Basic Energy Sciences
Materials Sciences and Engineering Division Overview

November 29, 2018

Linda Horton
Materials Sciences and Engineering Division
Office of Science, Basic Energy Sciences
To understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels

BES fulfills its mission through:

– Supporting basic research to discover new materials and design new chemical processes that underpin a broad range of energy technologies
– Operating world-class scientific user facilities in x-ray, neutron, and electron beam scattering as well as in nanoscale research
– Managing construction and upgrade projects to maintain world-leading scientific user facilities
Office of Basic Energy Sciences (BES)

Office of Basic Energy Sciences
Harriet Kung, Director

Materials Sciences and Engineering Division (MSE)
Linda Horton, Director
- Materials Discovery, Design and Synthesis
- Condensed Matter and Materials Physics
- Scattering and Instrumentation Sciences

Scientific User Facilities Division (SUF)
Jim Murphy, Director
- X-ray and Neutron Scattering Facilities
- Nanoscience and Electron Microscopy Centers
- Facility Construction and Major Items of Equipment

Chemical Sciences, Geosciences and Biosciences Division (CSGB)
Bruce Garrett, Director
- Fundamental Interactions
- Photochemistry and Biochemistry
- Chemical Transformations

Research grouped by scientific topics, not by specific energy technologies
DOE Office of Basic Energy Sciences: Scientific User Facilities
Nearly 16,000 users in FY 2017

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

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)

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)

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

http://www.science.doe.gov/bes/suf/user-facilities
BES By the Numbers – FY 2017

**BES Research Spans**
- More than 150 academic, nonprofit, and industrial institutions
- 17 DOE national laboratories
- 47 states and Washington, D.C.

**SUPPORTED RESEARCHERS**
- ~5,600 Ph.D. scientists
- ~1,800 students

**$724 Million Research Budget**

**$915 Million Scientific User Facility Operating Budget**

**BES by the Numbers FY 2017**

BES supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels.

- ~15% Average new grant success rate
- Over 1,000 core research projects
- Nearly 16,000 users at 12 BES facilities

**$233 Million Facility Upgrades, Construction Budget**

**36 Energy Frontier Research Centers**

**2 Energy Innovation Hubs**
Materials Sciences and Engineering Research
Broad Portfolio of Grand Challenge and Use-Inspired Fundamental Research

Scattering and Instrumentation Sciences:
Investigation of photon, neutron, and electron interactions with matter to characterize structures, dynamics, and functionality

Division-wide themes
Quantum materials
Theory, modeling & simulation
Nano- and meso-scale science
Advanced instrumentation
Materials synthesis

Materials Discovery Design and Synthesis:
Understanding design and synthesis to discover new materials via physical, chemical, and bio-molecular routes
BES-Supported Research Activities

- **Core Research (＞1,000 projects, ＄550M/yr)**
  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; typically 3-year awards. Annual FOA open year-round. Includes awardees under the SC Early Career Research Program (5-yr awards, separate FOA with annual proposal due dates).

- **Energy Frontier Research Centers (＄110M/yr)**
  ＄2-4 million/year research centers for 4-year award terms; focus on fundamental research described in Basic Research Needs Workshop reports. Recompetition completed in FY 2018

- **Computational Materials & Chemical Sciences (＄26M/yr)**
  ＄2-4 million/year research centers for 4-year award terms; focus on delivering open-source software for materials and chemistry by design in preparation for exascale computing. Recompetition anticipated in FY 2019 for CMS.

- **Energy Storage and Fuels from Sunlight & Batteries Hubs (＄39M/yr)**
  Research centers for 5-year award terms, established in 2010 (＞＄15-25M/year), engage in research topics that have proven challenging for traditional funding modalities and in which success could be transformative to science and technology. Project goals, milestones, and management structure are a significant part of the proposed Hub plan.
Recent Strategic Planning Workshops and Roundtables Cross the Breadth of the MSE Division

- Quantum Science
- Theory, Modeling and Computation
- Characterization
- Synthesis
- Cross-Cutting Energy

Forthcoming – Basic Research Needs for Microelectronics
Two Roundtable Reports (October 2017) defined a BES research agenda for emerging quantum systems and computing research opportunities:

**BES Science for Quantum Systems**

- Advance artificial quantum-coherent systems
- Enhance creation and control of coherence in quantum systems
- Novel approaches for quantum-to-quantum transduction
- New quantum methods for advanced sensing and process control

