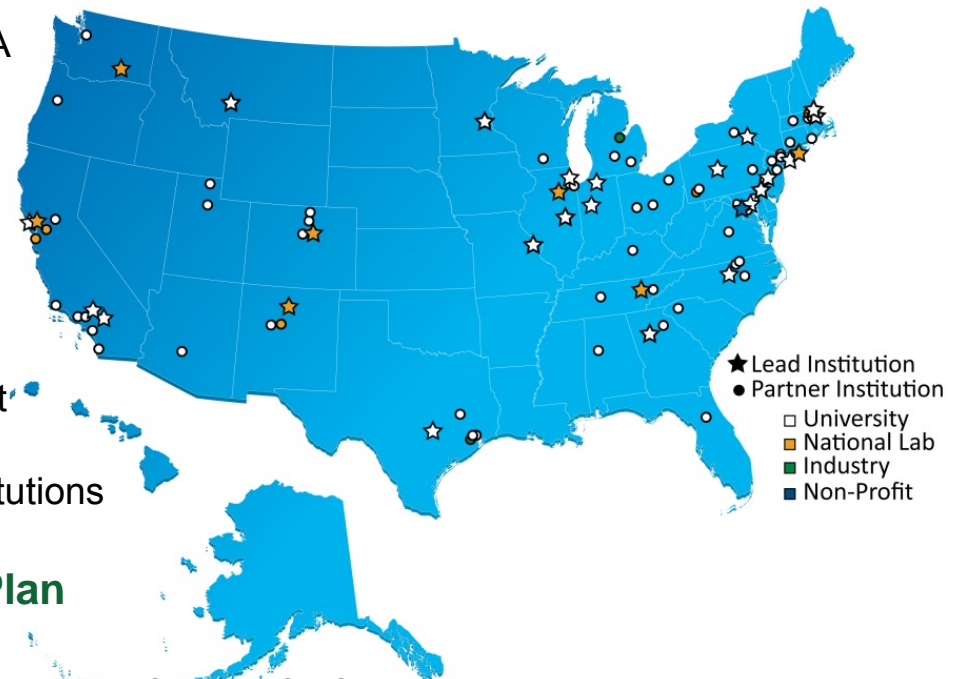
Energy Frontier Research Centers, 2009 - present

FY 2009 46 EFRCs were launched

- \$777M for 5 years, \$100M/year base + \$277M ARRA

FY 2014 Recompetition Results

- \$100M/year base
- 32 EFRCs in 32 States + Washington D.C.
(22 renewals+ 10 new)
- Each \$2-4M/yr for up to 4 years
- Led by 23 Universities, 8 DOE Labs, and 1 non-profit
- ~525 senior investigators and ~900 students, postdoctoral fellows, and technical staff at ~100 institutions



