Basic Energy Sciences Update

Board on Physics and Astronomy

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For Basic Energy Sciences

25 April 2019
FY 2017 – FY 2020 BES Budget

FY 2017 Enacted: $1.871B
FY 2018 Enacted: $2.09B
FY 2019 Enacted: $2.166B
FY 2020 Request: $1.858B

Priorities:

- Continue support of core research areas, EFRCs, Hubs, and CMS/CCS
- Continue support of 12 scientific user facilities at near optimal operation level
- Expand quantum information science (an SC-wide initiative) and other research priorities following strategic planning reports
- Support facility upgrades per 2016 BESAC prioritization study
BES strategic planning activities provide the foundation for program strategy

- **Science for Discovery**
- **Science for National Needs**

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

[https://science.energy.gov/bes/community-resources/reports/](https://science.energy.gov/bes/community-resources/reports/)
Basic Energy Sciences At a Glance (2018)

BES RESEARCH SPANS
MORE THAN 150 ACADEMIC, NONPROFIT, AND INDUSTRIAL INSTITUTIONS
15 DOE NATIONAL LABORATORIES
45 STATES AND WASHINGTON, D.C.

SUPPORTED RESEARCHERS
~6,200 Ph.D. SCIENTISTS
~2,100 STUDENTS SUPPORTED

BES BY THE NUMBERS
FY 2018
BES supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels.

$787 MILLION RESEARCH BUDGET

~26% AVERAGE NEW GRANT SUCCESS RATE

OVER 1,100 CORE RESEARCH PROJECTS

$934 MILLION SCIENTIFIC USER FACILITY OPERATING BUDGET
45% OPERATIONS FOR SCIENTIFIC USER FACILITIES
17% FACILITY UPGRADES, CONSTRUCTION
38% RESEARCH
49% UNIVERSITIES
51% DOE LABS

$369 MILLION FACILITY UPGRADES, CONSTRUCTION BUDGET

46 ENERGY FRONTIER RESEARCH CENTERS

MORE THAN 16,000 USERS AT 12 BES FACILITIES

2 ENERGY INNOVATION HUBS
Basic Energy Sciences - Research
FY 2018 Highlights

Research

- FY 2018 appropriation provided new funds for FOAs in key topical areas:
  - **Quantum computing and quantum systems** research ($28M in FY 2018, 27 awards for 3 years)
  - **Ultrafast Chemical and Materials Sciences** ($10M in FY 2018, 10 awards for 3 years)
  - **Computational Chemical Sciences** ($5M in FY 2018, 10 awards for 3 years)
- Energy Frontier Research Centers were recompeted ($100M in FY 2018, 42 awards for 2 or 4 years).
- The Batteries and Energy Storage Hub, JCESR, was renewed for 5 years ($24M/year for 5 years).
- BES supported 40 **Early Career awards** ($26M in FY 2018), up from 21 awards in FY 2017 (5-year awards).
- 82 supplemental funds to 10 National Laboratories ($21M) to add inflationary increases to projects and equipment awards to enhance specific capabilities.
TITLE IV—DEPARTMENT OF ENERGY QUANTUM ACTIVITIES
SEC. 401. QUANTUM INFORMATION SCIENCE RESEARCH PROGRAM.

(a) In General.—The Secretary of Energy shall carry out a basic research program on quantum information science.

(b) Program Components.—In carrying out the program under subsection (a), the Secretary of Energy shall—

(1) formulate goals for quantum information science research to be supported by the Department of Energy;

(2) leverage the collective body of knowledge from existing quantum information science research;

(3) provide research experiences and training for additional undergraduate and graduate students in quantum information science, including in the fields of—

(A) quantum information theory;

(B) quantum physics;

(C) quantum computational science;

(D) applied mathematics and algorithm development;

(E) quantum networking;

(F) quantum sensing and detection; and

(G) materials science and engineering;

(4) coordinate research efforts funded through existing programs across the Department of Energy, including—

(A) the Nanoscale Science Research Centers;

(B) the Energy Frontier Research Centers;

(C) the Energy Innovation Hubs;

(D) the National Laboratories;

(E) the Advanced Research Projects Agency; and

(F) the National Quantum Information Science Research Centers; and

(5) coordinate with other Federal departments and agencies, research communities, and potential users of information produced under this section.

