U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences Overview

MRS Spring Meeting

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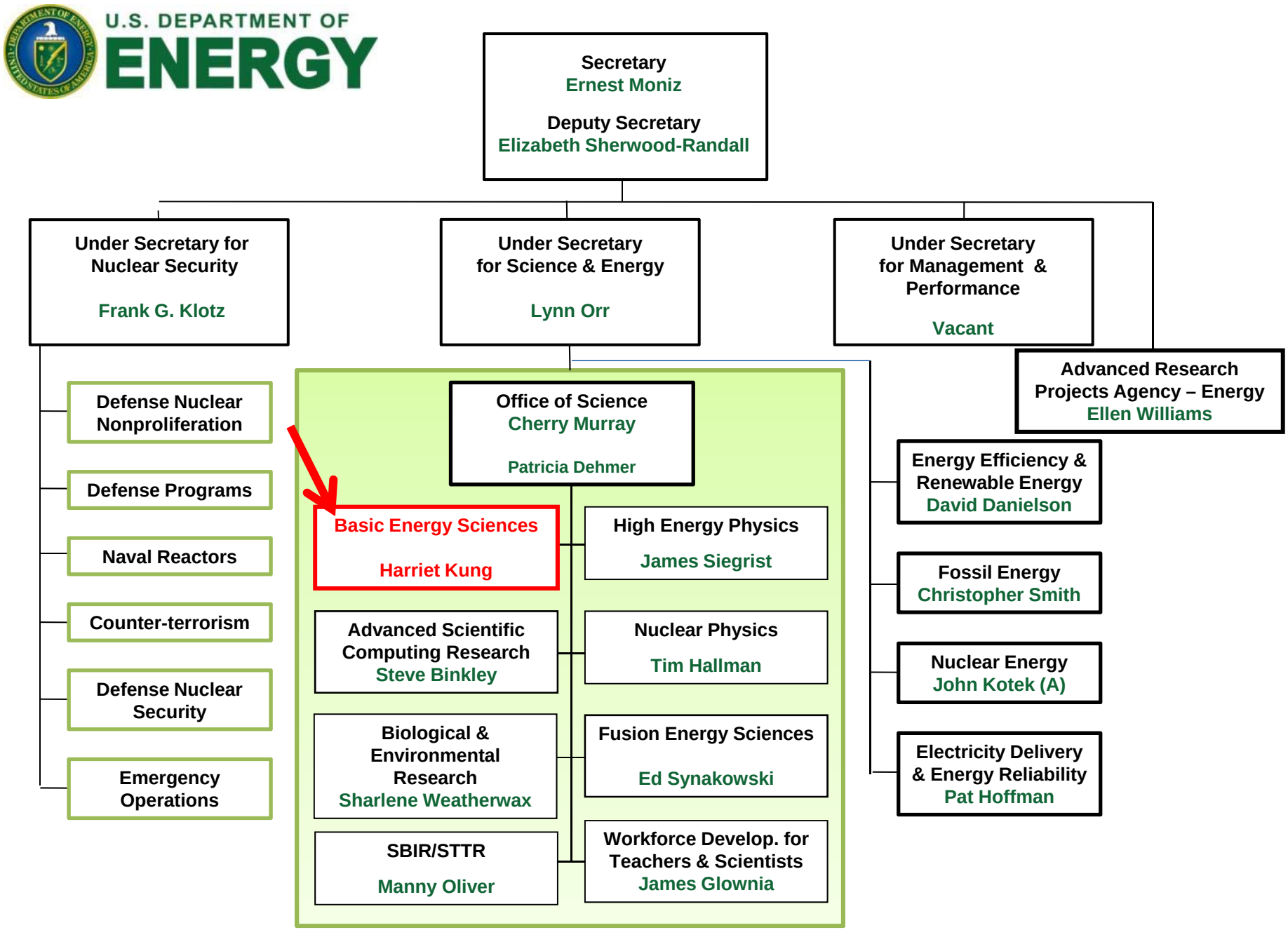
Department of Energy

Outline

- DOE and BES Overview
- BES Strategic Planning
- Funding Modalities and Opportunities
  - Core Research Program
  - Early Career Research Program
  - Energy Frontier Research Centers
  - Computational Materials & Chemical Sciences
  - Graduate Student Research Program
- BES User Facilities
- Where to Find More Information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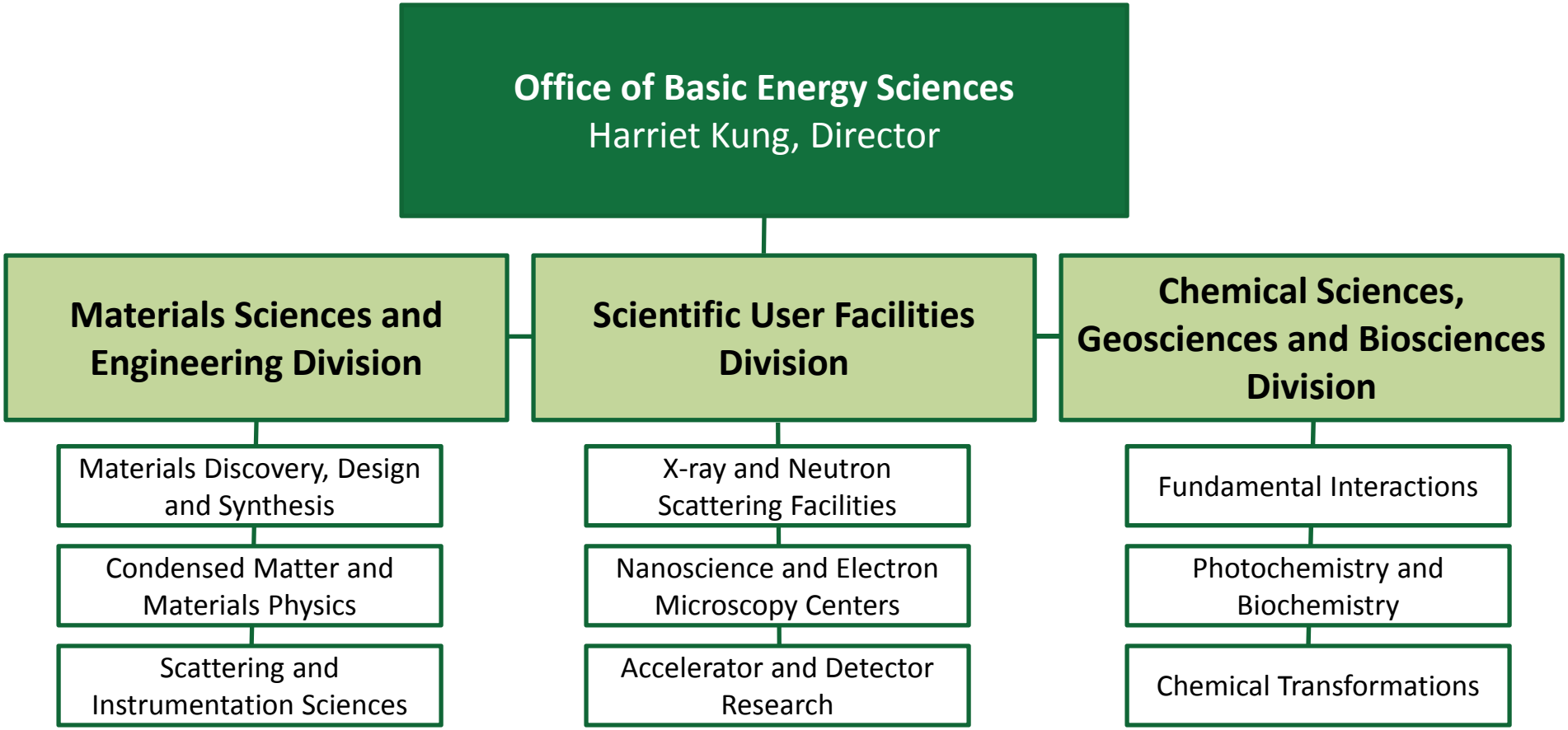
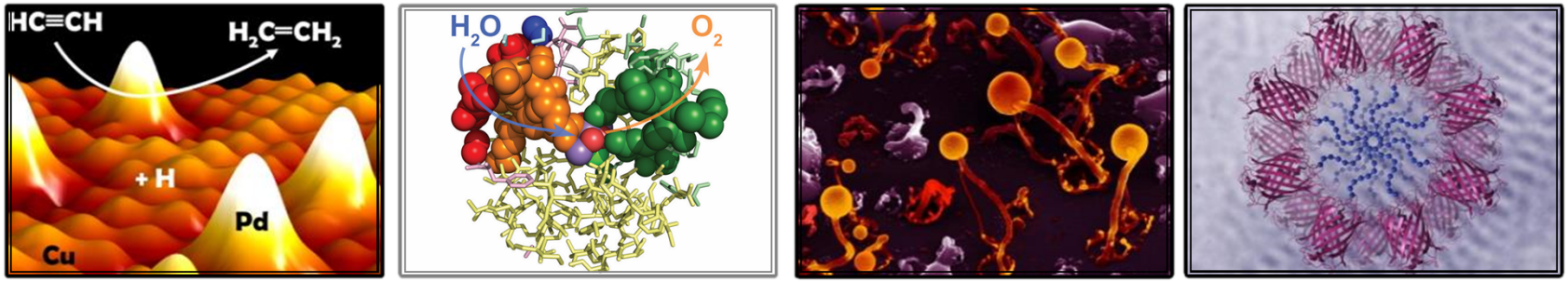