FY 2015 – FY 2016 Review and Management Plan

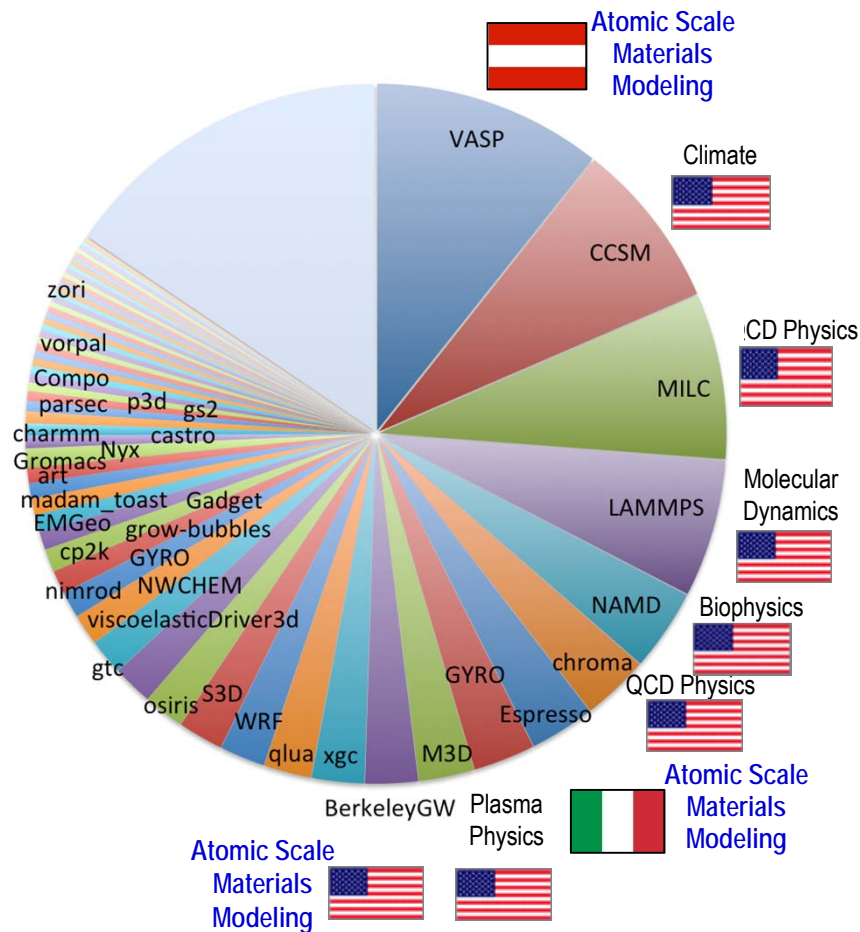
- Management review of new centers in FY 2015.
- Full mid-term progress review for all centers in FY 2016, with funding for final two years contingent upon review outcome.

FY 2016 Funding and New Solicitation

- Funding for EFRCs increases \$10M (FY 2015 = \$100M; FY 2016 = \$110M).
- Open call for new EFRC proposals with topical areas that complement current portfolio and that are informed by new community workshops.
- The EFRC program will transition to a biennial solicitation cycle starting in FY 2016.



Increase for Computational Materials Sciences



2013 Top Application Codes at NERSC

Funding

- FY 2015 included \$8M for new awards. FOA announced in January 2015 for proposals for 4-year research projects to be funded at \$2-4M per year.
- FY 2016 Request of \$12M will continue support for the 2015 awards and will fund additional awards to broaden the technical scope of the research.

Why computational materials sciences? The U.S. trails competitors in computational codes for materials discovery and engineering

- At NERSC, the most used code is VASP, a commercial Austrian atomic scale materials modeling code requiring purchase of license.
- (Quantum) Espresso, a popular materials modeling code, was developed by Italy.
- Top codes for other fields used at NERSC were developed in the U.S. and are all free, community codes.



Computational Materials Sciences

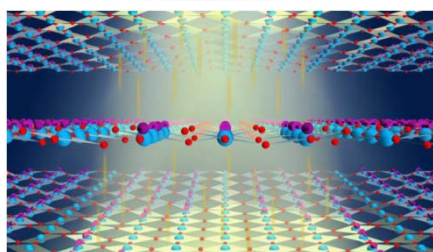
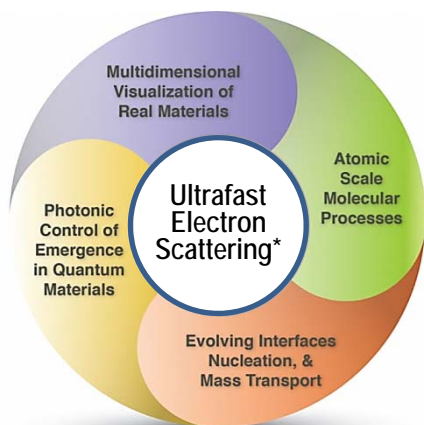
What is Different?

