

Basic Energy Sciences Overview

High Energy Physics Advisory Panel Meeting December 1, 2017

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BES Organizational History: A 40-Year Legacy



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: <u>http://science.energy.gov/bes/about/organizational-history/</u>

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.



The Energy Crises: 1973 and 1979

- Significant reshaping of R&D priorities to include
 - To improve fossil energy utilization
 - Expand use of non-fossil energy technologies, e.g., solar, renewables, energy efficiency, etc.
 - Physical sciences research extends into nonnuclear energy technologies

Historical context:

- 1973 Oil Embargo
- Energy Research & Development Administration (ERDA) established (January 1975).
- Department of Energy (DOE) established (August 1977).





ERDA to DOE Transition

Source: Foreword of Materials Sciences Program Summary (1977)

During FY 1977 a new Department of Energy was proposed by the President and approved by Congress. This Department is now (August, 1977) scheduled for activation about October 1, 1977. The Energy Research and Development Administration will be transferred to the Department of Energy together with other agencies and parts of agencies within the Federal government. Also during FY 1977 the Division of Physical Research of ERDA was reorganized into two Divisions, one called Basic Energy Sciences and one called High Energy and Nuclear Physics. At the time of this writing the organizational structure of the new Department of Energy has been established only at the functional levels. However, it is expected that the Divisions of Basic Energy Sciences and High Energy and Nuclear Physics will report to the Director of the D.O.E. Office of Energy Research. The Director of this Office will be appointed by the President with Senate consent. The Director shall advise the Secretary on the physical research program transferred to the Department from ERDA; monitor the Department's R&D programs; advise the Secretary on management of the multipurpose laboratories under the jurisdiction of the Department excluding laboratories that constitute part of the nuclear weapon complex; and advise the Secretary on basic and applied research activities of the Department.





Science

Office of Science Organization Structure (2017)



Basic Energy Sciences (2017)





BES Program Overview

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

Research: condensed matter and materials physics, chemistry, geosciences, and aspects of biosciences—to discover new materials and design new chemical processes that touch virtually every important aspect of energy resources, production, conversion, transmission, storage, efficiency, and waste mitigation.

Facilities: x-ray light sources, neutron sources, nanoscale science research centers for the atomic-level visualization and characterization of materials of all kinds, including biological molecules. Construction of the next-generation facilities to maintain international competitiveness.



FY 2017 BES \$1.87 B











BES Strategic Planning Activities:

Serving the Present; Shaping the Future

Engaging BES Advisory Committee and Scientific Community in planning for:

Science for Discovery



Science for National Needs



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





BESAC Grand Science Challenges Report:

Directing and Controlling Matter and Energy



- Synthesize, atom by atom, new forms of matter with tailored properties
- Synthesize man-made nanoscale objects with capabilities rivaling those of living things
- Control the quantum behavior of electrons in materials
- Control emergent properties that arise from the complex correlations of atomic and electronic constituents
- Control matter very far away from equilibrium







Basic Research Needs for Quantum Materials for Energy Relevant Technology February 8-10, 2016

Workshop Chair: Associate Chairs: Collin Broholm (JHU) Ian Fisher (SLAC/Stanford) Joel Moore (UC-Berkeley/LBNL) Margaret Murnane (UC-Boulder)

SC Technical Leads: Linda Horton and Jim Horwitz (BES)



CHARGE: Identify basic research needs and priority research directions for quantum materials with a focus on new, emerging areas with potential for transformative scientific advances and for impact on energy technologies. The phenomena of quantum materials are examined in the broad categories of: (1) superconductivity and charge-related order, (2) magnetism and spin, (3) transport and non-equilibrium dynamics, (4) electronic topology, (5) nano-structure or heterogeneity.

