



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Basic Energy Sciences Update

BES Advisory Committee Meeting

July 11, 2019

Harriet Kung
Associate Director of Science
Basic Energy Sciences

Outline

- **Staffing Update**
- **FY 2020 Budget Request and HEWD Mark**
- **Program News**
 - SC QIS Notice of Intent/Request for Information
 - BES/ASCR Collaboration to Address Data Challenges @ BES Facilities
 - LCLS-II
 - SC Website Update
 - Upcoming strategic planning



Director of DOE Office of Science



Dr. Christopher Fall was confirmed as DOE Office of Science Director on May 23, 2019.

He previously served as the Principal Deputy Director of Advanced Research Projects Agency-Energy (ARPA-E).

Dr. Fall also served in the White House Office of Science and Technology (OSTP) and in the Office of Naval Research, including as acting chief scientist and research division lead.

Dr. Fall received his B.S. in mechanical engineering and a Ph.D. in neuroscience from University of Virginia.



Office of Basic Energy Sciences

Harriet Kung, Director

BES Budget and Planning

Donetta Herbert, Financial Management
Natalia Melcer, Program Manager
Thomas Russell, Senior Technical Advisor

BES Operations

Teresa Crockett, Program Analyst
Robin Hayes, Program Manager
Kerry Hochberger, Program Support Specialist
Katie Runkles, Program Analyst / BESAC*
Andy Schwartz, Senior Technical Advisor for EFRCS*