- Will move theory and computation from research-use by experts to more general use by the community --- then industry
- Will fund teams of theorists and experimentalists with the express purpose of accelerating the development of multiscale, validated computational software
 - Fill in theoretical and scientific knowledge gaps
 - Current codes fail for strategic functional materials – magnets, thermal materials, superconductors, advanced semiconductors, membranes
 - Includes development of experimental and theoretical databases for functional materials with community input
 - Open source software, maintained for broad-use
 - Enhance speed and complexity by taking full advantage of super computers at the petascale and beyond
- Builds on the current portfolio of theory research and experimental characterization facilities, including user facilities
 - Seamlessly integrate codes with databases of validated information from both theory and experiments
- Will provide U.S. computational software for materials discovery – restoring the U.S. as a leader in the field

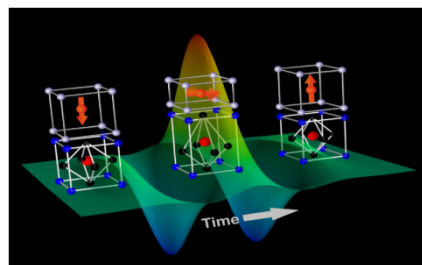


Midscale Instrumentation

Ultrafast Electron Diffraction, Imaging, and Spectroscopy



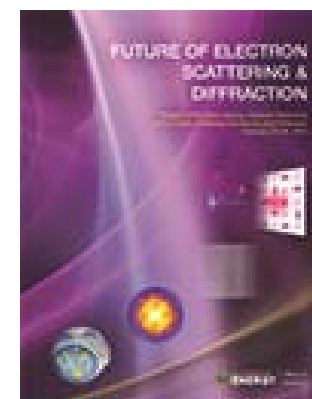
Photonic control in Quantum Materials



THz coupling to ferroelectric polarization

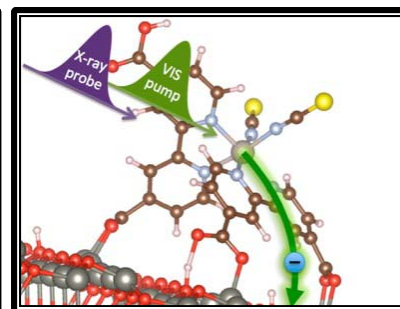
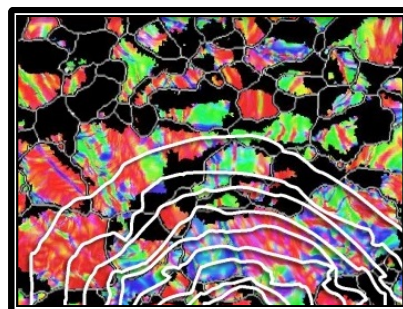
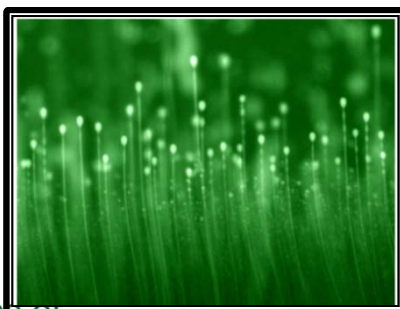
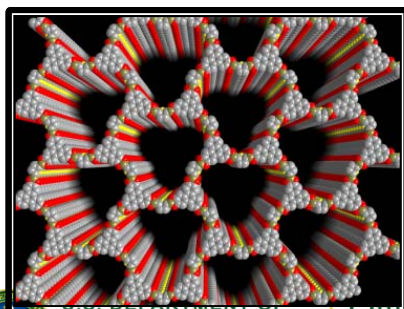
- Ultrafast electron diffraction, imaging, and spectroscopy are poised to enable major scientific advances by characterizing and controlling of physical and chemical processes in real-time and real-space:
 - Molecular dynamics of chemical reactions,
 - Photonic control related to quantum phenomena,
 - Mesoscopic materials and chemistry.