**Quantum Computing for BES Science**

- Control the quantum dynamics
- Unravel the physics and chemistry of strongly correlated electron systems
- Embed quantum hardware in classical frameworks
- Bridge the classical–quantum computing divide
Quantum Information Science: Opportunities for Basic Research for Next Generation Quantum Systems

Roundtable in October 2017 defined a BES research agenda for quantum systems for QIS and provided input on priority research opportunities:

- **Advance artificial quantum-coherent systems with unprecedented functionality**
  - Develop new capabilities for synthesis that couple theoretical predictions and real-time measurements of targeted quantum characteristics, including coherence
  - Explore robotic synthesis of layered materials, design of quantum properties for hybrid (organic and inorganic) systems, creation of topological states of matter, and precise control to position atomic defects

- **Enhance creation and control of coherence in quantum systems**
  - Understand scaling of coherence lengths and times with system size and complexity, and identify new signatures of quantum states in artificial quantum-coherent systems
  - Investigate mechanisms to prevent decoherence, leading to discovery and exploitation of novel entangled excitations

- **Discover novel approaches for quantum-to-quantum transduction**
  - Advance new capabilities for coherent transfer of complete wavefunctions between disparate physical systems, the core of quantum measurement and information processing
  - Develop new techniques for generation and stabilization of nonclassical states of light and matter; high fidelity transfer of quantum wavefunctions; and quantum state replication and entanglement

- **Implement new quantum methods for advanced sensing and process control**
  - Design new quantum-based sensors, detectors, and imaging systems for precise measurements of time, space, and fields to probe material properties and chemical processes
  - Create novel methods to use squeezed states for metrology and understand the connections of entanglement, thermodynamics, and many-body localization/diffusion
Roundtable in October 2017 defined a BES research agenda for emerging quantum computing and provided input on priority research opportunities:

• **Controlling the quantum dynamics of nonequilibrium chemical and materials systems**
  – Elucidate the fundamental principles underlying chemical reactions and catalytic pathways; discover dynamical phases of matter; and understand how to prepare entangled states across many quantum degrees of freedom

• **Unraveling the physics and chemistry of strongly correlated electron systems**
  – Enable a correct description of the quantum behavior of strongly entangled electrons to allow discovery of the principles controlling superconductivity, magnetic states and the dynamics of electronic states

• **Embedding quantum hardware in classical frameworks**
  – Develop efficient hybrid algorithms that embed quantum computing for strongly correlated quantum components in classical computing for more weakly correlated parts, thus enabling simulations of molecular and materials problems containing thousands of atoms

• **Bridging the classical–quantum computing divide**
  – Improve the efficiency of quantum computing using approximate results from classical computing as input, and improve the accuracy of classical computing using high-accuracy results from quantum computing to parameterize and optimize complex models
Roundtable in October 2017 defined a BES research agenda for ultrafast science with XFELs and provided input on priority research opportunities:

- **Probing and controlling electron motion within a molecule**
  - Understand how molecules are formed and transformed through interactions among their constituent atoms and electrons; combine time resolution and specificity necessary to follow the motion of the electrons and determine how this movement influences atomic rearrangement, thus permitting an unparalleled view of the steps in chemical transformation

- **Discovering novel quantum phases through coherent light-matter coupling**
  - Explore the frontier of quantum matter to create novel phases of matter, with properties that do not exist in equilibrium; enable the creation and control of light-induced phases of matter and the discovery of general principles needed to design novel states of quantum matter; explore interplay governing the properties and phases of quantum materials

- **Capturing rare events and intermediate states in the transformation of matter**
  - Understand the transformation of matter by identifying and characterizing the underlying ultrafast dynamics of molecules and materials that occur spontaneously; enable a detailed understanding of the intricate pathways by which phase transformations and chemical reactions occur; capture the complex processes involved in molecular and material transformations
Research programs

- Core Research will emphasize quantum materials and chemistry, ultrafast science, and BRN topics ($551M; Δ=+$62.9M).
- Computational Materials and Chemical Sciences continue ($26M)
- Energy Frontier Research Centers continue ($110M)
- Funding continues for Energy Innovation Hubs (JCAP & JCESR) ($39M).