The bill directs the President to implement a 10-year National Quantum Initiative Program.

The bill defines QIS as the storage, transmission, manipulation, or measurement of information that is encoded in systems that can only be described by the laws of quantum physics.
Department of Energy

The Committee recognizes DOE’s capabilities, research infrastructure, and expertise in materials science, physics, applied mathematics, and computer science provide a foundation for significant advances in QIS research and technological development. In particular, the DOE National Laboratories, which operate world class, open-access user facilities around the country, provide access to the supercomputers, x-ray light sources, photon sources, and neutron sources that are necessary to conduct ground-breaking quantum research. … The Committee supports DOE’s current efforts to increase investment in QIS across the Office of Science, including for proposed programs in Biological and Environmental Research, High Energy Physics, Nuclear Physics, Basic Energy Sciences, and Advanced Scientific Computing Research (ASCR), as requested in the President’s fiscal year 2019 Budget.

Sec. 402. National Quantum Information Science Research Centers

This section directs the DOE Office of Science to establish and operate up to five National Quantum Information Science Research Centers to conduct basic research to accelerate scientific breakthroughs in quantum information science and technology. This section also outlines criteria for establishment, collaborations, and other requirements. The Centers are directed to carry out activities for a period of five years. This section authorizes appropriations of $625,000,000 over five years for the Office of Science to carry out this section, which shall include $125,000,000 for each fiscal years 2019 through 2023.

https://www.congress.gov/115/bills/hr6227/BILLS-115hr6227enr.pdf
Quantum Information Science Activities in BES

- **Next Generation Quantum Systems**: Develop understanding leading to control of quantum phenomena in chemical and materials systems to advance quantum-based science and technology.

- **Quantum Computing**: Develop quantum computing algorithms and utilize emerging quantum computing capabilities to address major scientific problems in chemical and materials sciences.

- **User Capabilities**: Research and infrastructure at the Nanoscale Science Research Centers, enabling next-generation qubit concepts, innovative quantum and classical architectures.

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**BES Contributions to QIS**

- Fundamental Science
- DOE Community Resources
- Tools, Equipment, Instrumentation

**QIS Applications for BES**

- Quantum Computing
- Analog Quantum Simulation
- Quantum Sensing and Microscopy
Energy Frontier Research Centers

Accomplishments (Aug 2009 – May 2018)
- Over 10,500 peer-reviewed scientific publications
- ~100 companies have benefited from EFRC research
- At least 160 patents issued

Current EFRC Members
- ~670 senior investigators and ~1,100 postdoctoral associates, graduate students, undergraduate students, and technical staff at 115 institutions

FY 2020 Funding Opportunity Announcement (~$40M)
- Recompetition of four-year EFRC awards made in FY2016, which focused on science relevant to DOE’s environmental management mission.
- Solicitation of proposals for new EFRCs that are responsive to recent BES workshop reports, including use-inspired science relevant to advanced microelectronics and quantum information science (QIS).
Topical Distribution of 46 Current EFRC Awards

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

**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.

**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.

**Environmental Management** – Scientific understanding to improve the cleanup and long-term storage of nuclear waste.

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

**Quantum Materials** – Novel materials for innovative electronics, sensors, and communications.
DOE Office of Basic Energy Sciences: Scientific User Facilities

- 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)

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

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

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
More than 300 companies from various sectors of the manufacturing, chemical, & pharmaceutical industries conducted research at BES scientific user facilities. Over 30 companies were Fortune 500 companies.
Successful Demonstration of Fastest Electron Detector Ever Made (Feb 12, 2019)

Accomplishment
Successful installation and testing of the new 4D Camera that can produce continuous electron images every 11 microseconds. That’s about 60X faster than what was possible with previous high speed electron detectors.