- FY 2016 request (\$5M) will support developing instrumentation to enable ultrafast electron characterization for BES chemical and materials sciences research activities
 - Detectors
 - Electron optics and sources
 - Sample environments



Summary of FY 2016 President's Request for BES

- Increased funding for additional **Energy Frontier Research Centers (EFRCs)** ($\Delta = +\$10,000\text{K}$)
- Increased funding for **computational materials sciences** research to expand technical breadth of code development for design of functional materials ($\Delta = +\$4,000\text{K}$)
- New funding for **mid-scale instrumentation** for ultrafast electron scattering ($\Delta = \$5,000\text{K}$)
- **Energy Innovation Hubs:**
 - Joint Center for Energy Storage Research (JCESR) will be in its 4th year. (FY 2015 = \$24,175K; FY 2016 = \$24,137K)
 - Joint Center for Artificial Photosynthesis (JCAP) is under review for renewal starting in September 2015. (FY 2015 = \$15,000K; FY 2016 = \$15,000K)
- **National Synchrotron Light Source-II (NSLS-II)** begins its 1st full year of operations.
- **Linac Coherent Light Source-II (LCLS-II)** construction continues.
- BES **user facilities** operate at near optimum levels (~99% of optimal).
- Two **major items of equipment**: NSLS-II Experimental Tools (NEXT) and Advanced Photon Source Upgrade (APS-U) are underway.



ENERGY

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MSE and CSGB New and Renewal Success Rates – FY 2014 Implementation of Full Funding of Financial Assistance Awards

To comply with full funding of all awards under \$1M*, the two research divisions are making a concerted effort to use all available options, including shortened budget periods, “terminal renewals,” and no cost extensions (NCE) to maintain quality and portfolio balance. There are noticeable reductions in success rates in FY14 largely attributable to full funding requirement.

MSE	New Grant Success Rate	Renewal Grant Success Rate
2006 - 2008	24%	84%
2009 - 2011	22%	82%
2012 - 2014	18%	71%
2014	15%	65%

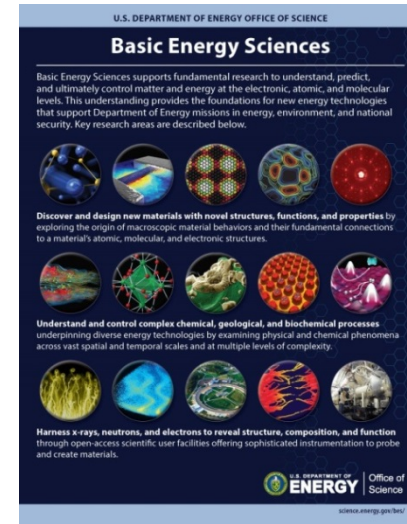
CSGB	New Grant Success Rate	Renewal Grant Success Rate
2005 - 2007	38%	76%
2008 - 2010	49%	82%
2011 - 2013	36%	74%
2014	19%	68%

* Consolidated and Further Continuing Appropriations Act, 2015 (H.R. 83), SEC. 307. Notwithstanding section 301(c) of this Act, none of the funds made available under the heading “Department of Energy—Energy Programs—Science” may be used for a multiyear contract, grant, cooperative agreement, or Other Transaction Agreement of \$1,000,000 or less unless the contract, grant, cooperative agreement, or Other Transaction Agreement is funded for the full period of performance as anticipated at the time of award.

BES Communications

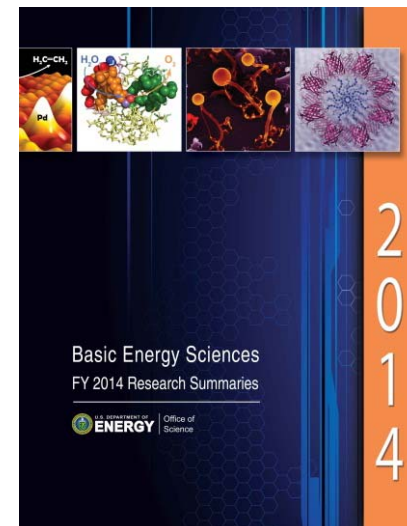
■ BES Brochure

- 11”x17” brochure describing BES-supported research, tools, and facilities
- Examples illustrate BES investments in:
 - research ranging from discovery science to science for energy technologies, and
 - tools including laboratory equipment, theory and experiment, and large user facilities.