Scientific user facilities

- Operations of 12 facilities at ≥ 95% optimal level ($898.6M; Δ=+$21.3M)
- $1M Lujan equipment disposition; $8.5M Long Term Surveillance and Maintenance

Construction/MIE*  Δ=+$131.5M

- Last year of funding for LCLS-II ($200M)
- Advanced Photon Source Upgrade($93M)
- Three new starts: LCLS-II-HE ($10M) and ALS-U ($30M); PPU ($36M)

FY 2018 Appropriation: $2090.0M
(+$218.5M or +11.7% from FY 2017)
Research programs

- Core Research will emphasize quantum materials and chemistry, ultrafast science, and BRN topics.
- Computational Materials and Chemical Sciences continue ($26M)
- Funding continues for Energy Innovation Hubs (JCAP & JCESR) ($39M).
- Energy Frontier Research Centers continue ($110M)

Scientific user facilities

- Operations of 12 facilities at 95% optimal level
- No funding is requested for Lujan equipment disposition or Long Term Surveillance and Maintenance

Construction

- Last year of funding for LCLS-II ($45M)
- Advanced Photon Source Upgrade ($17.5M)
- Two new starts: LCLS-II-HE ($7M) and ALS-U ($12M)
FY 2018 – FY 2019 BES Research Priorities

- **Quantum Information Science (QIS)**
  - By exploiting the intricate quantum mechanical phenomena, QIS will create fundamentally new ways of obtaining and processing information and open new vistas of science discovery and technology innovation. Research priorities were identified in two QIS roundtables held in October 2017.

- **Ultrafast Science**
  - Ultrafast science remains a priority in both research divisions to position the U.S. leadership in this critical field of science and in anticipation of the completion of the LCLS-II construction project. Research priorities were identified in a roundtable held October 2017.

- **Computational Materials and Chemical Sciences**
  - Computational Materials Sciences (CMS) and Computational Chemical Sciences (CCS) are maintained in support of the Exascale Computing Initiative. CCS was funded in FY 2017 and is moved to a new budget line in the FY 2019 Request.

- **Materials and Chemical Sciences for Future Nuclear Energy**
  - Research will be supported to achieve a multi-scale spatial and temporal understanding of fundamental physical and chemical processes that govern the properties and performance of novel material systems and fuels required for advanced reactors.

- **Priorities identified by Advisory Committee and Basic Research Needs Reports**
  - Both the core research and EFRCs will emphasize emerging high priorities identified by the Basic Energy Sciences Advisory Committee and recent Basic Research Needs workshop reports.
Energy Frontier Research Centers
FY 2017, 2018 Enacted = $110M; FY 2019 President’s Request = $110M

Current EFRCs ($110M)
- 36 awards, $2-4M per year for 4 years
- Lead institutions by type: **26 universities; 9 DOE national laboratories; 1 nonprofit organization**
- 120 participating institutions, located in 35 states plus the District of Columbia

EFRC Members
![EFRC Members](image)

FY 2018 Recompetition
- The EFRC program was recompeted, soliciting both renewal proposals for centers with awards that end in 2018 and proposals for new EFRCs. The recompetition focused on transformative opportunities and research priorities identified in recent BESAC and Basic Research Needs reports.
- Awards were recently announced: 31 four-year Awards (22 New, 9 Renewals) plus 11 two-year extensions of existing centers.

FY 2019 Request
- Provides the fourth year of funding for four EFRCs established in 2016, and the second year of funding for awards resulting from the 2018 recompetition.

Website: [http://science.energy.gov/bes/efrc/](http://science.energy.gov/bes/efrc/)
Topical Distribution of 42 EFRCs

**Catalysis** – Enhanced selectivity and efficiency in production of fuels and chemicals.

**Energy Storage** – New materials and chemistries for next-generation electrical energy storage.

**Nuclear** – Advanced fuels and radiation-tolerant materials for future nuclear energy.

**Quantum Materials** – Novel materials for innovative electronics, sensors, and communications.

**Subsurface** – New geophysics and geochemistry for enhanced oil/gas and geothermal applications.

**Solar** – Cutting-edge innovation for the capture of solar energy and conversion into electricity and fuels.

**Separations** – Advances to enhance gas separations and address energy-water issues.

**Synthesis/Mat-Chem by Design** – Foundational science underpinning materials and chemical synthesis for broad energy applications.

**4 additional EM-related EFRCs funded 2016-2020**
BES QIS Funding Opportunity Announcement (1)

**Materials and Chemical Sciences Research for Quantum Information Science**

DE-FOA-0001909 and LAB 18-1909

Fundamental research in materials and chemical sciences to:
- Advance understanding of quantum phenomena in systems that could be used for QIS
- Use today’s quantum computers for chemical and materials sciences research.
- Topics related to BES roundtable reports on QIS.