Breakout Sessions and Chairs:

Superconductivity and charge order: Adriana Moreo (U Tennessee) and John Tranquada (BNL) Magnetism and spin: Meigan Aronson (Texas A&M) and Allan MacDonald (U Texas Austin) Transport and non-equilibrium dynamics: Dimitri Basov (UCSD) and Jim Freericks (Georgetown) Topological quantum materials: Eduardo Fradkin (U of Illinois) and Amir Yacoby (Harvard) Heterogeneous and nano-structured quantum materials: Nitin Samarth (PSU) and Susanne Stemmer (UCSB)

Priority Research Directions:

- Control and exploit fluctuations in quantum matter for the design of bulk materials with novel functionality
- Harness topological states for groundbreaking surface properties
- Drive and manipulate quantum effects (coherence, entanglement) in nanostructures for transformative technologies
- Design revolutionary tools to accelerate discovery and technological deployment of quantum materials



Basic Research Needs for Quantum Materials for Energy Relevant Technology

Control and exploit fluctuations in quantum matter for the design of bulk materials with novel functionality

Looking beyond the standard paradigms of simple metals and semiconductors, how do stronglyinteracting electrons organize themselves in quantum materials, and how can this be controlled for energy-relevant technologies?

- Understand and control competing, coexisting, and intertwined order
- Predict, realize, and probe new states of quantum magnets

Harness topological states for groundbreaking surface properties

Building on recent advances in the field of topological insulators, what new topological states of matter can be realized, what are their signatures, and how can these be used for energy-related applications?

- Discover new topological quantum materials
- Design new platforms to probe and exploit topology

Drive and manipulate quantum effects (coherence, entanglement) in nanostructures for transformative technologies

How can the extraordinary properties of coherent quantum states be controlled and utilized for energy-related applications?

- Employ nanoscale structuring to elucidate and exploit coherence and entanglement
- Understand transport in quantum materials
- Dynamically visualize and manipulate quantum materials

Design revolutionary tools to accelerate discovery and technological deployment of quantum materials

What new methodologies and tools are needed to advance synthesis of quantum materials and our ability to probe and predict their properties?

- Enhanced synthesis of quantum materials
- Develop new windows into quantum materials
- Develop efficient methods for static and dynamic states beyond 1-electron paradigms



BASIC RESEARCH NEEDS WORKSHOP ON Quantum Materials for Energy Relevant Technology



BES Roundtables on Quantum Information Sciences

- Opportunities for Basic Research for Next-Generation Quantum Systems
 - October 30-31, 2017 (1.5 days)
 - Chair David Awschalom (UChicago/ANL)

Co-chair – Hans Christen (ORNL)

 Identify opportunities for basic materials and chemical sciences, including nanoscale research, to enable the next-generation of quantum devices and systems.

Opportunities for Quantum Computing in Chemical and Materials Sciences

- October 31 November 1 (1.5 days)
- Chair Joel Moore (UC-Berkeley/LBNL)

Co-chair – Alan Aspuru-Guzik (Harvard U)

 Identify opportunities for quantum computing (QC) to enable significant and impactful advances in understanding of important fundamental challenges in chemical and materials sciences



BES & Quantum Information Science

- Quantum materials and chemistry supported by BES core research and EFRCs are foundational to exploring and controlling novel quantum behaviors.
- BES Nanoscale Science Research Centers capabilities are key to nano-to-micro-scale electronic/ photonic quantum structure fabrication. Integration and testing will couple closely with theory, design and systems efforts.
- Research will enable next-generation qubit concepts, innovative quantum and classical architectures (beyond ion traps, quantum dots, nitrogen vacancies, donor centers, etc.)



Office of Science Released Dear Colleague Letter on QIS Nov. 29, 2017





BES Scientific User Facilities

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





BES User Facilities Hosted Nearly 16,000 Users in FY 2017



Fiscal Year

- The newly constructed NSLS-II started early operations in FY 2015 (hosted 110 users); NSLS closed on 9/30/14.
- The three electron beam microcharacterization centers were merged administratively with their respective neighboring NSRCs in FY 2015.
- BES operations at the Lujan Neutron Scattering Center ceased operations in FY 2014.