■ BES Research Summaries

- Report describing over 1200 BES-supported research projects in FY 2014
- Each entry includes the title, senior investigators, number of students and postdocs, institutions, funding level, program scope, and FY 2014 highlights.



Funding Opportunities: FAQs

- How do I get DOE/BES support?
 - Respond to “FY 2015 Continuation of Solicitation for the Office of Science” -- **Read all FOAs carefully!!**
 - Hypothesis driven, fundamental science project - energy relevance
 - All proposals are peer reviewed
- Can I contact the program manager?
 - Discussion of your research ideas with the program managers is encouraged
 - **White papers/pre-proposals are encouraged**
 - **Can be sent to the program manager or submitted through the Portfolio Analysis and Management System (PAMS) – see the FOA for details**
- What is the typical support level?
 - Peer review will assess the requested budget versus research needs
 - Typical support levels are 1 month of summer support plus graduate student/postdoctoral fellow
 - Multiple PI grants are also supported –program managers can provide more information



FY 2015 – Annual FOA

- FY 2015 Continuation of Solicitation for the Office of Science Financial Assistance Program
(http://science.energy.gov/~media/grants/pdf/foas/2015/SC_FOA_0001204.pdf)
- Read the FOA carefully for program specific limitations, for example:
 - Materials Chemistry: Research primarily aimed at the optimization of synthetic methods or properties of materials for applications, and research with a primary goal of device fabrication and testing will be discouraged.
 - Biomolecular Materials: Research aimed at optimization of materials properties for any applications, device fabrication, sensor development, tissue engineering, and biomedical research will be discouraged.
 - Experimental Condensed Matter Physics: Proposals emphasizing conventional superconductivity and semiconductor physics will not be considered.
 - Mechanical Behavior: Proposals emphasizing mechanics of materials, rather than materials science, will not be considered responsive.

FY 2015 – Annual FOA (continued)

- Read the FOA carefully for program specific emphasis areas, for example:
 - Many programs: The activity will expand research on....
 - Synthesis and Processing Science: The program has an increasing focus on understanding of kinetics and mechanisms of materials growth including: bulk material processes, organic and inorganic film deposition, plasma mediated nanoparticle synthesis and the organization of mesoscopic assemblies across a range of length scales, especially relating to use inspired clean energy research.
 - Experimental Condensed Matter Physics: Growth in research support is expected in the areas of spin physics, magnonics, and topological states of matter.
- FY 2015 applications that do not include a Data management plan will be returned without review



DOE Response to OSTP Memo

Increasing Access to the Results of Federally Funded Scientific Research

http://www.whitehouse.gov/sites/default/files/microsites/ostp/ostp_public_access_memo_2013.pdf

EXECUTIVE OFFICE OF THE PRESIDENT
OFFICE OF SCIENCE AND TECHNOLOGY POLICY
WASHINGTON, D.C. 20502

February 22, 2013

MEMORANDUM FOR THE HEADS OF EXECUTIVE DEPARTMENTS AND AGENCIES

FROM: John P. Holdren *JPH*
Director

SUBJECT: Increasing Access to the Results of Federally Funded Scientific Research

1. Policy Principles

The Administration is committed to ensuring that, to the greatest extent and with the fewest constraints possible and consistent with law and the objectives set out below, the direct results of federally funded scientific research are made available to and useful for the public, industry, and the scientific community. Such results include peer-reviewed publications and digital data.

Scientific research supported by the Federal Government catalyzes innovative breakthroughs that drive our economy. The results of that research become the grist for new insights and are a source of progress in areas such as health, energy, the environment, agriculture, and national security.