**Awards:**
- Single investigator/small group and team proposals: $150K to $1.5M per year, up to 3 year awards
- 27 projects, ~$28 M in FY 2018 funding (~$74M over 3 years)
- 21 awards led by universities; 6 by national laboratories
- 8 awards for use of quantum computing; 19 awards to advance QIS quantum systems
FOA Scope:

Research Infrastructure: includes funding for metrology, fabrication, and prototypes (measurement science instrumentation, modeling and simulation, and shared DOE-lab based user facilities).

Research: Topics related to BES roundtable reports on QIS.

Awards

- A maximum of 3 pre-applications were accepted per Nanoscale Science Research Center
- Team proposals: $500K - $2M per year, up to 3 year awards
- 7 awards and $12M in FY 2018 funding ($32M over 3 years)
Computational Materials Sciences

FY 2018, FY 2019 Request $13M

Computational Materials Sciences -- ensuring U.S. leadership in computing for materials design and discovery

- Research focuses on predictive design of functional materials, taking full advantage of current leadership computers and future exascale capabilities
- Supports integrated theory-computational-experimental teams to perform the basic research required to deliver open-source community codes and the associated experimental and theoretical databases
- Advance tools to predict and validate electronic, magnetic, and strain properties for energy conversion, correlated materials, layered materials, and excited-state phenomena
- **In FY 2019**, a funding opportunity will:
  - Consider applications for renewal of awards that have successfully completed 4-years of research
  - Focus on applications for new awards in the area of predictive design of quantum materials for quantum information science

Ab-initio theory of decay of an optically excited electron-hole pair (red) into 2 lower energy pairs (blue), while conserving spin

Calculation of the correct electronic charge density of anatase TiO$_2$ using quantum Monte Carlo and including temperature dependence
Computational Materials Sciences – FY 2019 Solicitation

- Funding Opportunity Announcement DE-FOA-0002040 posted Nov. 26, 2018
- Supports Single investigator/small group (SI/SG) and larger team awards

Deliver robust, open-source community software and databases for predictive design of functional materials within the Materials Genome Initiative for Global Competitiveness and the Office of Science Exascale activities:

- Takes full advantage of leadership computers ranging from peta- to exascale performance
- Supports integrated theory-computation-experimental teams to perform the basic research required to deliver open-source community codes and the associated experimental and theoretical databases with necessary verification and validation
- Software tools will emphasize strong correlations, multiscale properties, excited states, transport, electronic or optical properties

- Award size: up to $750K (SI/SG) or $2M (Team) annually over four years
- Pre-Application due: December 21, 2018
- Application due: February 28, 2019
- A parallel, companion announcement Lab 19-2040
- Full details available at: https://science.energy.gov/bes/funding-opportunities/
EPSCoR Implementation Grants

- Funding Opportunity Announcement DE-FOA-0002023 posted November 13
- Applicants limited to EPSCoR jurisdictions
- The FOA contains information on topical areas of interest, etc.

- Award size: up to $3,000,000 over two years
- Pre-applications due December 20
- Responses provided for pre-applications January 25, 2019
- Applications due March 27
- Full details available at: [https://science.energy.gov/bes/funding-opportunities/](https://science.energy.gov/bes/funding-opportunities/)
Office of Science Early Career Research Program – Started in FY 2010

• Purpose: To support individual research programs of outstanding scientists early in their careers and to stimulate research careers in the disciplines supported by the Office of Science

• Eligibility: Within 10 years of receiving a Ph.D., either untenured academic assistant or associate professors on the tenure track or full-time DOE national lab employees

• 5-Yr Awards: University grants $150,000/yr, National lab awards $500,000/yr min

FY 2017 Program

• 700 Office of Science proposals received, 21 Basic Energy Sciences (19 universities, 2 Labs) awards out of a total of 59 awards for the Office of Science (10 in BES-Materials Sciences and Engineering)

FY 2018 Program

• Awards announced – see website for more information.

• Annual FOA will be released in FY 2019 for the next opportunity. FOAs cover different topics than the annual FOA for BES – important to read the details!

Office of Science Graduate Student Research (SCGSR) Program

Prepare graduate students for STEM careers critically important to the DOE Office of Science mission. (~ 100-120 participants)

- Graduate students conduct a part of their graduate thesis research at a DOE lab with a collaborating principal investigator.
- Award terms range from 3 months to 1 year and can begin any time between the earliest and latest start dates specified in the solicitation.
- Graduate students pursuing Ph.D. degrees in areas of physics, chemistry, material sciences, biology (non-medical), mathematics, engineering, computer or computational sciences, or specific areas of environmental sciences that are aligned with the mission of the Office of Science are eligible to apply for the supplemental research awards provided by the SCGSR program.
- Specific areas of interest deemed to be of high program priority/workforce need. The areas may change slightly from year to year, depending on program determinations of workforce need.