Unique Advances Enabled
87,000 frames/second, optimized for high dynamic range through speed and sensitivity

Impact of the New Capability
- Acquisition of pixelated images during high resolution STEM imaging without slowing down the electron probe, leading to real-time phase contrast ptychographic imaging
- Drift mitigation and improvements in signal/noise for beam-sensitive samples (ie- biomolecules)
- Breakthroughs in nanoscale strain mapping and quantification of materials using scanning electron diffraction imaging methods at high resolution
- All data will be streamed in real time via a 400 Gbps 1 km optical link to the Cori supercomputer at NERSC for inline processing and analysis.

Light Sources: Global Race to the Top
60+ Facilities Worldwide and Growing

Many other new & upgraded facilities are in the design stage...
Take Away Message: It’s a very competitive landscape!

APS
ALS
NSLS-II
SSRL
LCLS
BES Light Sources
Ring Upgrades

Japan: SPring-8-II
Germany: PETRA 3/4
Brazil: SIRIUS, 2019
France: ESRF II, 2022
Sweden: MAX-IV, 2016

China: BLS

SACLA FEL 2011
8.5 GeV, 30 Hz NC
PAL XFEL 2016
10 GeV, 60 Hz NC
EU XFEL 2017
17.5 GeV, 3000 x 10 Hz SC

Upgraded & New FELs
New Rings
Ring Upgrades
LCLS is a 2-mile long atomic & molecular camera with a femtosecond “shutter speed”

LCLS operates 24 hours/day with 95% beam availability as an open-access User Facility for the DOE Office of Science.
Future Outlook: LCLS-II will increase the X-ray repetition rate from 120 Hz to 1 MHz, bringing transformative capabilities to the fields of atomic, chemical, material and plasma science.
<table>
<thead>
<tr>
<th>Project</th>
<th>ANL APS-U</th>
<th>LBNL ALS-U</th>
<th>ORNL SNS PPU</th>
<th>ORNL SNS STS</th>
<th>SLAC LCLS-II</th>
<th>SLAC LCLS-II-HE</th>
</tr>
</thead>
</table>

**Current Status of Facility**

<table>
<thead>
<tr>
<th>Worldwide Competition</th>
<th>Status Q2/19</th>
<th>FY19 Approp</th>
</tr>
</thead>
<tbody>
<tr>
<td>EU ESRF Germany PETRA3,4 Japan SPring-6 China HEPS</td>
<td>CD-2 CD-3B</td>
<td>✔</td>
</tr>
<tr>
<td>Sweden MAX-IV Brazil SIRIUS CH SLS-II</td>
<td>CD-1</td>
<td>✔</td>
</tr>
<tr>
<td>EU ESS Japan JPARC China CSNS UK ISIS</td>
<td>CD-1 CD-3A</td>
<td>✔</td>
</tr>
<tr>
<td>EU ESS Japan JPARC China CSNS UK ISIS</td>
<td>CD-0</td>
<td>✔</td>
</tr>
<tr>
<td>EU XFEL Japan SACLA Korea PAL XFEL CH Swiss FEL</td>
<td>CD-3</td>
<td>✔</td>
</tr>
<tr>
<td>EU XFEL China SCLF</td>
<td>CD-1</td>
<td>✔</td>
</tr>
</tbody>
</table>
### SC Critical Decision Matrix