Access to digital data sets resulting from federally funded research allows companies to focus resources and efforts on understanding and exploiting discoveries. For example, open weather

DOE Public Access Plan is available on the DOE Open Government website

<http://energy.gov/downloads/doe-public-access-plan>

Public Access Plan



U.S. Department of Energy
July 24, 2014

ENERGY.GOV



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Office of Science Statement on Digital Data Management

All proposals submitted to the Office of Science for research funding will be required to include a Data Management Plan

- Requirements will be included in all solicitations for research funding starting Oct, 1st, 2014. This includes the *Annual FOA*.

- Detailed requirements and further information on:

<http://science.energy.gov/funding-opportunities/digital-data-management/>

- Suggestions for what to include in a Data Management Plan
- Supplemental guidance and requirements from SC Program Offices
- Links to information about data management resources at SC user facilities
- Definitions of key terms
- FAQs

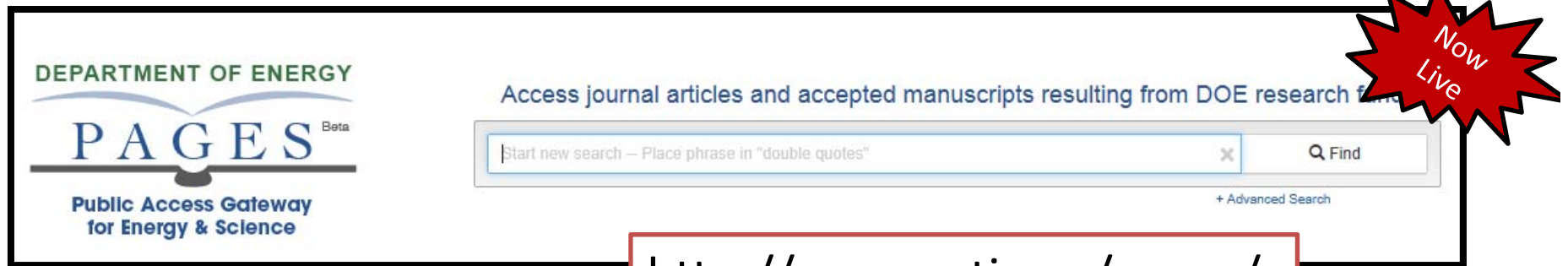


Other DOE offices will have
DMP requirements by FY 2016



Public Access Gateway for Energy and Science (PAGES^{Beta})

- Full text versions of peer-reviewed articles resulting from DOE supported research are publicly accessible through PAGES^{Beta}
- DOE-supported researchers will be **required** to submit metadata for peer-reviewed publications and full text or links to accepted manuscripts starting in FY 2015
- PAGES^{Beta} will link to full-text accepted manuscripts or articles after a 12-month post-publication administrative interval.
- Researchers should acknowledge DOE funding appropriately <http://science.energy.gov/funding-opportunities/acknowledgements/>



DEPARTMENT OF ENERGY
PAGES^{Beta}
Public Access Gateway
for Energy & Science

Access journal articles and accepted manuscripts resulting from DOE research funding

Start new search -- Place phrase in "double quotes"

+ Advanced Search

Now Live

<http://www.osti.gov/pages/>

Funding Opportunities: FAQs

- Can I visit DOE-BES in person?
 - Yes - Initial contact by email and phone is required – contact information is on the website for every program manager
 - DOE-BES is located in Germantown, MD – secure facility, requires planning and additional information from foreign nationals.
- How long will it take for me to find out if my project is funded?
 - The Open Call is a continuous process (no fixed deadline for submission of applications)
 - Reviews take 4 – 6 months to complete, awards are made based on strength of the merit review, programmatic priorities, and available resources
 - Proposals can be held up to one year for consideration
- I want to support my research group with multiple federal grants – what are the requirements?
 - You must have separate research proposals that can “stand alone” with respect to research performed and research output