Users by Discipline at the Light Sources



Linac Coherent Light Source at SLAC



Science

Linac Coherent Light Source at SLAC

Injector (35°) at 2-km point

Existing 1/3 Linac (1 km) (with modifications)

New e- Transfer Line (340 m)

Transport Line (200 m)

Undulator (130 m) Argonne Near Experiment Hall (underground)

Far Experiment Hall (underground)

Light Sources: A Global Race to the Top



Three categories of facilities were considered in the prioritization:

Ring-based x-ray light sources

ANL Advanced Photon Source Upgrade (APS-U) LBNL Advanced Light Source Upgrade (ALS-U)

Free electron laser based x-ray light sources SLAC LCLS-II High Energy Upgrade (LCLS-II-HE) (i.e., additional cryomodules in existing tunnel)

Spallation-based neutron scattering sources

ORNL Spallation Neutron Source Proton Power Upgrade (SNS PPU) ORNL Spallation Neutron Source Second Target Station (SNS STS)



2016 BESAC Facility Prioritization Report

Summary Table of Assessment

Facility Upgrade	Contribution to World- leading Science	Readiness to Proceed with Construction		
APS-U	Absolutely Central	Ready to initiate construction		
ALS-U	Absolutely Central	Ready to initiate construction		
LCLS II-HE	Absolutely Central	Ready to initiate construction		
SNS Proton Power Upgrade	Absolutely Central	Significant scientific/engineering challenges to resolve before initiating construction		
SNS Second Target Station	Absolutely Central	Significant scientific/engineering challenges to resolve before initiating construction		



The Power of Light Sources

Seeing the Invisible in Real Materials

Where are the Atoms?



Direct measurements of "pure" ac spin currents (flow of spin angular momentum without flow of charge)

Office of

Science

spin current l

Time (ps)

125 250 375 500

S. DEPARTMENT OF

(b) 0 LCP

PRL (2016)

Capturing the transient behavior of catalytic bond formation

Science (2015)

25



Goal: Control Matter & Energy on These Scales!

LCLS-II and APS-U Construction Projects

Linac Coherent Light Source-II (LCLS-II)

- When completed, LCLS-II will provide high-repetitionrate, ultra-bright, transform-limited 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.
- The upgrade adds a 4 GeV superconducting linac; an electron injector; and two undulators, which will provide x-rays in the 0.2–5 keV energy range.

Advanced Photon Source Upgrade (APS-U)

- FY 2018: R&D, design, prototyping, testing, fabrication, site preparation, installation, and long lead procurements.
- APS-U will provide an x-ray source with world-leading transverse coherence and extreme brightness.
- The upgrade provides a new storage ring incorporating a multi-bend achromat lattice, new insertion devices, superconducting undulators, and new or upgraded beamlines.







Advanced Light Source Upgrade (ALS-U) at LBNL

Goal:

High coherent flux in soft x-ray region (~50-2,000 eV) necessary to resolve nanometerscale features and enable real-time observation of chemical processes and materials as they function



Comparison of the beam profiles of ALS (left) and ALS-U (right).

Map nano-objects' 3D electronic, chemical, & magnetic structure

Understand Roles of Heterogeneity

 Connect spatial, chemical, and temporal heterogeneity with real-time movies



 Potential benefit – optimize material processes & properties, e.g., low carbon footprint concrete

Control chemical kinetics in confined spaces

Master Hierarchical Architectures

- Reveal relationships between nanoscale chemical structures & the kinetic processes they support
- Potential benefit chemical catalytic reactors, solar fuel production, water purification

Deploy spin, quantum, and topological materials

Harness Coherence in Light & Matter

 Probe electronic structure of single domains and gated structures of complex materials



 Potential benefit – ultralow-power computing, new classes of sensors, spin-based devices



LCLS-II High Energy (LCLS-II-HE) at SLAC

<u>Goal:</u>

■ To deliver ultrafast, coherent x-rays with Angstrom resolution (≥12 keV) at high average power to enable spectroscopic analysis of additional key elements in the periodic table, deeper penetration into materials, enhanced resolution of experiments, and studies of structural dynamics at the atomic scale.