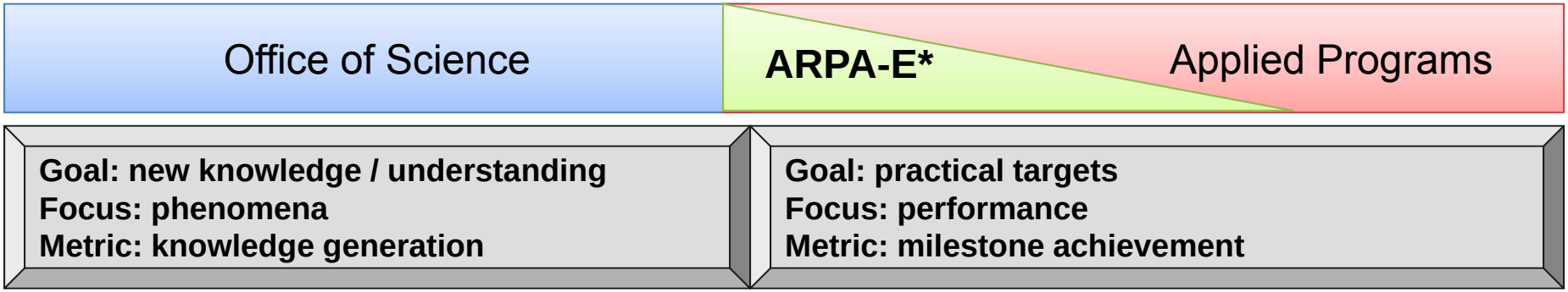
Research grouped by scientific topics -- not by specific energy technologies – theory, modeling, and simulation crosscuts programs and are often integrated with experimental research

Basic Energy Sciences Mission

- Fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels
- Provide the foundations for new energy technologies to support DOE's missions in energy, environment, and national security
- Plan, construct, and operate world-leading scientific user facilities for the Nation



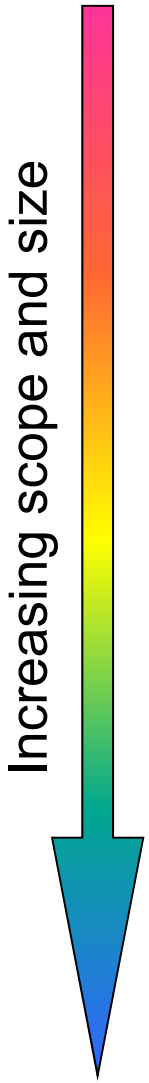
Continuum of Research, Development, and Deployment in DOE



- Basic research to address fundamental gaps in current theories and descriptions of nature at the level of electrons, atoms, and molecules
- Basic research for discovery and fundamental new understanding of chemical, physical, material, geological, and biological systems that may lead to revolutionary new energy technology in the future
- Basic research with the goal of addressing scientific showstoppers to real-world applications in energy technologies
- Proof of new, higher-risk concepts
- Prototyping of new technology concepts
- Explore feasibility of scale-up of demonstrated technology concepts in a "quick-hit" fashion
- Research with the goal of meeting *technical milestones*, with emphasis on the development, performance, cost reduction, and durability of materials and components or on efficient processes
- Scale-up research
- Small-scale and at-scale demonstration
- Cost reduction
- Manufacturing R&D
- Deployment support, leading to market adoption
- High cost-sharing with industry partners

* ARPA-E: targets technology gaps, high-risk concepts, aggressive delivery times

BES Research Activities



- **Core Research (>1,300 projects)**
  Single investigators ($150K/year) and small groups ($500K-$2M/year) engage in fundamental research related to any of the BES core research activities. Investigators propose topics of their choosing.

- **Energy Frontier Research Centers (32)**
  $2-4M/year research centers for 4-year award terms; focus on fundamental research described in the Basic Research Needs Workshop reports.

- **Computational Materials and Chemical Sciences (3)**
  $2-4M/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

- **Energy Innovation Hubs (2)**
  Research centers for 5-year award terms, established in 2010 ($15-25M/year), engage in basic and applied research, including technology development, on a high-priority topic in energy that is specified in detail in an FOA. Project goals, milestones, and management structure are a significant part of the proposed Hub plan.

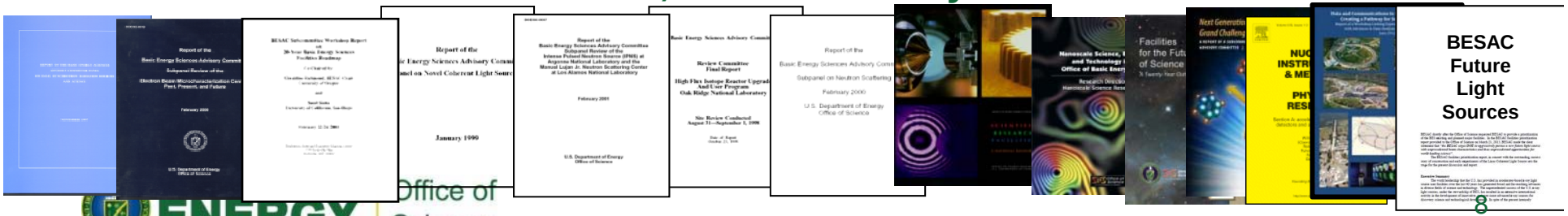
BES Strategic Planning Activities

- **Science for Discovery**

2015

- **Science for National Needs**

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



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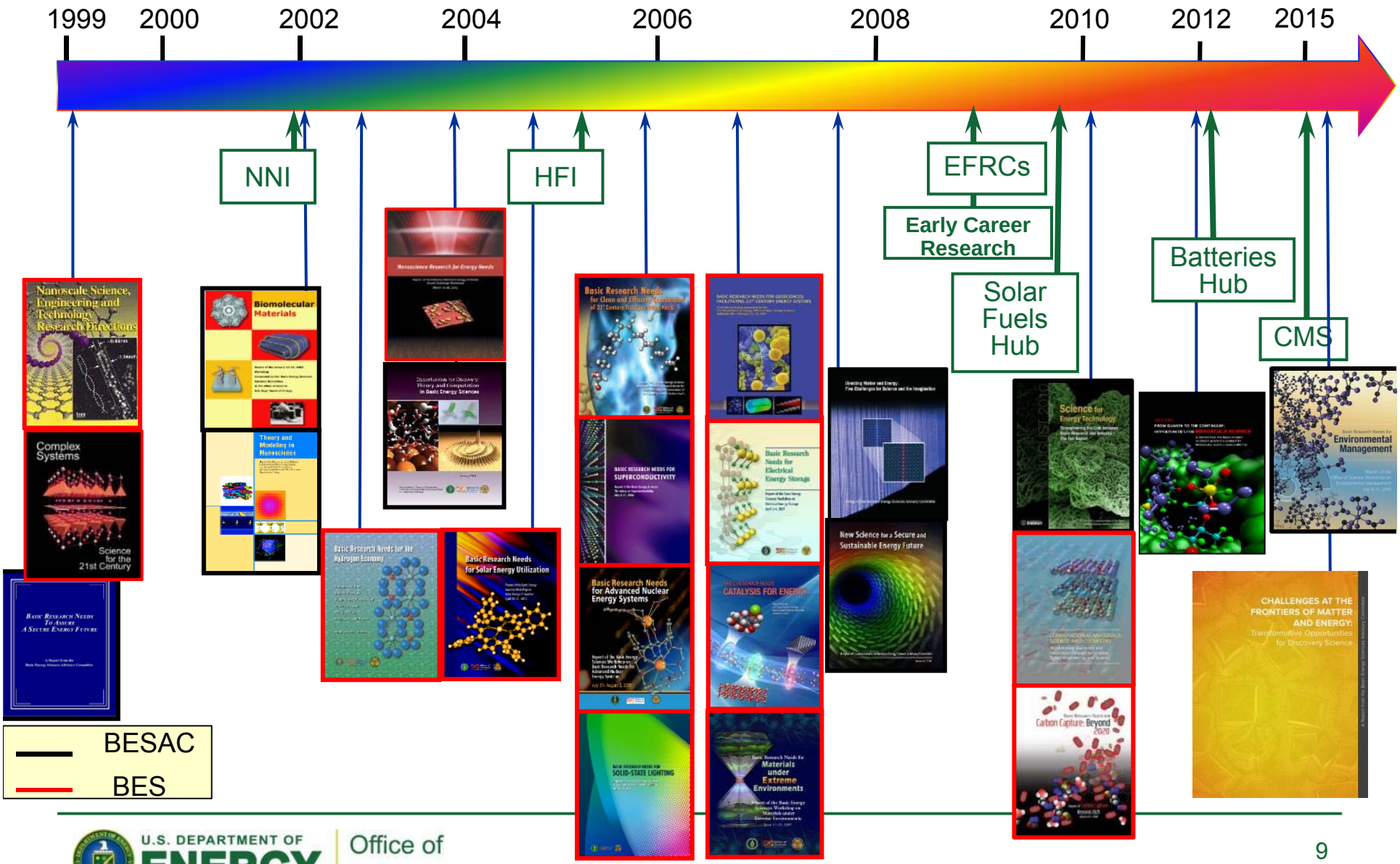
http://science.energy.gov/bes/news-and-resources/reports/