* Basic Energy Sciences Advisory Committee
* Energy Frontier Research Centers

Materials Sciences and Engineering Division

Linda Horton, Director

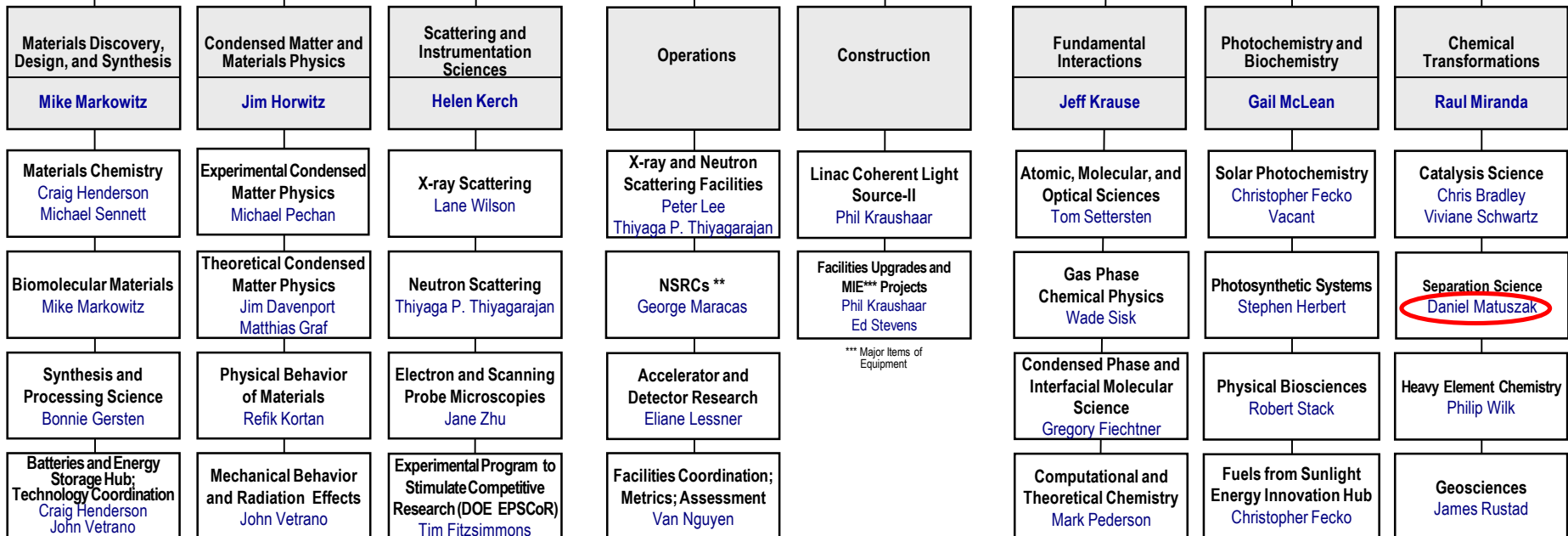
Scientific User Facilities Division

James Murphy, Director

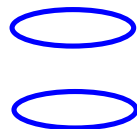
Rocio Meneses, Program Assistant

Chemical Sciences, Geosciences, and Biosciences Division

Bruce Garrett, Director

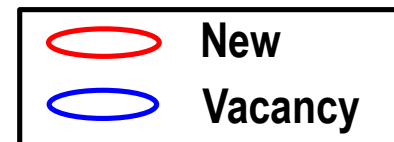


** Nanoscale Science Research Centers



Quantum Information Science Program Manager

Neutron Facilities Program Manager



July 2019

Posted July 1, 2019



Dr. Daniel Matuszak

Program Manager, Separations Science
Office of Basic Energy Sciences

9+ years at DOE HQ

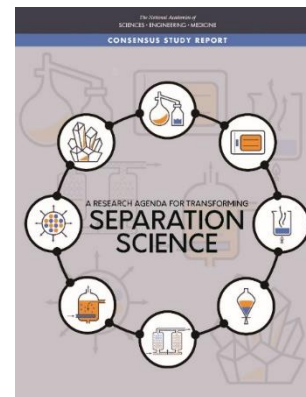
Expertise

- Molecular Thermodynamics of Fluids
- Gas Separation and Conversion
- Nanoporous & Nano-structured Systems

Experience

- Office of Fossil Energy: Program Manager for carbon utilization
- ARPA-E: Technical Manager for “Innovative Materials and Processes for Advanced Carbon Capture Technologies”
- Johns Hopkins University, Ph.D.

New program opportunity as guided by NAS study



<http://nas-sites.org/dels/studies/separations/>



Dr. Emily Smith

AAAS Science and Technology Policy Fellow
Office of Basic Energy Sciences

Expertise

- Spectroscopy and imaging
- Characterization of nanomaterials, thin films, cell membranes and biomass
- Analytical instrument development

Joining BES in September 2019

Experience

- Faculty member: Iowa State University, Department of Chemistry, Ames Iowa since 2006
- Faculty Scientist: Ames Laboratory since 2007 (courtesy appointment)
- University of Wisconsin-Madison, Ph.D.



