Basic Energy Sciences
Materials Sciences and Engineering
Overview of Research Opportunities

April 2, 2018

Linda Horton
Materials Sciences and Engineering Division
Office of Science, Basic Energy Sciences
Basic Energy Sciences

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

Scientific User Facilities—the largest collection of facilities for electron, x-ray, and neutron scattering in the world

In FY 2017, BES supported:

- ~5,600 Ph.D. scientists and ~1,800 students
- Research at over 150 academic institutions in 46 states and at 17 DOE laboratories.
- Over 1,000 research projects in 25 core research areas
- 36 Energy Frontier Research Centers
- Fuels from Sunlight & Batteries and Energy Storage Hubs
- Nearly 16,000 users at 12 BES facilities
- New grant success rates ~15%

In FY 2017, BES invested ~$724 M in research, ~$915 M in operations for world-class, open-access scientific user facilities; and ~233 M in facility upgrades and construction.

Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels
DOE Office of Basic Energy Sciences: Scientific User Facilities
Nearly 16,000 users in FY 2017

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

**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)

http://www.science.doe.gov/bes/suf/user-facilities
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, ~$500M/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. Annual FOA open year-round. Includes awardees under the SC Early Career Research Program (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 underway 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.

- **Fuels from Sunlight & Batteries and Energy Storage 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.
Science Research – The bill includes $6.26 billion for science research – an increase of $868 million above the 2017 enacted level. This funding supports basic energy research, the development of high performance computing systems, and research into the next generation of energy sources. These investments lay the groundwork for a more secure energy future, helping to reduce the nation’s dependence on foreign oil and ensuring continued economic growth.
- EFRCs, CMS, CCS, and both Hubs are all fully funded.
- Light sources increase by 0.2%, neutron facilities increase by 5.6%, and NSRCs increase by 6.7% over FY 2017.
- Construction: LCLS-II fully funded. APS-U ramps up. Three new projects funded: SNS PPU ($36M), ALS-U ($30M), LCLS-II-HE ($10M) including OPC.
- EPSCoR funded at $20M.
- $7M for Long Term Surveillance and Maintenance at BNL.

Source: [http://docs.house.gov/floor/](http://docs.house.gov/floor/)
EPSCoR State National Laboratory Partnerships

- Funding Opportunity Announcement DE-FOA-0001897 posted March 28
- Limitations—applicants from EPSCoR jurisdictions, one letter of intent/one application per institution

- Award size: up to $750,000 over three years
- Letters of Intent due April 25
- Applications due May 16
- Full details available at: https://science.energy.gov/bes/funding-opportunities/
Energy Frontier Research Centers
FY 2017, 2018 Enacted = $110M; FY 2019 President’s Request = $110M

Current EFRCs ($110M in FY 2017)
- 36 awards of $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
- 617 Senior Investigators
- 779 Graduate Students
- 125 Undergraduate Students
- 184 Technical Staff
- 558 Postdocs

FY 2018 Plans
- BES is recompeting the EFRC program in FY 2018, soliciting both renewal proposals from current centers with project periods that end in 2018 as well as proposals for new EFRCs. The recompetition focuses on transformative opportunities and research priorities identified in recent BESAC and Basic Research Needs reports.
- Awards expected to be announced in July 2018.

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/)
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.
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 (Ion traps, quantum dots, nitrogen vacancies, donor centers, etc.)
In light of significant progress in QIS over the past several years, SC components have held a variety of workshops to define the scientific needs and opportunities. QIS has now been identified as an important cross-cutting topic with potential impact across all SC program offices. To accelerate development of QIS and apply advances in quantum computing, sensing, and other areas to fundamental research questions, quantum information and materials have been emphasized in the DOE SC Fiscal Year 2018 Budget Request. Recent specific FY 2017 program announcements were also issued for National Laboratory-led exploration of hardware approaches to quantum testbeds and development of quantum algorithm teams.

**Through this Dear Colleague Letter, DOE SC encourages submission of innovative research ideas in QIS via any appropriate existing mechanism.** This letter does not add to the scope of any published announcement and it does not change the review criteria of any published announcement, but it should be taken as a statement of interest in encouraging activity in this field. DOE SC recommends that researchers contact program managers within the most relevant SC program office for details on appropriate programs and specifics on proposal submission; however, it is recognized that many efforts in this area are interdisciplinary and thus may undergo co-review or other joint evaluation by multiple program offices. Activities are particularly encouraged that involve collaboration between academia and DOE National Laboratories, and/or take advantage of the unique resources available in the National Laboratory system.

