

Basic Energy Sciences Overview

Fusion Energy Sciences Advisory Committee Meeting February 2, 2017

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Basic Energy Sciences (BES)

The Program:

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

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

Scientific User Facilities—5 X-ray light sources, 2 neutron sources, and 5 Nanoscale Science Research Centers -- 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



BES Strategic Planning Activities – Engaging BES Advisory Committee and Scientific Community

Science for Discovery



Science for National Needs



National Scientific User Facilities, the 21st century tools of science







Science for National Needs:

BESAC & BES "Basic Research Needs (BRN) ... " Workshops (2002 --)

BRN to Assure a Secure Energy Future (BESAC)

- BRN for Hydrogen Economy (2003)
- BRN for Solar Energy Utilization (2005)
- BRN for Superconductivity (2006)
- BRN for Solid State Lighting (2006)
- BRN for Advanced Nuclear Energy Systems (2006)
- BRN for Geosciences (2007)
- BRN for Clean and Efficient Combustion (2007)
- BRN for Electrical Energy Storage (2007)
- BRN for Catalysis for Energy Applications (2007)
- BRN for Materials under Extreme Environments (2007)
- BRN for Carbon Capture (2010)
- New Science for Sustainable Energy Future (2008)
- **Computational Materials Science and Chemistry (2010)**
- Science for Energy Technology (2010)
- Controlling Subsurface Fractures and Fluid Flow (2015)
- BRN for Environmental Management (2016)
- BRN for Quantum Materials (2016)





https://science.energy.go v/bes/communityresources/reports/

BES Research and Funding Modalities

Core Research (>1,000 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, including the Early Career Research Awards and SciDAC Awards (joint with ASCR).

Energy Frontier Research Centers (36, 2009 --)

\$2-4M/year research centers for 4-year award terms; focus on fundamental research described in the Basic Research Needs Workshop reports.

Computational Materials Sciences (5, 2015 --)

\$2-4M/year research centers for 4-year award terms; focus on delivering open-source software for materials by design in preparation for exascale computing

Energy Innovation Hubs (2, 2010 --)

Research centers for 5-year award terms, established in 2010 (\$15-25M/year), engage in basic and applied research, including technology development, on a highpriority 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 Frontier Research Centers (EFRCs)



 HISTORY: 20 community workshops since early-2000s with over 2,000 participants describing "basic research needs" for energy applications and "grand-challenge science"

ESTABLISHMENT OF EFRCs IN 2009

- 46 awards: 30 funded at \$100M/year; 16 fully funded by ARRA at \$277M
- \$2-5M/year each for a 5-year term

RECOMPETITION IN 2014

- 32 awards funded at \$100M/year (22 renewal, 10 new)
- \$2-4M/year each for a 4-year term, with competitions now every 2 years
- Solicitation topics were informed by additional community workshop reports including mesoscale science and computational materials and chemistry.

Targeted FOA in 2016

- 4 new awards funded at \$10M/year
- \$2-4M/year each for a 4-year term
- Solicitation topics in environmental management research areas as informed by BRN-EM (2016) 7

Energy Frontier Research Centers Status as of August 2016 (36 EFRCs)



Over 110 participating institutions, located in 34 states plus the District of Columbia



Accomplishments since 2009

- Over 8,200 peer-reviewed papers (> 360 in Science and Nature Journals)
- 24 PECASE and 26 DOE Early Career Awards
- 44 EFRCs have created over 380 US and 250 foreign patent applications, more than 490 patent/invention disclosures, and at least 100 licenses
- ~90 companies have benefited from EFRC research
- (May 2014) EFRC students and staff now work: > 300 university faculty and staff; > 475 industrial; > 200 national labs, government, and non-profit



FY 2016: EFRC Partner Institutions



NorthEast Center for Chemical Energy Storage (NECCES)

M. Stanley Whittingham, Binghamton University



EFRC Communications

The 2016 EFRC booklet describes the history and outcomes from the first seven years of the EFRC program, including representative scientific highlights, academic publications, intellectual property, and science commercialization.