International Competition:

- SACLA (Japan) has been in operation since 2011 (5-20 keV, 60 Hz)
- EuXFEL is now operational but not yet at full capability (designed for 0.2-25 keV, 28 kHz in 10 Hz bursts)
- PAL XFEL (Korea, designed for 0.3-20 keV, 60 Hz) and SwissFEL (Switzerland, designed for 0.2-12 keV, 100 Hz) are now online but not yet at full capability

<u>Heterogeneity</u> & complexity in ground & excited states

- Correlate catalytic reactivity and structure
- Real-time evolution with chemical specificity and atomic resolution



<u>Dynamics</u> of biomolecules and molecular machines

- Study large scale conformational changes via solution scattering
- Physiological conditions



Fluctuations in the ground state and spontaneous evolution

- Characterize statistically dynamic systems without long-range order
- Inform directed design of energy conversion and storage materials



US Response based on 2016 BESAC Prioritization Report

	Storage Rings		FEL		
Project	ANL APS-U	LBNL ALS-U	SLAC LCLS-II	SLAC	
Project Scope	Hard X-ray ~Diffraction Limited 6 GeV MBA Ring	Soft X-ray ~Diffraction Limited 2 GeV MBA Ring	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	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 PETRA 3,4 Japan SPring-6 China HEPS	Sweden MAX-IV Brazil SIRIUS CH SLS-II China NSRL-U	EU XFEL Japan SACLA Korea PAL XFEL CH Swiss FEL	EU XFEL China SCLF	
Dark Time	~1 yr	~0.75 yr	~1 yr	Cu Linac: No Dark Time SRF Linac: ~ 1 yr	
Status FY2017	CD-3b	CD-0	CD-3	CD-0	

The ALS-U, APS-U & LCLS-II-HE proposals were each deemed "absolutely central to contribute to world leading science & ready to initiate construction"

BES Detector Research

Development of higher-precision, more efficient detectors capable of acquiring data several orders of magnitude faster than state-of-the-art detectors

- More efficient sensors
- Improvements in time-resolved imaging
- Improvements in data acquisition, visualization tools, and analysis workflows







Mixed-Mode Pixel Array for high energy X-rays

- -- 1 kHz frame rate
- -- high dynamic range
- S. Gruner (Cornell U)



"Day 1" LCLS-II Soft X-ray Detector 5-10 kHz, high QE Coherent Imaging, Scattering and Diffraction; Inelastic Scattering *P. Denes (LBNL); G. Carini (SLAC)*



Nanofabricated Smart Tip Detectors Coaxial metal-insulator-metal tip detectors as probe in synchrotron x-ray STM V. Rose (ANL) – Early Career FY12



Fast, high-efficiency superconducting X-ray detector using transition-edge sensors Energy accuracy ~1 eV K. Irwin (SLAC); A. Miceli (APS)



FLORA: Fermilab-LCLS CMOS High dynamic range; fast frame > 10 kHz G. Deptuch (Fermi); G. Carini (SLAC)



High-speed Scanning Transmission Electron Microscope Detector – 100 kHz

- Massive data rates workflow
- Records a *diffraction pattern* at every scan point