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 strongly-interacting 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
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
Opportunities for Basic Research at the Frontiers of XFEL Ultrafast Science

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
Funding Opportunity Released Today

- Research at the Frontiers of X-Ray Free Electron Laser Ultrafast Chemical and Materials Science
- FOA number DE FOA-0001904 and National Lab Announcement 18-1904
- Focus: small groups of investigators for support of experimental and theoretical efforts to advance ultrafast chemical and materials sciences that utilize x-ray free electron lasers
- Applications must focus on XFEL-based research and address the Priority Research Opportunities identified in the recent BES Roundtable Report, “Opportunities for Basic Research at the Frontiers of XFEL Ultrafast Science.”
- Only two applications per institution are permitted
- Funding: $300K per year to $1,500K per year for up to 3 years.

<table>
<thead>
<tr>
<th>FOA Issue Date:</th>
<th>April 2, 2018</th>
</tr>
</thead>
<tbody>
<tr>
<td>Submission Deadline for Required Letters of Intent:</td>
<td>April 30, 2018 at 5 PM Eastern Time</td>
</tr>
<tr>
<td>Submission Deadline for Applications:</td>
<td>May 21, 2018 at 5 PM Eastern Time</td>
</tr>
</tbody>
</table>
Ensure sustained U.S. leadership in the development of computational chemistry codes by

- Leveraging current leadership in a systematic effort to develop computational chemistry codes that are well adapted to anticipated exascale architecture
- Delivering open-source community codes to accurately model chemical processes using current petascale and future exascale computers

Funding

- FY 2017 included $13 M that funded 6 multi-PI awards (2 led by National Labs and 4 led by universities) and 11 single-PI university awards
- FY 2018 funding of $13M will allow continuation of current projects and initiation of 3-4 new multi-PI efforts
- FY 2019 funding of $13M will allow continuation of previously started projects
- Ongoing 4-year cycle will allow new solicitations in FY 2021 and FY 2022, pending funding availability
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

Calculation of the correct electronic charge density of anatase TiO$_2$ using quantum Monte Carlo and including temperature dependence

Ab-initio theory of decay of an optically excited electron-hole pair (red) into 2 lower energy pairs (blue), while conserving spin
Enable design of revolutionary molten salt coolants & liquid fuels
How can we characterize and predict the structure, dynamics, and energetics of molten salts including evolving chemical composition across length and time scales?

Master the hierarchy of materials design and synthesis for complex, reactor environments
How do we design, synthesize, and process superior materials able to function and perform over decades in the extreme environments of advanced nuclear reactors?

Tailor interfaces to control the impact of nuclear environments
How can the multitude of inextricably linked chemical and physical processes that occur at interfaces be controlled?

Reveal multiscale evolution of spatial and temporal processes for coupled extreme environments
How can computational and experimental techniques be integrated to bridge spatial, temporal, and energy scales that underpin materials’ behavior and chemical transformations in coupled extreme environments?

Identify and control unexpected behaviors from rare events and cascading processes
How do we identify, anticipate and control rare events that initiate cascading processes and cause aberrant properties and materials responses?
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**

- Preproposals review completed, full proposals for encouraged preproposals are due on April 4
- 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/
**Advanced Scientific Computing Research (ASCR)**

- (a) Applied Mathematics
- (b) Computer Science

**Basic Energy Sciences (BES)**

- (a) Accelerator and Detector R&D
- (b) Nuclear Chemistry and Radiochemical Separations
- (c) Neutron Scattering Research and Instrumentation
- (d) Predictive Materials Science and Chemistry
- (e) Fundamental Electrochemistry related to energy transduction, storage, chemical conversion, and corrosion
- (f) Crystal Growth
- (g) Ultrafast Materials and Chemical Sciences
- (h) Electron and Scanning Probe Microscopy Research and Instrumentation
- (i) Basic Geosciences
- (j) Gas Phase Chemical Physics
- (k) Radiation Effects in Materials
- (l) Catalysis Science with NMR Spectroscopy and Neutron Scattering
- (m) Highly Ionizing Radiation in Chemistry
- (n) Energy Transfers in Large Proteins and Protein Complexes

**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
- (e) Environmental Systems Science
- (f) Atmospheric System Research
- (g) Earth System Modeling

**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

---

**SCGSR Program: Applications are due on May 15**

*Topics based on SC’s Assessment of Workforce Development Needs and evolving needs of SC programs*
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
Funding Opportunities: FAQs

• **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 awards are allowed
  – National Lab awards are always multiple PI, except for early career

• **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

• **Delineation from other grants...**
  – You must have separate research proposals that can “stand alone” with respect to research output
On Line Resources

- **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 Report Brochures**

[Link to Online Resources]
https://science.energy.gov/bes/community-resources/overview-brochures/
Questions?