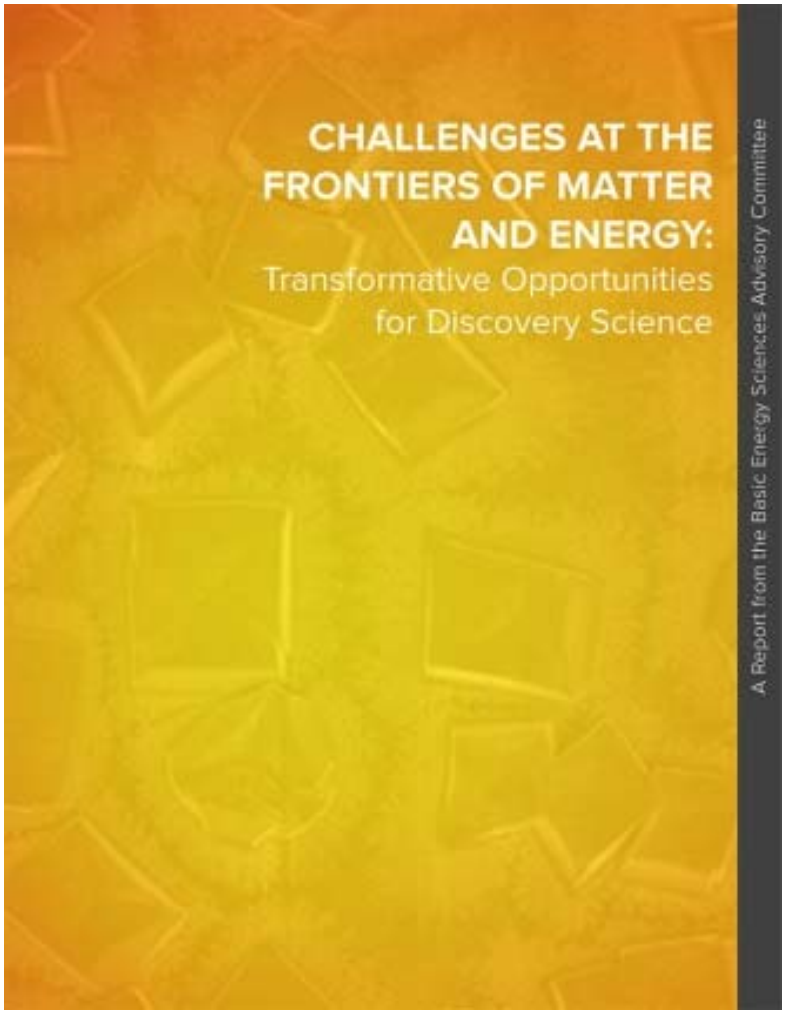
BES Strategic Planning and Program Development



http://science.energy.gov/bes/news-and-resources/reports/

Challenges at the Frontiers of Matter and Energy:
Transformative Opportunities for Discovery Science

"The most exciting phrase to hear in science, the one that heralds new discoveries, is not 'Eureka!' but 'That's funny...'" —*Isaac Asimov*



Mastering Hierarchical Architectures and Beyond-Equilibrium Matter

Beyond Ideal Materials and Systems: Understanding the Critical Roles of Heterogeneity, Interfaces and Disorder

Harnessing Coherence in Light and Matter

Crosscutting Opportunities

Revolutionary Advances in Models, Mathematics, Algorithms, Data, and Computing

Exploiting Transformative Advances in Imaging Capabilities Across Multiple Scales

Follow-up Basic Research Needs Workshops

February 8 – 10, 2016

- Basic Research Needs for Quantum Materials for Energy Relevant Technology

May 2016

- Basic Research Needs for Synthesis Science

June 2016

- Basic Research Needs for Innovation and Discovery of Transformative Experimental Tools

Fall 2016

- Basic Research Needs for Efficient Energy Conversion and Use

FY 2016 BES Budget Appropriation

Research programs

- Energy Frontier Research Centers ($110M; Δ = +$10M)
- Computational Materials Sciences ($12M; Δ = +$4M)
- Core Research & Hubs at ~FY 2015 level ($558.5M)
- Ammonia synthesis ($3M) FOA for university awards to come in April

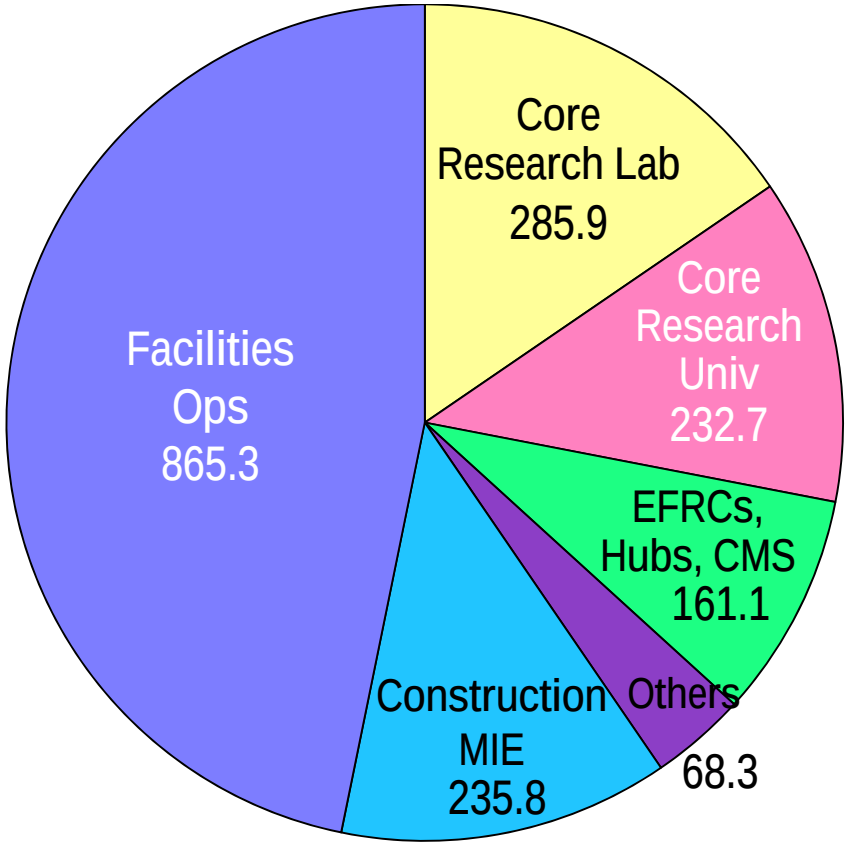
Scientific user facilities

- All full operating facilities at near optimal operations ($865.3M)
- NSLS-II 1st year of full operations ($110M)

Construction and instrumentation

- NSLS-II instrumentation (NEXT) ($15.5M)
- Advanced Photon Source Upgrade ($20M)
- Linac Coherent Light Source-II ($200.3M; Δ = +$52.3M)

FY 2016 Appropriation: $1,849 M (+$115.8M from FY 2015)



MSE and CSGB New and Renewal Success Rates –
FY 2014 Implementation of Full Funding of Financial Assistance Awards

To comply with full funding of all awards under $1M*, the two research divisions are making a concerted effort to use all available options, including shortened budget periods, "terminal renewals," and no cost extensions (NCE) to maintain quality and portfolio balance. There are noticeable reductions in success rates in FY14 largely attributable to full funding requirement.

MSE	New Grant Success Rate	Renewal Grant Success Rate
2006 - 2008	24%	84%
2009 - 2011	22%	82%
2012 - 2014	18%	71%
2014	15%	65%

CSGB	New Grant Success Rate	Renewal Grant Success Rate
2005 - 2007	38%	76%
2008 - 2010	49%	82%
2011 - 2013	36%	74%
2014	19%	68%

* Consolidated and Further Continuing Appropriations Act, 2015 (H.R. 83), SEC. 307. Notwithstanding section 301(c) of this Act, none of the funds made available under the heading "Department of Energy—Energy Programs—Science" may be used for a multiyear contract, grant, cooperative agreement, or Other Transaction Agreement of $1,000,000 or less unless the contract, grant, cooperative agreement, or Other Transaction Agreement is funded for the full period of performance as anticipated at the time of award.

Office of Science Early Career Research Program

Office of Science Early Career Research Program – Started in FY10

- **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
- **Awardees**: Over 6 years, BES has made 158 awards out of a total of 356 awards for the Office of Science.

Overall demographics of BES Awards:

- 30% female and 70% male
- 73% university and 27% DOE lab awards
- Average 5.5 years post Ph.D.
- Average success rate of 4.8%

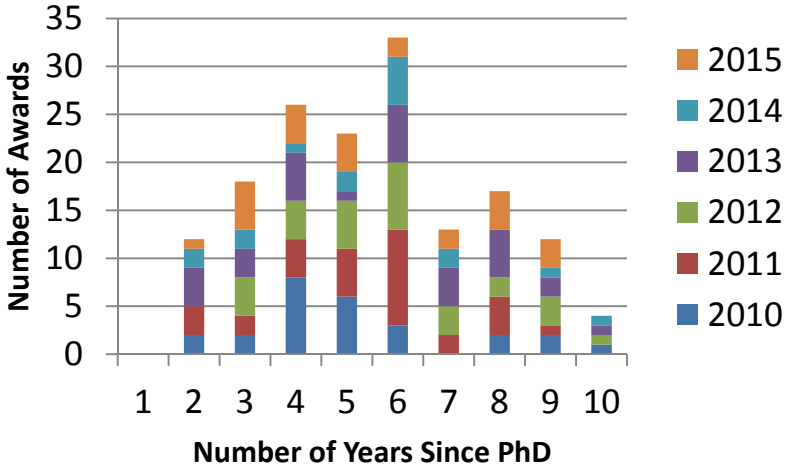
Early Career Research Program Timeline

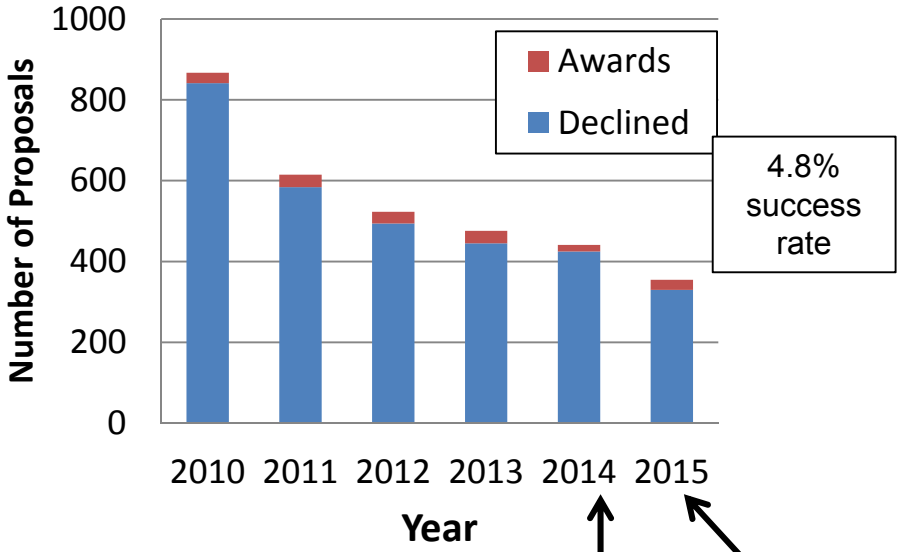
Step	Date	Time	Notes
Issue Solicitation:	Jul 31, 2015		mid-summer
Due date for Preproposals:	Sep 10, 2015	5 PM Eastern	6 weeks for PIs to write preproposals
Encourage / Discourage Decisions:	Oct 8, 2015	5 PM Eastern	4 weeks for DOE to decide
Due date for Proposals:	Nov 19, 2015	5 PM Eastern	8 weeks for PIs to write proposals
Target Award Start Date:	Jul 15, 2016		