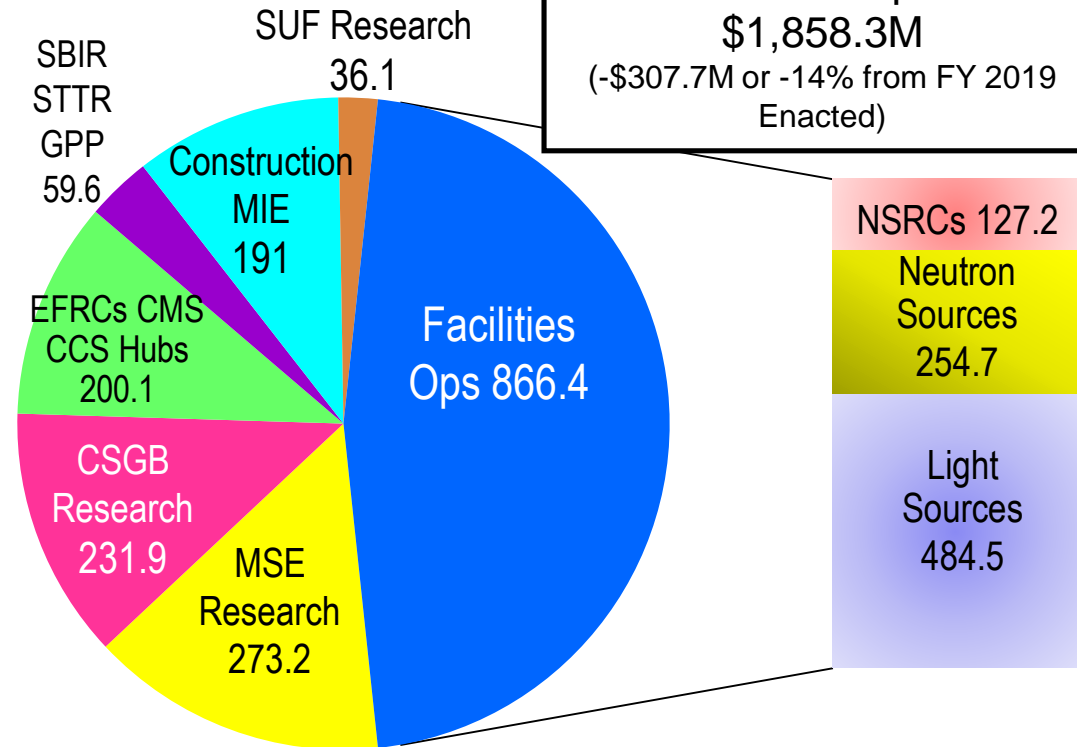
FY 2020 BES Budget Request

Research programs

- Core Research will emphasize quantum information science (QIS), including co-sponsoring **QIS center** with ASCR and HEP, **microelectronics** (\$531.1M).
- Computational Materials and Chemical Sciences continue (\$26M)
- Energy Frontier Research Centers continue (\$130M)**
- Energy Innovation Hubs, including re-competition for **Solar Fuels Hub** (\$44.1M).
- Data analytics for BES facilities (\$10M)**

Scientific user facilities

- Operations of operating facilities at ~87% optimal level (\$866.4M)
- LCLS at 97% starting at 2Q FY 2020

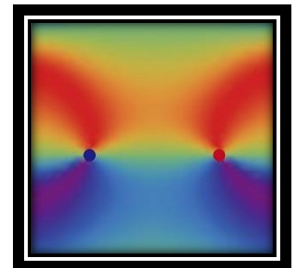
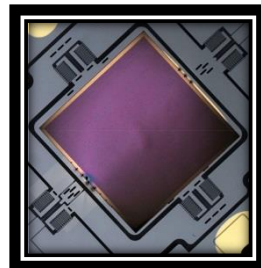
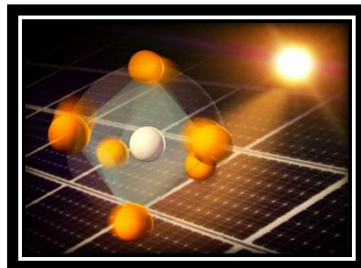
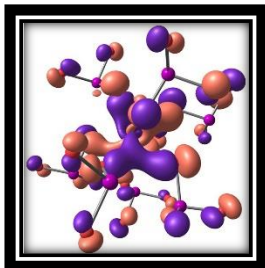
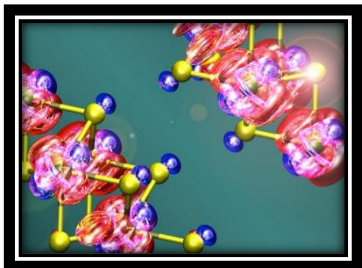


Construction

- No funding for LCLS-II ($\Delta = -\$129M$)
- APS-U ($\Delta = +20M$); PPU ($\Delta = +\$5M$), STS (\$1M)
- ALS-U ($\Delta = -\$47M$) and LCLS-II-HE ($\Delta = -\$14M$)
- Two new starts: NEXT-II (\$1M) and NSRC-recap (\$1M)