**TOTAL PROJECT COST (TPC)**

<table>
<thead>
<tr>
<th>DECISION / REQUIREMENTS / APPROVAL</th>
<th>Prior to CD0, Approve Mission Need Statement</th>
<th>Delegation Allowed</th>
</tr>
</thead>
<tbody>
<tr>
<td>$750M or more</td>
<td>Reviewed by SC-28 (SC-28)</td>
<td>Reviewed by SC-28</td>
</tr>
<tr>
<td>Less than $750M to $400M</td>
<td>Approved by SC-1</td>
<td>Approved by SC-1</td>
</tr>
<tr>
<td>Less than $400M to $100M</td>
<td>Reviewed by SC-28 (SC-28)</td>
<td>Reviewed by SC-28</td>
</tr>
<tr>
<td>Less than $100M to $50M*</td>
<td>Approved by SC-1</td>
<td>Approved by SC-1</td>
</tr>
<tr>
<td>Less than $50M* to $20M</td>
<td>Reviewed by SC-28 (SC-28)</td>
<td>Reviewed by SC-28</td>
</tr>
<tr>
<td>Less than $20M to $10M**</td>
<td>Delegation Allowed</td>
<td>Reviewed by SC-28</td>
</tr>
</tbody>
</table>

**PRIOR TO CD-4—PROJECT COMPLETION**

<table>
<thead>
<tr>
<th>CRITICAL DECISIONS</th>
<th>Changes to TPC</th>
<th>Deviations</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD-0—APPROVE MISSION NEED</td>
<td>SC-1</td>
<td>SC-1</td>
</tr>
<tr>
<td>CD-1—APPROVE ALTERNATIVE SELECTION AND COST RANGE</td>
<td>SC-1</td>
<td>SC-1</td>
</tr>
<tr>
<td>CD-2—APPROVE PERFORMANCE BASELINE</td>
<td>SC-2</td>
<td>SC-2</td>
</tr>
<tr>
<td>CD-3—APPROVE START OF CONSTRUCTION</td>
<td>SC-1</td>
<td>SC-1</td>
</tr>
<tr>
<td>CD-4—APPROVE START OF OPERATIONS OR PROJECT COMPLETION</td>
<td>SC-1</td>
<td>SC-1</td>
</tr>
</tbody>
</table>

**BASELINE MANAGEMENT**

- No TPC Change
- Routine / Project / Event
- Changes to TPC

<table>
<thead>
<tr>
<th>CRITICAL DECsISIONS</th>
<th>No TPC Change</th>
<th>Routine Change</th>
<th>Changes to TPC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mission Validation Independent</td>
<td>SC-AD</td>
<td>Team External to Project</td>
<td></td>
</tr>
<tr>
<td>Design Review Prior to CD-1</td>
<td>SC-AD</td>
<td>Team External to Project</td>
<td></td>
</tr>
<tr>
<td>Conduct Independent Project Prior to CD-2</td>
<td>SC-AD</td>
<td>Team External to Project</td>
<td></td>
</tr>
<tr>
<td>SC-AD Request Annual Peer Review</td>
<td>SC-AD</td>
<td>Team External to Project</td>
<td></td>
</tr>
<tr>
<td>Performance Baseline Deviation</td>
<td>SC-2</td>
<td>Team External to Project</td>
<td></td>
</tr>
</tbody>
</table>

**EVMS Review—Certification Prior to CD-3 & Bi-annual Surveillance (annual by contractor)**

<table>
<thead>
<tr>
<th>CRITICAL DECISIONS</th>
<th>SC-28</th>
<th>SC-28</th>
<th>SC-28</th>
<th>SC-28</th>
</tr>
</thead>
<tbody>
<tr>
<td>ORR/RA—Operational Readiness Review/Readiness Assessment Prior to CD-4</td>
<td>Team External to Project</td>
<td>Team External to Project</td>
<td>Team External to Project</td>
<td>Team External to Project</td>
</tr>
<tr>
<td>Technology Readiness Assessment (TRA) prior to CD-2 and 3 by SAE or AE</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Project Definition Rating Index (PDRI) by APM</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>Hazard Cat. 1, 2, 3 Nuclear Facility—Technical IPR Prior to CD-3</td>
<td>PSO</td>
<td>PSO</td>
<td>PSO</td>
<td>PSO</td>
</tr>
</tbody>
</table>