Solar concentrators based on quantum dots

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



Accurately modeling materials for energy applications

Optimal method identified for multiscale simulations of carbon nanostructures

GY FRONTIER RESEARCH CENTERS



Building precision nanobatteries by the billions

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



Examining the enzyme complex that makes cellulose fibrils

Imaging and computational modeling revealed new structural insights



Viability of long-term carbon sequestration in the subsurface

The Bravo Dome gas field was used to estimate CO_2 dissolution rates over milennia



Nanoscale control of uranium for solvent-free recovery

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



EFRC Workforce Development Opportunities



http://www.energyfrontier.us/newsletter



Graduate Student and Postdoctoral Researcher Competition



http://www.energyfrontier.us/content/2 015-student-and-postdoc-competition

Poetry of Science Contest



http://www.energyfrontier.us/ poetry-winners

Life at the Frontiers of Energy Research Video Contest



http://www.energyfrontier.us/video-contest



Ten Hundred and One Word Challenge



http://www.energyfrontier.us/1001word-challenge-winners

Ionization Induces Healing of Defects in Silicon Carbide



Projected scanning transmission electron microscopy images of predamaged crystal (top) and improved structural order after 21 MeV Ni ion irradiation (bottom).

Y. Zhang, R. Sachan, O.H. Pakarinen, M.F. Chisholm, P. Liu, H. Xue, and W. J. Weber, "Ionization-induced annealing of preexisting defects in silicon carbide," *Nature Commun.* **6**, 8049 (2015). DOI: 10.1038/ncomms9049

Scientific Achievement

Energy transferred to electrons in silicon carbide (SiC) by energetic ions via ionization can effectively heal preexisting defects and restore structural order.

Significance and Impact

Because SiC is a critical material for nuclear applications and power electronics for space applications, ionizationinduced self-healing may contribute to increased radiation tolerance in extreme radiation environments.

Research Details

- Defects were introduced into single-crystal SiC by implantation with 900 keV Si ions.
- Irradiation of these samples with ions having high electronic energy loss (4.5 MeV C to 21 MeV Ni) healed pre-existing defects.
- Healing was validated by ion channeling, scanning transmission electron microscopy and atomistic simulations.
- Energy transfer of 1.4 keV/nm to electrons was sufficient to activate this process.









Computational Materials Sciences



2015 Top Application Codes at NERSC

- High-accuracy software is needed to understand how the behavior of atoms and molecules (or quantum effects) impacts energy conversion and materials synthesis.
- At NERSC, the most used materials and chemistry research codes were developed by foreign countries, (e.g., VASP -- a commercial Austrian atomic scale modeling code requiring purchase of license).
- Top codes used at NERSC for other fields were developed in the U.S. and are all free, open-source community codes.
- BES support began in 2015, and is currently supporting 5 teams at \$12M/yr to develop research codes and data for design of functional materials to be used by academia, labs, and industry – as part of the Exascale crosscut.

The U.S. trails other countries in development of computational codes in chemistry and materials sciences.







- Fuels from Sunlight:
 - Awarded to the Joint Center for Artificial Photosynthesis (JCAP); 1st phase award (2010 2014) funded at ~ \$25M/yr for hydrogen fuels research, including prototype development.
 - Based on peer review outcomes, JCAP was renewed for the 2nd term in 2015 at \$15M/yr to conduct research on CO₂ reduction to produce chemical fuels – a grand science challenge.
 - Led by Caltech with participating institutions: LBNL, UCI, UCSD, and SLAC.
- Batteries and Energy Storage Hub:
 - Awarded to the Joint Center for Energy Storage Research (JCESR) and commenced operations in December 2012 at ~ \$25M/yr.
 - JCESR focuses on discovery science to enable next generation batteries—beyond lithium ion—and energy storage for transportation and the grid.
 - Led by ANL with participating institutions: LBNL, SNL, SLAC, PNNL,UI-UC, NWU, UCh, UI-C, UMich, MIT, Utah, United Tech, Dow, AMAT, JCI, CET.



Cross-sectional SEM image of a protected photoelectrode (Verlage, et. al. *Energy Environ. Sci.* 2015)



Theoretical predictions of Mg deposition (from MgCl) on a Mg metal surface



BES Scientific User Facilities

Unique research facilities *and* scientific expertise for ultra high-resolution characterization, synthesis, fabrication, theory and modeling of advanced materials



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)

Neutron Sources

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



* Available to all researchers <u>at no cost</u> 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 Lightsource (SLAC)

BES User Facilities Hosted Over 15,000 Users in FY 2016



- The newly constructed NSLS II started early operations in FY 2015.
- The three electron beam microcharacterization centers were merged administratively with their respective neighboring NSRCs in FY 2015.
- The BES operations at the Lujan Neutron Scattering Center ceased operations in FY 2014.