FY 2020 BES Budget Request

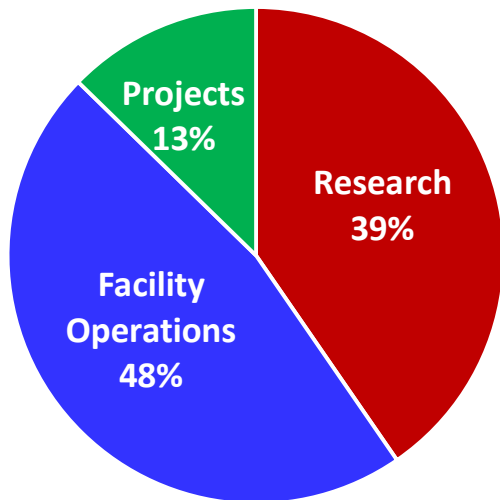
- The BES FY 2020 Request of **\$1,858M** focuses resources toward the highest priorities in early-stage fundamental research, in operation and maintenance of scientific user facilities, and in facility upgrades.
- Core research priorities in the FY 2020 Request include quantum information science (QIS), next-generation microelectronics, data analytics and machine learning for data-driven science, and computational materials and chemical sciences as part of the Exascale Computing Initiative
- **BES will partner with Advanced Scientific Computing Research (ASCR) and High Energy Physics (HEP) to establish at least one multi-disciplinary QIS center** to promote basic research and early stage development to accelerate the advancement of QIS through vertical integration between systems and theory and hardware and software.
- The Request increases funding for the **Energy Frontier Research Centers (EFRCs)** with a planned solicitation in FY 2020 to expand the portfolio in key topical areas including QIS, microelectronics, and other program priorities. The solicitation will also re-compete funding for science relevant to the Department's environmental management mission.
- The **Fuels from Sunlight Energy Innovation Hub** will complete its second five-year term with FY 2019 funding. FY 2020 funding will continue to support early-stage fundamental research on solar fuels generation that builds on the Hub's unique capabilities and accomplishments to date. BES will issue an **open competition in FY 2020** for research to address emerging new directions as well as long-standing challenges in this transformational area of energy science.
- The **BES user facilities** continue operations at approximately **87% of optimal**. Linac Coherent Light Source (**LCLS**) **operations will resume in the second quarter of FY 2020** on completion of installation of LCLS-II accelerator components. All five Nanoscale Science Research Centers (NSRCs) are supported with funding designated for QIS research and related tools development.
- The FY 2020 Request provides continued support for the **Advanced Photon Source Upgrade (APS-U)** project, the **Advanced Light Source Upgrade (ALS-U)** project, the **LCLS-II High Energy (LCLS-II-HE)** project, the **Proton Power Upgrade (PPU)** project, and the **Second Target Station (STS)** project. Two new Major Item of Equipment projects are initiated: the **NSLS-II Experimental Tools-II (NEXT-II)** project to continue the phased build-out of beamlines at NSLS-II, and the **NSRC Recapitalization** project.



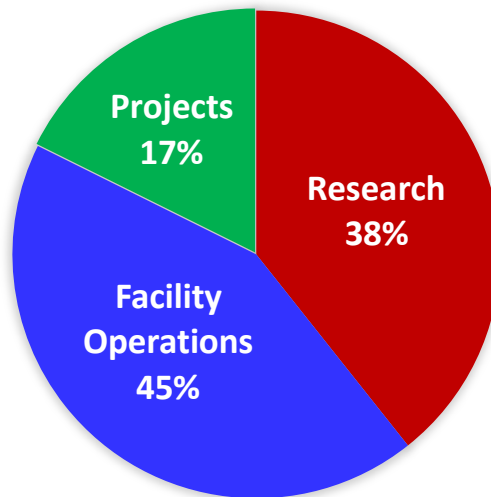
BES Budget by Budget Element: 2017 - 2020

	FY 2017 Enacted	FY 2018 Enacted	FY 2019 Enacted	FY 2020 President's Request	FY 2020 House Mark
Research	755,669	821,403	815,600	799,877	858,000
Facility Operations	877,331	898,597	922,000	866,408	944,000
Projects (Construction + MIE)	237,500	369,000	427,400	191,000	340,000
Other	1,000	1,000	1,000	1,000	1,000
Total	1,871,500	2,090,000	2,166,000	1,858,285	2,143,000