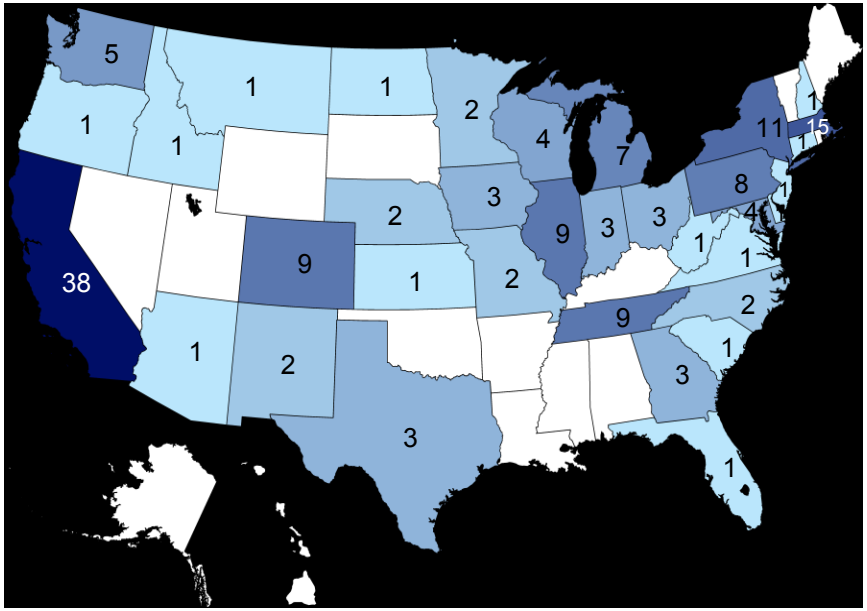
The schedule above is fairly typical of the Early Career Research Program, so look for the FY2017 solicitation in summer 2016.

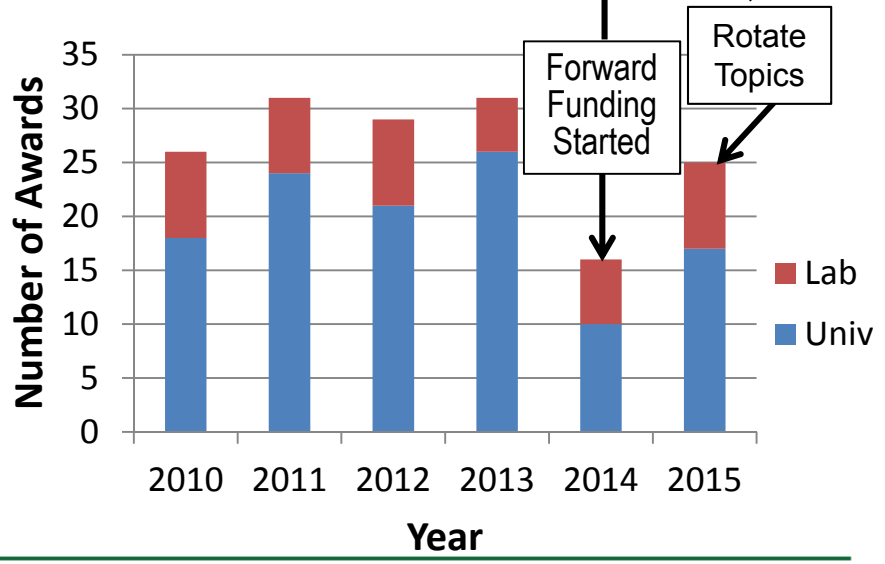
Snapshot of BES Early Career Research Program Awards

158 Awards in 35 States, 12 National Laboratories, and 64 Universities





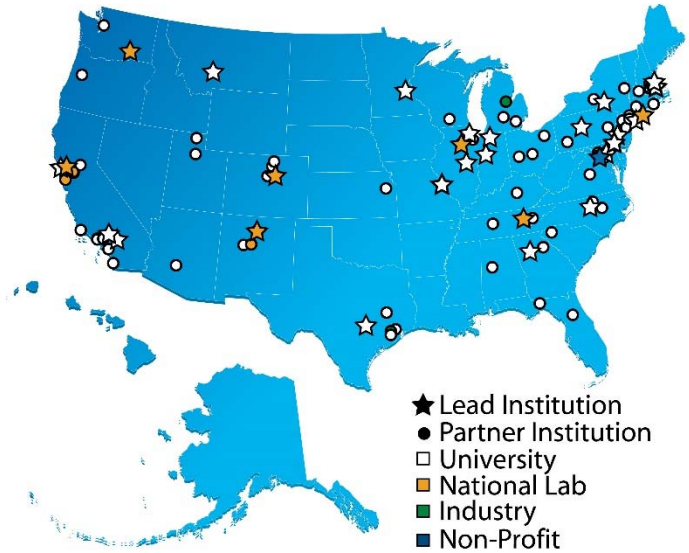




Energy Frontier Research Centers
History and Current Status

Current EFRCs ($100M in FY 2015)

- 32 awards of $2-4M per year for 4 years (22 renewal, 10 new centers)
- Lead institutions by type: 23 universities; 8 DOE National Laboratories; 1 nonprofit organization
- Over 100 participating institutions, located in 33 states plus the District of Columbia



EFRCs 2009 – 2014 ($100M/year + $277M ARRA)

- 46 EFRCs of $2-5M per year for 5 years

Current EFRC Members

- 530 senior investigators and at least 1250 additional researchers, including postdoctoral associates, graduate students, undergraduate students, and technical staff
- >200 scientific advisory board members from 12 countries and 39 companies

Accomplishments since 2009

- Over 6,500 peer-reviewed papers
- 41 EFRCs have created over 335 US and 210 foreign patent applications, more than 125 patent/invention disclosures, and at least 80 licenses
- ~85 companies have benefited from EFRC research
- EFRC students and staff now work in:
  >425 university faculty and staff positions;
  >550 industrial positions;
  >225 national labs, government, and non-profit positions

Competition in FY 2016: $10M for new EFRCs

Characteristics of a Successful EFRC

A compelling mission
that everyone understands and embraces

Active management
to evaluate progress and redirect resources in response to promising new opportunities

Team-based basic research
that would not be attempted by individual investigators

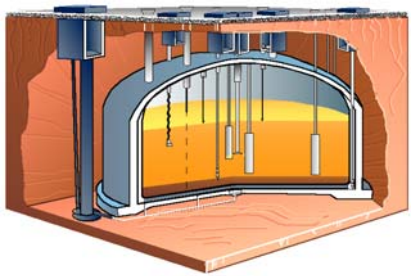
Synergy
among researchers working toward collectively developed objectives.

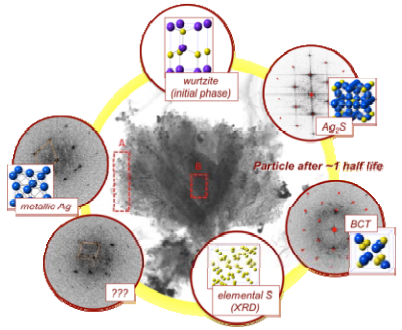
Accelerated success and failure
enabling adjustments and key decisions that lead to the most impactful science

Training the next generation of scientists
in collaborative research, including students, postdocs and other early-career scientists.

Energy Frontier Research Centers FOA ($10M)

- Intent of the FOA is to support multi-disciplinary basic research teams in two topical areas of relevance to the DOE environmental management mission:
  - Novel and innovative methods for characterization, transformation, and separation of nuclear waste
  - New materials for long-term storage of nuclear waste, including waste forms
- Applications must:
  - Address relevant Priority Research Directions identified in the *Basic Research Needs for Environmental Management* report
  - Address BESAC "grand challenges" and embody "transformative opportunities"
- Funding level per Award: $2M to $4M per year for 4 years
- One Letter of Intent/Application per institution and per lead PI/Director
- Important dates:
  - **Required Letter of Intent Due: 3/9/2016**
  - **Application Due: 4/19/2016**



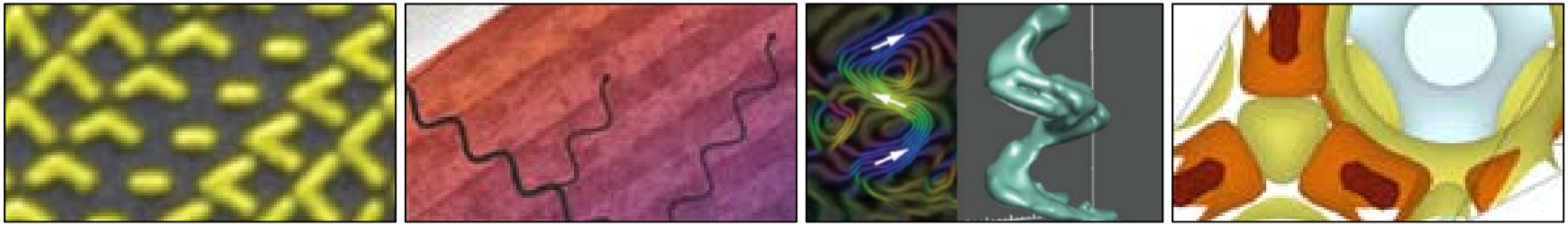


Theory and Computational Materials Science

- Part of DOE's contribution to the Materials Genome Initiative for Global Competitiveness (MGI).
- Improved theory and computational methods validated by experiments.
- Software and databases will be usable by a broad community in universities, government and the private sector.