Users by Discipline at the Light Sources





Light Source User Demographics for FY 2015



BES X-ray Free Electron Laser Source: Linac Coherent Light Source (LCLS)





MEC provides a unique set of tools that utilize the combined LCLS ultra fast high brightness x-ray beams and high power optical laser beams to study the transient behavior of matter in extreme conditions. Key scientific areas include warm dense matter physics, high pressure studies, and shock physics.

BES Reactor Neutron Source

BES operates the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory

- 85 MW light-water moderated and cooled reactor
- Principal mission Neutron scattering
 - Secondarily produces a variety of isotopes for medical and industrial applications
 - Also provides a significant materials irradiation capability due to its unique flux trap design providing an intense fast neutron flux
- <u>More than 100</u> HFIR irradiation capsules have been completed for fusion since the 1970s
- Between <u>5,000-10,000 specimen</u> have been exposed over the last decade





Several specimen types to be loaded into the irradiation capsules in lower left



Nanoscale Science Research Centers



Synthesis

- Quantum dots, nanowires
- Functionalized nanoparticles
- High mobility & quantum materials
- Nanocrystalline diamond
- Ordered nanoparticle assemblies
- Combinatorial nanomaterials

Fabrication

- E-beam lithography
- Dip pen, STM lithography
- Nanopatterned block copolymers
- Atom scale fabrication
- Nanometer scale 3D printing

Characterization

- Atomic resolution electron microscopy
- Ultrafast & THz optical
- X-ray scattering
- In-situ and in-operando
- Neutron scattering

Modeling/Prediction

 Comprehensive suite of codes on clusters and HPC integrated with experiments



Los Alamos National Laboratory &

Sandia National Laboratory



4 Nobel Prizes in 10 Years Using Light Source User Facilities

- 2003: Roderick MacKinnon (Chemistry) for "structural and mechanistic studies of ion channels." Used NSLS beamlines X25 and X29.
- 2006: Roger Kornberg (Chemistry) "for his studies of the molecular basis of eukaryotic transcription." Used SSRL macromolecular crystallography beamlines.
- 2009: Venkatraman Ramakrishnan, Thomas A. Steitz, and Ada E. Yonath (Chemistry) "for studies of the structure and function of the ribosome." Used all 4 DOE light sources.
- 2012: Robert J. Lefkowitz and Brian K. Kobilka (Chemistry) "for studies of G-protein-coupled receptors." Used APS beamline 23-ID.



The overall view of a voltage-dependent potassium ion channel.



The visualized transcription process.



The 50S subunit structure at 2.4Å resolution.



The structure of the β2AR-Gs complex.



Lab-Industry Partnerships at the BES Scientific User Facilities Support U.S. Science and Economy



Maintaining World Leadership in BES Facilities

- Engage BES Advisory Committee in setting priorities
- Be mindful of international competitions
- Take a long view in planning: ~ 10 years for major upgrades

Status of Upgrade Planning:

Ring-based x-ray light sources

ANL Advanced Photon Source Upgrade (APS-U) (CD-1/3B) LBNL Advanced Light Source Upgrade (ALS-U) (CD-0)

Free electron laser based x-ray light sources

SLAC LCLS-II (CD-3) SLAC LCLS-II High Energy Upgrade (LCLS-II-HE) (CD-0)

Spallation based neutron scattering sources

ORNL Spallation Neutron Source Proton Power Upgrade (CD-0) ORNL Spallation Neutron Source Second Target Station (CD-0)



CD-0: Mission Need CD-1: Alternatives Analysis CD-3B: Long Lead Procurement CD-3: Construction Start

LCLS-II and APS-U Underway

Linac Coherent Light Source-II (LCLS-II)

- LCLS-II will provide high-rep-rate, ultra-bright, transformlimited femtosecond x-ray pulses with polarization control and pulse length control to ~1 femtosecond. The hard x-ray range will be expanded to 25 keV.
- Added are a 4 GeV superconducting linac; an electron injector; and two undulators to provide x-rays in the 0.2–5 keV energy range.
- FY 2016 = \$200,300K; FY 2017 = \$190,000K for R&D, design, prototyping, long lead procurement, and construction of technical systems.
- The project is on track and ~42% complete; first light is planned for Jan 2020

Advanced Photon Source Upgrade (APS-U)