**REPORTING**

<table>
<thead>
<tr>
<th>CRITICAL DECISIONS</th>
<th>Monthly PARS II Reporting (EVMS for Projects&gt;$20 M)</th>
<th>Monthly or Quarterly Project Reporting (QPR) or Meeting after CD-0</th>
</tr>
</thead>
<tbody>
<tr>
<td>SC-AD</td>
<td>SC-AD to invite SC-28</td>
<td>SC-AD to invite SC-28</td>
</tr>
<tr>
<td>APM</td>
<td>PSO</td>
<td>PSO</td>
</tr>
<tr>
<td>SC-2</td>
<td>PSO</td>
<td>PSO</td>
</tr>
</tbody>
</table>

**Project Status**

- After CD-0 and EV After CD-2
- After CD-0
- After CD-0

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**CD-0 Approve Mission Need**

**CD-1 Approve Alternative Selection and Cost Range**

**CD-2 Approve Performance Baseline**

**CD-3 Approve Start of Construction**

**CD-4 Approve Start of Operations or Project Completion**

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Note: If performance, scope, schedule, or cost baseline at CD-2 cannot be met, then SC-1 and SC-2 must be notified & a determination made to terminate the project or establish a new performance baseline.
BES Construction/MIE Funding Profile 1984 – 2019
I am asking BESAC to form a subcommittee to assess the scientific justification for a U.S. domestic high-performance reactor-based research facility, taking into account current international plans and existing domestic facility infrastructure.

- What is the merit and significance of the science that could be addressed by a high performance, steady-state reactor, and what is its importance in the overall context of research in materials sciences and related disciplines?
- What are the capabilities of other domestic and international facilities, existing and planned, to address the science opportunities afforded by such a domestic research reactor?
- What are the benefits to other fields of science and technology and to industry of establishing such a capability in the U.S.? In particular, consider applications such as isotope production, materials irradiation, neutron imaging, dark matter research, and neutron activation for trace element analysis.
- What are the strengths and limitations of a steady-state research reactor compared to a pulsed spallation neutron source for science, engineering, and technology?
- Are there feasible upgrade paths for HFIR to provide world-leading capabilities in serving the Office of Science missions well into the future?
- Can Low Enriched Uranium (LEU) and High Assay LEU (HALEU) fuels (defined as<20% enriched U-235) replace Highly Enriched Uranium fuels in research reactors while preserving the needed characteristics of neutrons produced by steady-state reactors? What R&D would be needed to support LEU and HALEU fuels development?
Upcycling: the process of selectively converting waste materials into products with greater value as opposed to traditional recycling which typically converts waste into materials for reuse but with reduced properties (downcycling)

This Roundtable will focus on four challenges and research opportunities for chemical upcycling of polymers that build off the strengths in BES portfolio

- Design chemical mechanisms to deconstruct polymers and create targeted molecular intermediates that provide building blocks for new products
- Create integrated depolymerization-reassembly processes that target high-value end products from starting polymers
- Design next-generation polymeric materials that enable efficient depolymerization-reassembly
- Investigate crosscut opportunities for advancing experimental, computational and data science driven approaches for upcycling of polymers
Motivation for Chemical Upcycling of Polymers

- In the US, plastic materials contribute 13% (34.5M tons) to municipal solid wastes in 2015 with less than 10% recycled, approximately 15% combusted for energy recovery, and the remained sent to the landfill (75%)\(^1\)
- Most recycling of plastic wastes typically involves mechanical processes (primary or secondary recycling: sort, grind, wash, extrude) and is only applied to limited plastic types but the products are cheaper than new materials
- More energy is saved by recycling than recovered by burning plastic (heating value of plastics 36 MJ kg\(^{-1}\) while mechanical recycling conserves 60 – 90 MJ kg\(^{-1}\))
- On average, each tonne of plastic recycled saves the energy equivalent in the combustion of 22 barrels of oil\(^2\)
- Increased plastic recycling is an important pathway to reduce plastic waste and has clear energy, economic, and environmental impacts
- Opportunity exists for fundamental research to provide the foundational knowledge needed to design chemical reactions, processes, and materials that enable efficient, low-temperature conversion of discarded plastics to high-value chemicals or materials