Starting in FY 2015, "Computational Materials Sciences" supports research at $8M/year for four years.

- Research by integrated, multidisciplinary teams to develop validated software and data bases for predictive design of functional materials.
- Additional funds of $4M/year in FY 2016.



FY 2016 Computational Materials Sciences FOA ($4M)

Focus on materials and software not supported by 2015 awards

- Applications from integrated teams (materials theory, modeling, computation, synthesis, characterization) must:
  - Address a specific class of functional materials
    - *Explicitly excluded are structural, thermoelectric, and energy storage materials; structural properties; and synthesis of 2-D layered materials, assemblies of nanoparticles, isolated molecules, liquids (including ionic liquids), and homogeneous catalysts*
  - Support basic research that will deliver experimentally validated research codes and the associated experimental and theoretically derived data for the design of functional materials
    - *Explicitly excluded are proposals that emphasize density functional methods as currently implemented or semi-empirical approaches, dynamical mean field theory, and classical and first principles molecular dynamics*.
  - Provide a detailed plan for the full utilization of today's petascale and tomorrow's exascale leadership computing facilities
- Funding level per Application: $1.5M to $2.5M per year for 4 years
  - $4M appropriated for FY 2016
- Only one Letter of Intent/Application will be accepted from any institution and from any lead PI/Director
- Important dates: **Required Letter of Intent Due: 3/7/2016 at 5:00 PM ET**
  - Application **Due: 4/25/2016 at 5:00 PM ET**

DOE Office of Science
Graduate Student Research (SCGSR) Program

The SCGSR Program provides supplemental awards to outstanding graduate students to spend 3 to 12 months conducting part of their doctoral thesis/dissertation research at a DOE national laboratory in collaboration with a DOE laboratory scientist.

- Graduate students must apply online through the online application system.
- The application requires a research proposal and letters of support from both the graduate student's thesis advisory and the collaborating DOE laboratory scientist.
- Student's research and proposed SCGSR project must be aligned with one of the identified SCGSR priority research areas defined by the SC Program Offices and specified in the solicitation.
- Applications proposing to use an SC user facility must apply for user facility time separately.

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 Permanent Resident
- Qualified graduate program & Ph.D. Candidacy
- Graduate research aligned with an SCGSR priority research area
- Establishment of a collaborating DOE laboratory scientist at the time of application

2016 Solicitation 1 – Applications Due: May 11, 2016 5:00PM ET

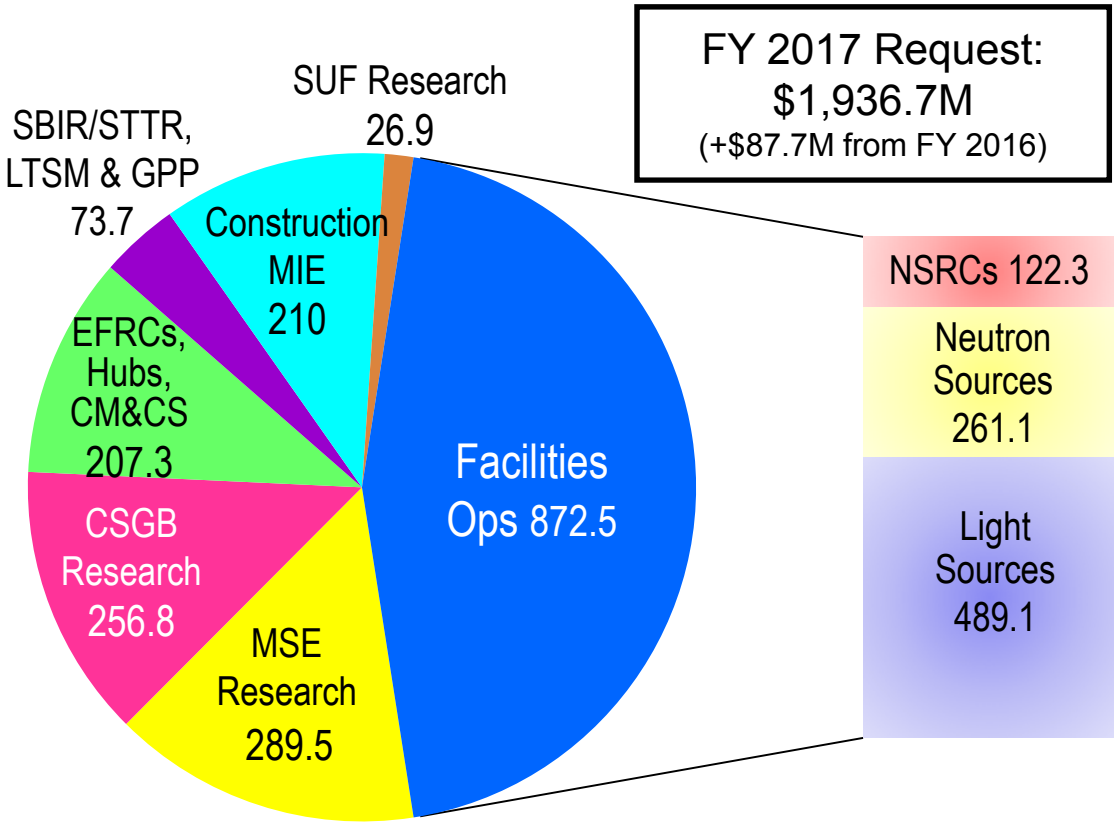
Full details, requirements, FAQs, and link to application at: http://science.energy.gov/wdts/scgsr/

FY 2017 Budget Request

FY 2017 BES Budget Request

Research programs (w/SBIR/STTR)

- Energy Frontier Research Centers (Δ = +$33.8M)
- Computational Chemical Sciences (new, $14M)
- Core Research* with increase for Mission Innovation and other new opportunities, including quantum materials, synthesis science, and subsurface science (Δ = +$52M)
- Energy Innovation Hubs & Computational Materials Sciences



Scientific user facilities (w/SBIR/STTR)

- All full operating facilities at optimal operations (Δ = +$7.5M)
- Accelerator and Detector Research (Δ = +$4.8M)

Construction and instrumentation

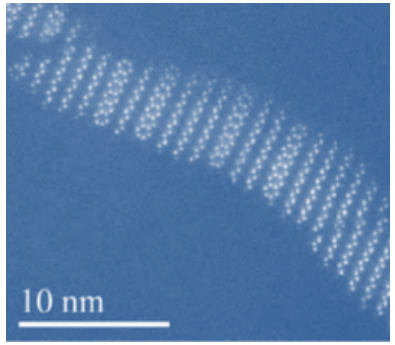
- Advanced Photon Source Upgrade
- Linac Coherent Light Source-II (Δ = -$10.3M)

*Includes EPSCoR

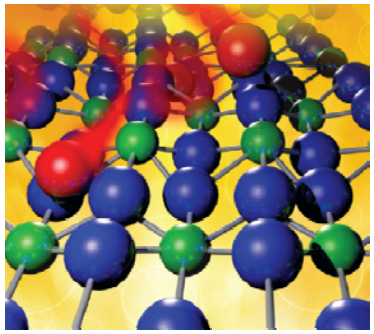
BES Core Research Contributes to Mission Innovation

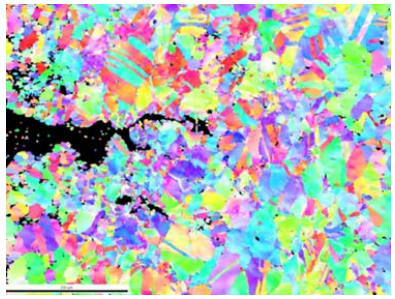
- **Energy efficiency**
  - Catalysts based on enzymes that can operate under lower temperatures and ambient conditions
  - Lightweight materials – hierarchical architectures and non-equilibrium structures beyond aluminum
  - Thermocaloric materials – understanding and predicting properties of new materials for energy-efficient energy applications

- **Extreme environments**
  - Next generation materials for corrosive and high radiation environments, including self-healing materials that exploit reactivity induced by the nuclear environment
  - Corrosion research for the electrochemical reactions in energy storage and utilization
  - Interfacial chemistry leading to new separation methods, new materials for waste forms, and new control of subsurface contamination



Structure of advanced lightweight alloy


Diffusion of oxygen atoms (red) into uranium dioxide


Analysis of cracks at the nanoscale

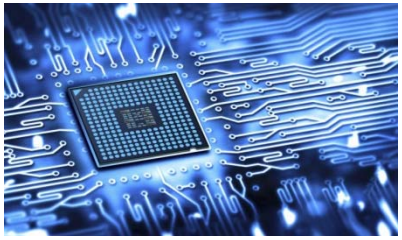
Quantum Materials

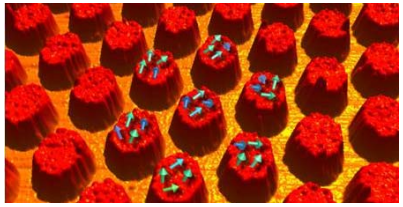
New materials are needed for next generation semiconductors, energy efficient electronics, and technological advances ranging from new magnets to superconductors to support energy technologies.