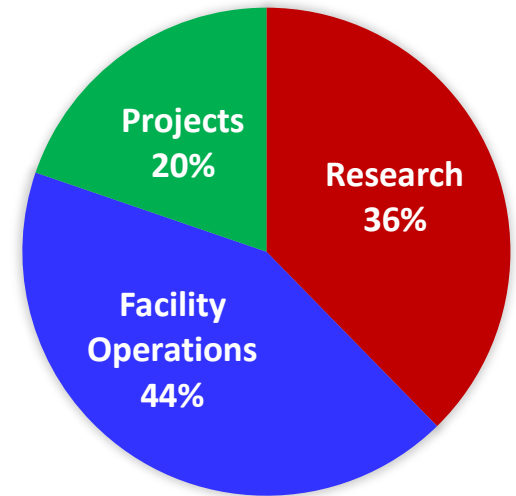
FY 2017



FY 2018



FY 2019



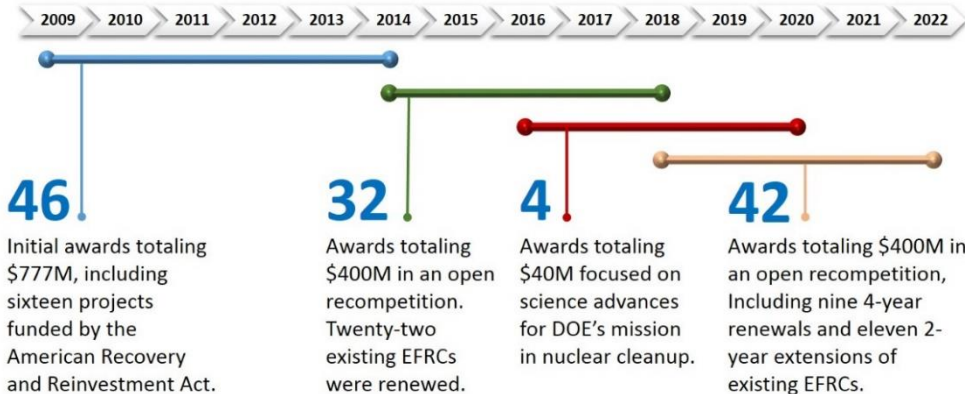
Summary of BES FY 2020 HEWD Mark

As compared with FY 2019 Enacted:

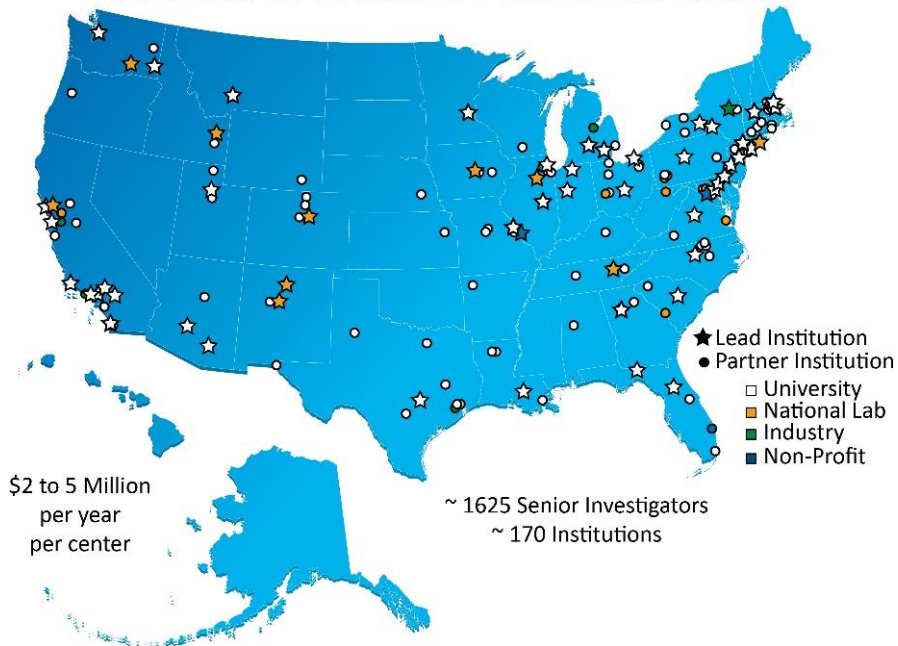
- Facility operations funding increases by \$22M – enabling optimal operations of X-ray light sources and Nanoscale Science Research Centers (+3% above FY19) and near optimal operations of neutron sources (+1% above FY19).
- Research increases by \$42M, including increases for EPSCoR (+\$5M), EFRCs (+\$10M), microelectronics (+\$25M), QIS Centers (+\$10M), data analytics (+\$7M), and Fuels from Sunlight Hub (+\$5M). These increases will be offset by a reduction in core research by \$20M.
- Construction and MIE funding is at or exceeds ideal profile levels for APS-U, ALS-U, LCLS-II-HE, PPU, STS, NEXT-II, and NSRC-Recap.