**Award Benefits:**
- A monthly stipend of up to $3,000/month for general living expenses
- Reimbursement of inbound/outbound traveling expenses to/from the DOE laboratory of up to $2,000.
(Award payments are provided directly to the student.)

**Eligibility:**
- U.S. Citizen or Lawful Permanent Resident
- Qualified graduate program & Ph.D. Candidacy
- Research aligned with a SCGSR priority research topic
- Establishment of a collaborating DOE laboratory scientist at the time of application

See website for details: https://science.energy.gov/wdts/scgsr/
SCGSR Program: Topics from Previous Calls

Topics based on SC’s Assessment of Workforce Development Needs and evolving needs of SC programs

Advanced Scientific Computing Research (ASCR)
(a) Applied Mathematics
(b) Computer Science

Basic Energy Sciences (BES)
(a) Neutron Scattering Research and Instrumentation
(b) Predictive Materials Science and Chemistry
(c) Fundamental Electrochemistry related to energy transduction, storage, chemical conversion, and corrosion
(d) Crystal Growth
(e) Ultrafast Materials and Chemical Sciences
(f) Electron and Scanning Probe Microscopy Research and Instrumentation

Basic Energy Sciences (BES)
(a) Neutron Scattering Research and Instrumentation
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(e) Ultrafast Materials and Chemical Sciences
(f) Electron and Scanning Probe Microscopy Research and Instrumentation

Biological and Environmental Research (BER)
(a) Computational Biology and Bioinformatics
(b) Novel in Situ Imaging and Measurement Technologies for Biological Systems Science
(c) Plant Science for Sustainable Bioenergy
(d) Soil Microbiology

Energy Transfers in Large Proteins and Protein Complexes

Fusion Energy Sciences (FES)
(a) Burning Plasma Science & Enabling Technologies
(b) Discovery Plasma Science

High Energy Physics (HEP)
(a) Theoretical and Computational Research in High Energy Physics
(b) Advanced Technology Research and Development in High Energy Physics
(c) Experimental Research in High Energy Physics

Nuclear Physics (NP)
(a) Medium Energy Nuclear Physics
(b) Heavy Ion Nuclear Physics
(c) Low Energy Nuclear Physics
(d) Nuclear Theory
(e) Nuclear Data and Nuclear Theory Computing
(f) Isotope Development and Production for Research and Applications
(g) Accelerator Research and Development for Current and Future Nuclear Physics Facilities
Funding Opportunities: FAQs
READ FOAs!

• Open call is a continuous process (no fixed deadline for submission)
  – Reviews take 4 – 6 months to complete, awards are made based on strength of the merit review and available resources
  – Proposals can be held up to one year for consideration

• White papers are encouraged
  – Respond to “Open Call For Proposals” (Special Calls may have different requirements – read these carefully)
  – Hypothesis driven, fundamental science project - energy relevance
  – White papers/ are encouraged but not required for academic research
  – All proposals are peer reviewed

• Funding levels
  – Peer review will assess requests versus research needs (10 CFR 605)
  – Typical academic awards are for 1 summer month plus students/postdoc
  – Multiple PI teams are allowed
  – National Lab awards are always multiple PI, except for early career

• Delineation from other grants...
  – You must have separate research proposals that can “stand alone” with respect to research output
For more information on BES Budgets
Office of Science Home Page


FY 2019 Budget Request to Congress (narrative 5.4MB)

- Funding by Appropriation
- Overview
- Funding by Congressional Control
- Advanced Scientific Computing Research
- Basic Energy Sciences
- Biological and Environmental Research
- Fusion Energy Sciences
- High Energy Physics
- Nuclear Physics
- Workforce Development for Teachers and Scientists
- Science Laboratories Infrastructure
- Safeguards and Security
- Science Program Direction
- Isotope Production and Distribution Program Fund
- Crosscuts
- General Provisions
On Line Resources

- **BES at 40**
  - Highlights on the impact of BES

- **BES Program Update**
  - Annual publication that describes updates to the BES program in FY 2017, including major new awards and strategic planning activities. It also describes select research highlights.

- **BRN Workshop and Roundtable Reports**

https://science.energy.gov/bes/community-resources/overview-brochures/
Questions?