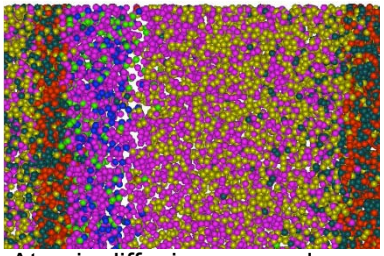
- Emerging quantum materials -- materials whose properties result from strong and coherent interactions of the constituent electrons with each other, the atomic lattice, or light.

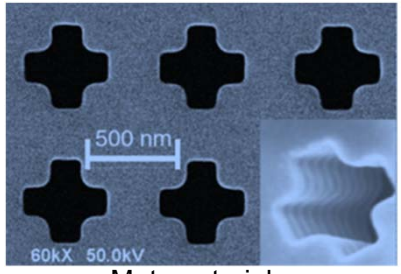
In FY 2017, additional research to discover new materials with unprecedented properties is proposed to take advantage of these phenomena and recent advances in the ability to manipulate and exploit coherence in light and matter.

- Discovery of entirely new materials and properties through atomic-level control of synthesis and design of materials to enable high quality, tailored interfaces, controlled heterogeneity, and coherent manipulation of charge, spin, strain, and lattice dynamics
- Application of combined characterization tools to understand diffusion at interfaces, control of spin, and correlation with structure and chemistry – including ultrafast timescales and near-atomic spatial resolution
- Predictive theory and modeling coupled with experiments to evaluate new phenomena


Semiconductor


Superconducting Islands


Atomic diffusion across layers



Metamaterials

Subsurface Grand Challenge: Advanced Imaging of Geophysical and Geochemical Signals in the Subsurface

Predicting and controlling geological response to perturbations from energy production and storage depends crucially on the arrangements of faults and fractures with respect to ambient subsurface stress.

Key Challenges

- Stress, which governs the overall repository/reservoir response, is obtained only indirectly from strain and rock plasticity
- Rocks have multi-scale fracture network structure - fractures cannot be individually resolved at all relevant scales
- Rock mechanics is strongly influenced by chemical-mechanical coupling via precipitation/dissolution in fractures and pores
- Requires tightly integrated field, laboratory, and computational approaches

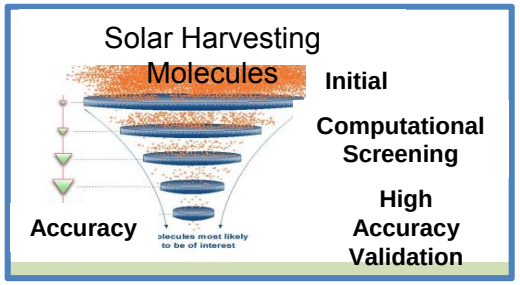
Implementation Plan

- $33.8M to fully fund up to 5 Energy Frontier Research Centers (EFRCs) for three years
- EFRCs will engage the grand challenge through development and use of new geophysical/geochemical imaging approaches and computational methods
  - Coupling with cross-cutting activities (computational/data analysis methods, new laboratory studies on imaging and chemical analysis)
  - Coupling with field-based projects (supported by DOE technology programs)

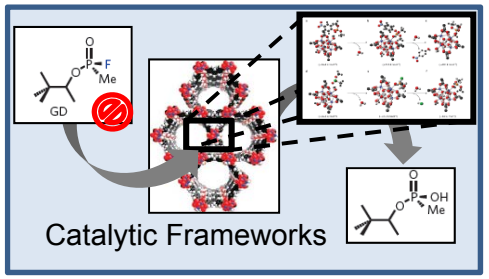
Computational Chemical Sciences
FY 2017 = $14M

Deliverable: Open-source modular chemistry codes and software packages that are automated, account for quantum/relativistic effects, and with sufficient accuracies for d- and f- electron systems

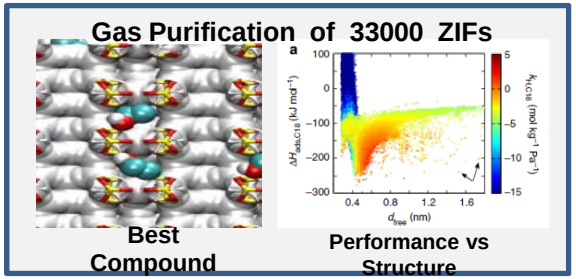
- A new activity -- $14M is requested to support 4-5 teams of researchers to capitalize on existing investments in quantum chemistry codes and upgrade them to be compatible with the current and future generations of high performance computers.
- Assemble teams of mathematical and computational chemists to develop open-source software with new algorithms to allow simulation of chemical processes of complex systems.
- Rewrite software and algorithms to fully realize the current and future gains in efficiency offered by massively parallel computing platforms.
- Deliver codes that treat electronic and spin effects in order to avoid case-by-case retooling of the model of electronic potential that is embedded in many current computational methods.



High-Accuracy Design of Catalysis



Artificial Photosynthesis



Field-Driven Chemical Rearrangements

BES User Facilities

DOE Office of Basic Energy Sciences: Scientific User Facilities

- 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)

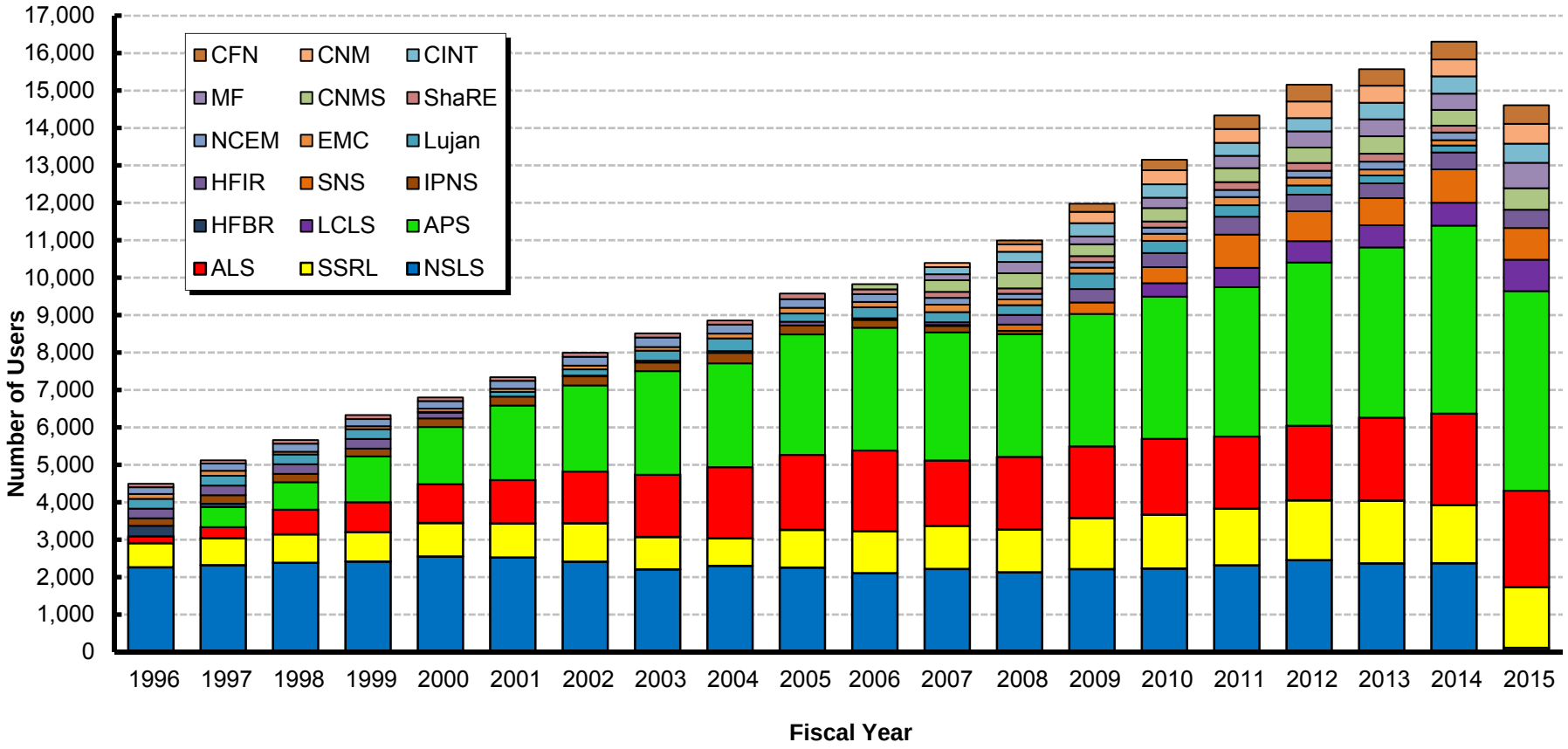
Light Sources

- 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)