P. Denes (LBNL)

Backup Slides



Overview of BES FY 2018 President's Request

- The BES FY 2018 Request of \$1,554.5 million is a decrease of \$317 million or 17% from the FY 2017 Enacted level.
- The overall research funding in FY 2018 is reduced by 18% from FY 2017, requiring a significant shift in
 priorities with targeted reductions of activities that extend to later-stage fundamental research. Both the core
 research and the EFRC program will emphasize emerging high priorities in quantum materials and
 chemistry, catalysis science, synthesis, and instrumentation science.
- No funding is requested for the two BES-supported Energy Innovation Hubs, Batteries and Energy Storage and Fuels from Sunlight, or for the DOE Experimental Program to Stimulate Competitive Research.
- All BES user facilities will operate at below optimal levels. Selected light source beamlines and neutron flight paths will be shut down. The Stanford Synchrotron Radiation Lightsource will operate up to the first quarter and then transition to a warm standby status. No funding is requested for two Nanoscale Science Research Centers: the Center for Functional Nanomaterials or the Center for Integrated Nanotechnologies.
- No funding is requested for Long Term Surveillance and Maintenance or for the disposition of unused equipment for the Lujan Neutron Scattering Center.
- To maintain international competitiveness of our facilities, BES will continue to support the Linac Coherent Light Source-II (LCLS-II) and Advanced Photon Source Upgrade (APS-U) projects. APS-U will transitions from a major item of equipment to a line item construction project.



FY 2018 HEWD Appropriations: Basic Energy Sciences July 11, 2017

	FY 2017 Enacted Approp.	FY 2018 President's Request	FY 2018 House Mark	FY 2018 H Mark vs. F Enacte	Y 2018 House ark vs. FY 2017 Enacted		FY 2018 House Mark vs. FY 2018 President's Request	
Research	1,681,500	1,352,400	1,612,400	-69,100	-4.11%	260,000	19.23%	
Construction 13-SC-10 Linac Coherent Light								
Source-II, SLAC	190,000	182,100	192,100	2,100	1.11%	10,000	5.49%	
18-SC-10 APS Upgrade, ANL	100.000	20,000	67,000	67,000	0.00%		235.00%	
Iotal, Construction	190,000	202,100	259,100	09,100	34.19%	57,000	20.20%	
Total	1,871,500	1,554,500	1,871,500		0.00%	317,000	20.39%	

- Core research increases ~1% over FY17.
- EFRCs, CMS, CCS, EPSCoR flat with FY17.
- No funding for the Hubs, but \$10M designated for competitive awards to continue similar research.
- All facilities funded at or near FY17 levels.
- APS-U increases to \$67M (+\$24.5M) and converts to line item construction.
- LCLS-II increases to \$200M, \$10M above FY17.

FY 2018 SEWD Appropriations: Basic Energy Sciences

	FY 2017 Enacted Approp.	FY 2018 President's Request	FY 2018 Senate Mark	FY 2018 S Mark vs. F Enact	Senate FY 2017 ted	FY 2018 Mark vs. President's	Senate FY 2018 s Request
Research	1,681,500	1,352,400	1,641,300	-40,200	-2.4%	+288,900	+21.4%
Construction							
LCLS-II, SLAC	190,000	182,100	200,000	+10,000	+5.3%	+17,900	+9.8%
APS Upgrade, ANL		20,000	93,000	+93,000	0.0%	+73,000	+365.0%
ALS Upgrade, LBNL			20,000	+20,000	0.0%	+20,000	0.0%
SNS Proton Power Upgrade, ORNL			26,000	+26,000	0.0%	+26,000	0.0%
Total, Construction	190,000	202,100	339,000	+149,000	+78.4%	+136,900	+67.7%
Total	1,871,500	1,554,500	1,980,300	+108,800	+5.8%	+425,800	+27.4%

- The Senate mark reduces the control point from Research and Construction (shown above) to individual activities (eg. EFRCs, Hubs, CMS, CCS, individual facilities).
- Core research increases ~1% over FY17.
- EFRCs, Hubs, CMS, CCS are flat with FY17.
- EPSCoR increases from \$15M in FY17 to \$20M in the Senate mark.
- All facilities funded at or near FY17 levels. No funding for Lujan D&D.
- LCLS-II increases to \$200M, \$10M above FY17.
- APS-U increases to \$93M (+\$50.5M over FY17) and converts to line item construction.
- New funds provided to start the ALS-U, PPU, and LCLS-II-HE projects.
- \$7M for Long Term Surveillance and Maintenance at BNL.