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\(^2\) Rahimi, A.; Garcia, J. M. Nat. Rev. Chem. 2017, 1, Article Number 0046
Globally Plastics are Growing

- If plastic production continues its current growth rate, then the plastics industry may account for 20% of the world’s total oil consumption.
- In 2015, global plastic waste disposal:
  - Discard: 55%; Recycle: 19.5%; Incineration: 25.5%


• Packaging is the largest use for plastics but single use:
  – Plastics used in packaging include: LDPE (30%), PET (23%), HDPE (21%), PP (18%), PS (5%), and PVC (2%)

• If current trends continue, by 2050, the ocean will contain more plastic than fish, by weight  
  (UNEP (2018). Single Use Plastic: A Road Map for Sustainability

Global Flow of Packaging Waste
40% Landfill
32% Leakage
14% Incinerated
14% Recycled

Majority of Plastics (87%) Fall into Categories 1-6
Recovery Rates for Plastic Recycling in US are Low

<table>
<thead>
<tr>
<th>Category</th>
<th>Common Products</th>
<th>Recycled Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>PETE</td>
<td>Polyethylene Terephthalate</td>
<td>clothing, carpet, clamshells, soda &amp; water bottles</td>
</tr>
<tr>
<td>HDPE</td>
<td>High-Density Polyethylene</td>
<td>milk jugs, detergent &amp; shampoo bottles, flower pots, grocery bags</td>
</tr>
<tr>
<td>PVC</td>
<td>Polyvinyl Chloride</td>
<td>cleaning supply jugs, pool liners, twine, sheeting, automotive product bottles, sheeting</td>
</tr>
<tr>
<td>LDPE</td>
<td>Low-Density Polyethylene</td>
<td>bread bags, paper towels &amp; tissue overwrap, squeeze bottles, trash bags, six-pack rings</td>
</tr>
<tr>
<td>PP</td>
<td>Polypropylene</td>
<td>yogurt tubs, cups, juice bottles, straws, hangers, sand &amp; shipping bags</td>
</tr>
<tr>
<td>PS</td>
<td>Polystyrene</td>
<td>to-go containers &amp; flatware, hot cups, razors, CD cases, shipping cushion, cartons, trays</td>
</tr>
<tr>
<td>OTHER</td>
<td>Other</td>
<td>Common types &amp; products: polycarbonate, nylon, ABS, acrylic, PLA; bottles, safety glasses, CDs, headlight lenses</td>
</tr>
</tbody>
</table>

| Recovery Rates | 19.5% | 10% | 0% | 5% | 1% | 1% | varies |

The single Recommendation from the BES40 report asked BES to be bold in choosing new research and facilities to support and experimenting with new funding mechanisms where appropriate. This recommendation is especially timely in view of intensifying globalization in research talent and resources. ... I am writing to ask BESAC to provide input on possible implementation strategies, especially in the context of keeping pace with international competition.

- Within the BES-supported topical research areas and facility capabilities, in which areas and capabilities is U.S. leadership most threatened, presently or in the foreseeable future?
- To preserve and foster U.S. leadership with resource constraints, what are the key efficiencies and balances that should be sought?
- For someone deciding whether to pursue a scientific career, or a mature scientist considering whether to stay in the U.S., how can BES programs and facilities be structured and managed to create incentives that will attract and retain talents? What are the key attractions and deterrents of a career in BES-supported science areas? How can the mix of research funding modalities be designed to enhance the attractions and minimize the deterrents?