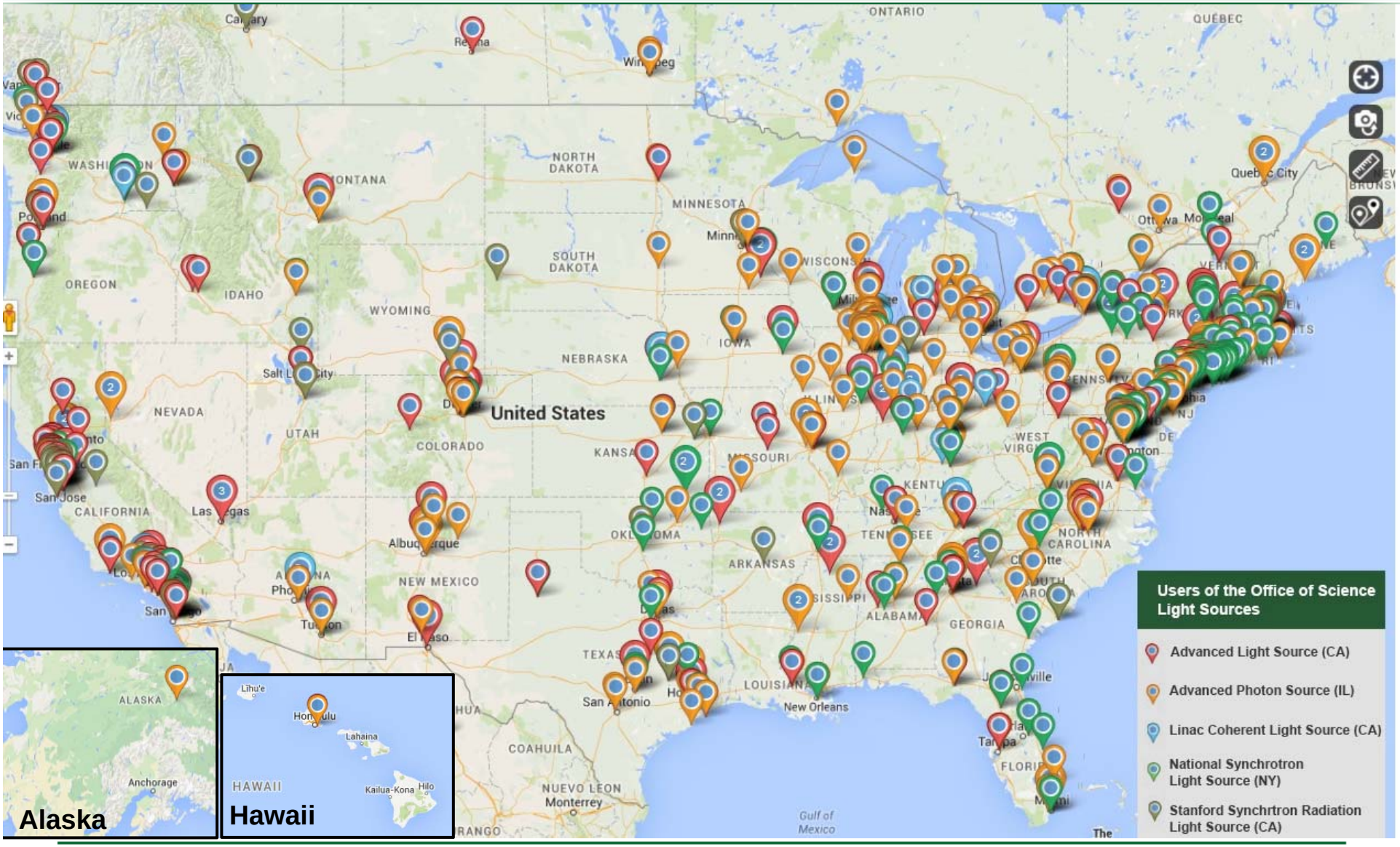
BES User Facilities Hosted Over 14,000 Users in FY 2015



- The newly constructed NSLS II started early operations in FY 2015 (hosted 110 users).
- The three electron beam microcharacterization centers were merged administratively with their respective neighboring NSRCs in FY 2015.
- The BES operations at the Lujan Neutron Scattering Center ceased operations in FY2014.

Where Do the U.S. Light Source Users Come From?

http://science.energy.gov/user-facilities/user-statistics/



FAQs and Web Resources

Core Program Funding Opportunities: FAQs

- How do I get DOE/BES support?
  - Respond to "FY2016 Continuation of Solicitation for the Office of Science Financial Assistance Program" Read all FOAs carefully!!
  - Hypothesis driven, fundamental science with energy relevance; discovery science and use-inspired basic research
  - All eligible/responsive proposals are peer reviewed

- Can I contact/visit a program manager?
  - Initial contact by email and phone is encouraged – contact information is on the website for every program manager
  - White papers/pre-proposals are encouraged – Can be sent to program manager or submitted through the PAMS system; see FOA for details
  - BES offices located in Germantown, MD – secure facility, requires planning and additional information from foreign nationals.

- How much support can I get?
  - Peer review will assess requested budget versus research needs
  - Typical is 1 month of summer support plus graduate student/postdoc
  - Multi-PI grants are also supported – talk with the program manager

FY 2016 – Annual FOA

- FY 2016 Continuation of Solicitation for the Office of Science Financial Assistance Program
  http://science.energy.gov/~/media/grants/pdf/foas/2016/SC_FOA_0001414.pdf

- Read the FOA carefully for program specific limitations, for example:
  - Materials Chemistry: Research primarily aimed at the *optimization* of synthetic methods or properties of materials for applications, and research with a primary goal of device fabrication and testing will be discouraged.
  - Theoretical Condensed Matter Physics: Soft matter physics, granular materials, quantum computing, and surface chemistry are not current priorities.
  - Neutron Scattering: In FY 2016, the program will not consider applications with a major focus on conventional and high temperature superconductivity, organic photovoltaics and nanoconfined fluids.

FY 2016 – Annual FOA (continued)

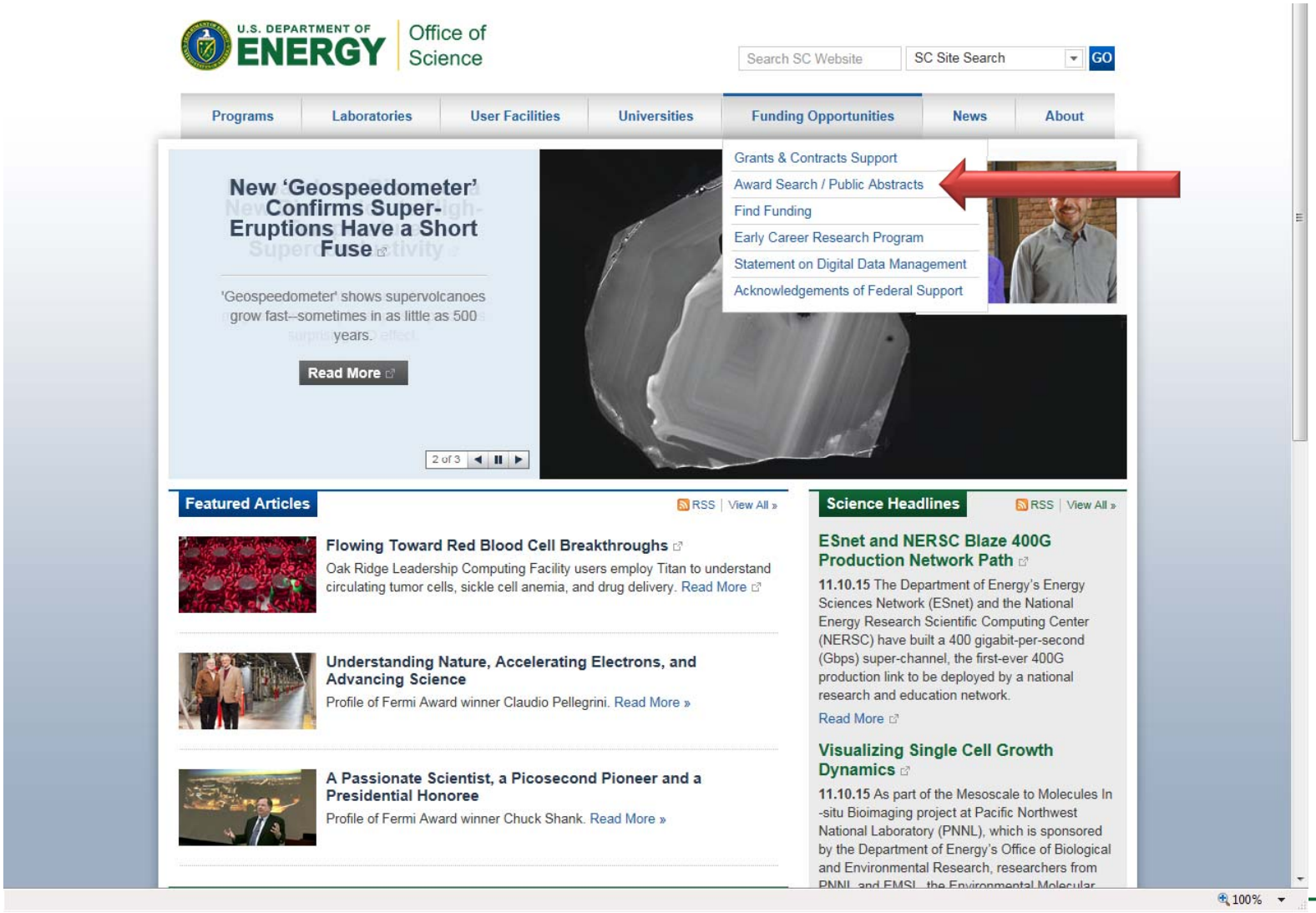
- Look for program specific areas of emphasis, for example:
  - Many programs: The activity will expand research on….
  - Synthesis and Processing Science: The program has an increasing focus on understanding of kinetics and mechanisms of materials growth including: bulk material processes, organic and inorganic film deposition, plasma synthesis and the organization of mesoscopic assemblies across a range of length scales, especially underpinning many energy related technological areas.
  - X-Ray Scattering: New investments in ultrafast science will focus on research that uses radiation sources associated with BES facilities and beam lines but also includes research performed with ultra-short pulse radiation probes created by tabletop laser sources.
- Applications that do not include a Data management plan will be returned without review.