- APS-U will provide a multi-bend achromat lattice to provide extreme transverse coherence and brightness.
- Initial conceptual design for the new lattice completed; conducting R&D and key component prototyping in support of the new design; beamline proposal selection complete
- FY 2016 = \$20,000K; FY 2017 = \$20,000K for R&D, design, and limited prototyping.
- CD-1 Refresh approved 2/2016; CD-3B, Long Lead Procurement approved 10/2016







X-ray Synchrotron Light Source Upgrade Multiple Bend Achromat Lattice Design



ERC

Science



International Landscape of X-ray Storage Ring Light Sources: New Constructions (3) and Upgrades (3)



Four Competing X-Ray FELs Begin/Continue Operation in 2017



SNS Will be Challenged by ESS



19 European countries are building the 5 MW European Spallation Source (ESS) in Sweden

ESS construction in 1/2017, ops in ~2019







Relative time structure for short pulse sources SNS FTS and STS, and J-PARC, and the ESS long pulse design.

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BESAC Report on Facility Upgrades (June 2016): Neutrons & Photons (Status as of Q1 CY2017)

Project	ANL APS-U	LBNL ALS-U	ORNL SNS PPU	ORNL SNS STS	SLAC LCLS-II	SLAC LCLS-II-HE
Proposed Project	Hard X-ray ~Diffraction Limited 6 GeV MBA Ring	Soft X-ray ~Diffraction Limited 2 GeV MBA Ring	Proton Power Upgrade to 2.5 MW (W Target) 1.3 GeV SC Linac	High Resolution Neutron Science; Second Target Station	High Rep-Rate, Soft X-ray FEL, 4 GeV SC Linac	High Rep-Rate, Medium Energy X-ray FEL, 8 GeV SC Linac
Current Status of Facility	APS is operational since 1996; ring will be replaced	ALS is operational since 1993; ring will be replaced	SNS Linac is operational since 2006 at 0.94 GeV	SNS is operational since 2006	LCLS is operational since 2010; LCLS-II is under construction	LCLS is operational since 2010; LCLS-II is under construction
Worldwide Competition	EU ESRF Germany PETRA3,4 Japan SPring-6 China HEPS	Sweden MAX-IV Brazil SIRIUS CH SLS-II	EU ESS Japan JPARC China CSNS UK ISIS	EU ESS Japan JPARC China CSNS UK ISIS	EU XFEL Japan SACLA Korea PAL XFEL CH Swiss FEL	EU XFEL
Dark Time	~1 yr	~0.75 yr	0 yr	~0.5 yr	~1 yr	0 yr
Status Q1/17	CD-3b	CD-0	CD-0	CD-0	CD-3	CD-0



f <u>https://science.energy.gov/~/media/bes/besac/pdf/Reports/BESAC_Facility_Upgrade_Assessment</u> <u>Approved_June_9_2016.pdf</u>

BES At-a-Glance



Relevant Websites

BES: <u>https://science.energy.gov/bes/</u>

Reports: <u>https://science.energy.gov/bes/community-resources/reports/</u>

Research: https://science.energy.gov/bes/research/

User Facilities: <u>https://science.energy.gov/user-facilities/user-facilities-at-a-glance/bes/</u>



Questions?

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BES Budget At-a-Glance



BES Organizational History



ERDA's 1976 R&D plan, A National Plan for Energy Research, Development, and Demonstration: Creating Energy Choices for the Future (April 15, 1976).

- The formation of BES was part of the *Department of Energy* Organization Act of 1977 to provide for basic energy research in non-nuclear areas.
- Basic research activities within the Energy Research and Development Administration (ERDA) were first grouped as the BES program in the FY 1977 Budget Request (released February 1976). The BES organization was formed in June 1977 in preparation for the creation of DOE in October 1977.
- While BES has gone through many changes in structure and program emphases, the mission of BES has not changed. As stated in 1976, "The primary purpose of the BES program is to increase knowledge of the physical phenomena relevant to the goal of meeting our nation's energy needs."

The research activities and subprograms of BES have undergone substantial changes over the past three decades. For a detailed evolution of the BES program, see: http://science.energy.gov/bes/about/organizational-history/

The origins of the federal research programs that became BES are rooted in the nation's research efforts to win World War II. The goals of the early U.S. science programs that evolved into BES were to explore fundamental phenomena, create scientific knowledge, and provide unique user facilities. In this sense, the BES program predates the establishment of the Atomic Energy Commission in 1946, which became part of ERDA on October 11, 1974, as a result of the Energy Reorganization Act of 1974.