Core Program Funding Opportunities: FAQs (continued)

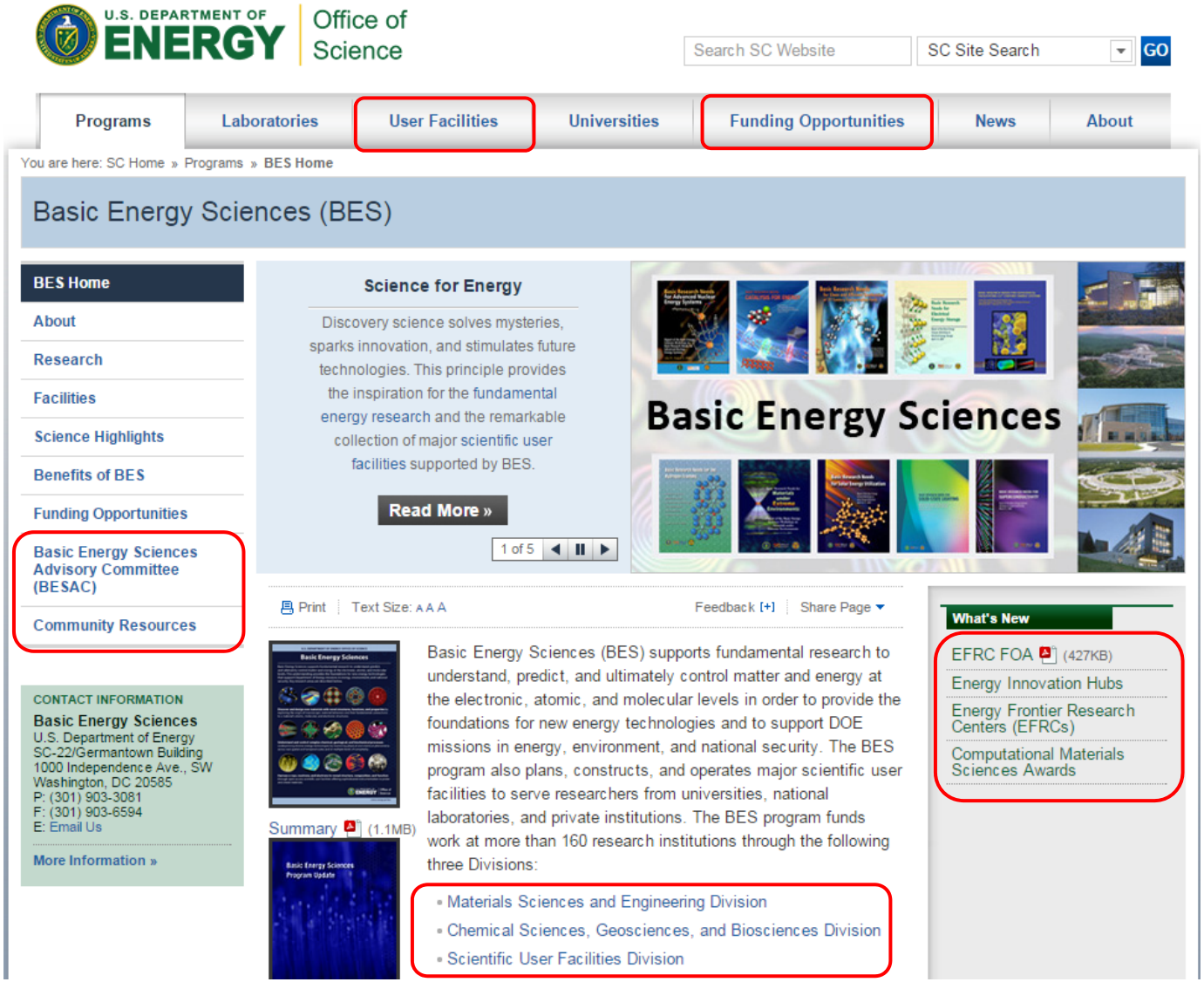
- How long will it take for me to find out if my project is funded?
  - The Open Call is a continuous process (no fixed deadline for submission of applications)
  - Reviews take 4 – 6 months to complete, awards are made based on strength of the merit review, programmatic priorities, and available resources
  - Proposals can be held up to one year for consideration

- I want to support my research group with multiple federal grants – what are the requirements?
  - You must have separate research proposals that can "stand alone" with respect to research performed and research output

A link to the DOE Office of Science Award Search can be found at science.energy.gov



http://science.energy.gov/bes/

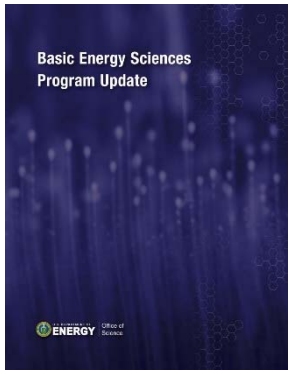


BES Publications

BES 2015 Program Update

http://science.energy.gov/bes/

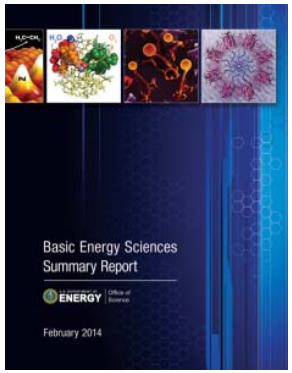
- Brochure describing changes in the BES program in FY 2015 and accessible research highlights



BES 2014 Summary Report

http://science.energy.gov/bes/research/

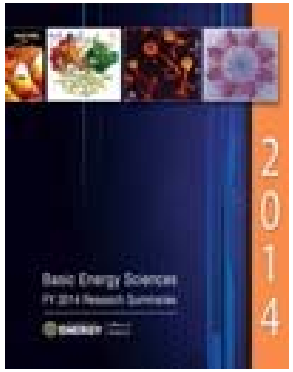
- Overview of BES
- How BES does business
- Descriptions and representative research highlights for 3 BES divisions, EFRCs, and Energy Innovation Hubs



BES FY 2014 Research Summaries

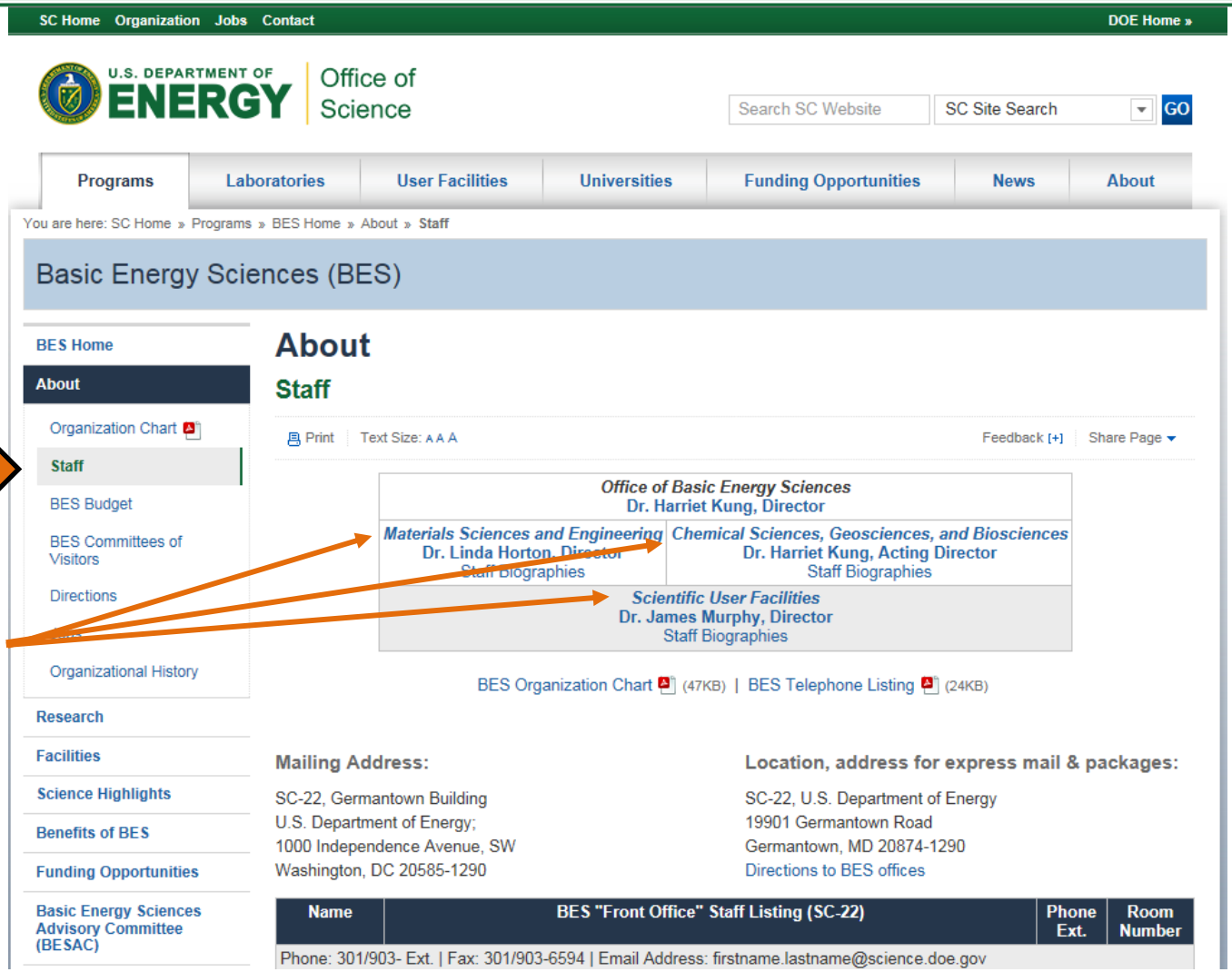
http://science.energy.gov/bes/research/

- Summaries of more than 1300 research projects across 3 BES divisions, including senior investigators, postdocs, graduate and undergraduate students, and a brief project description



Contact Information

Program descriptions and Program Manager Contact Info



http://science.energy.gov/bes/about/staff/