Energy Frontier Research Centers (2009 – 2019)

EFRC AWARDS HISTORY



82 EFRCs in 40 States + D.C. since 2009



Cumulative Investment (2009-2018): \$1.3B

Cumulative Accomplishments (Aug 2009 – May 2019)

- ❑ Over 11,600 peer-reviewed scientific publications
- ❑ ~110 companies have benefited from EFRC research
- ❑ Over 180 patents issued
- ❑ >1,600 senior investigators at ~170 institutions (university, lab, industry, non-profit)
- ❑ At least 5,000 students and postdocs trained in EFRCs

Energy Frontier Research Centers

FY 2020 Funding Opportunity Announcement (up to \$40M, pending appropriation)

- 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).

History of Biennial EFRC PI Meetings



PI Meeting and “EFRCs at Ten”

July 29-30, 2019

Invitation only

~800 attendees from EFRCs, DOE,
and other Federal agencies

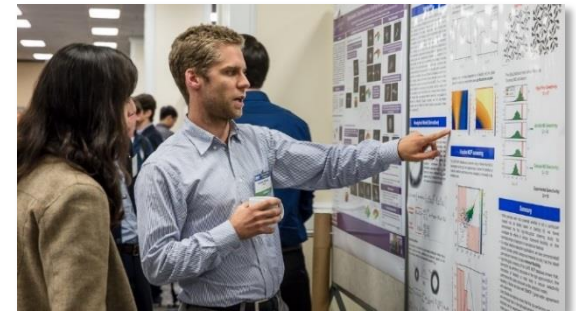
Summit and Forum

~1000 attendees

Open to public



PI Meetings
500-600 attendees



July 2019 EFRC PI Meeting Overview

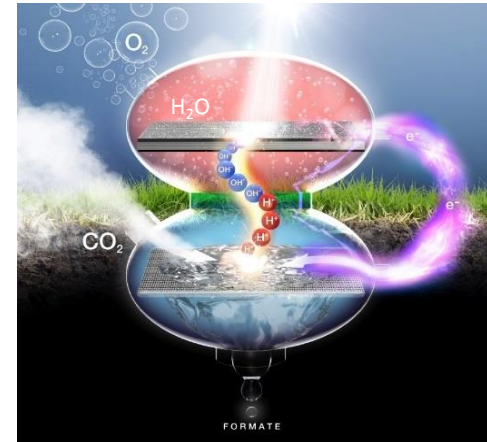
- **Day 1 (July 29): EFRCs at Ten**
 - Plenary Speakers
 - Under Secretary Dabbar (confirmed)
 - Mr. Norm Augustine, Lockheed Martin - retired (confirmed)
 - Prof. Esther Takeuchi, Stony Brook Univ./BNL (confirmed)
 - Dr. Kelvin Droegemeier, OSTP (confirmed)
 - Award announcements (Ten at Ten and Video Contests)
 - Lunchtime panel (organized by Early Career Network)
 - Moderated Panel Discussion on Science to Technology Transition with DOE technology offices
 - Two Moderated Panel Discussions on EFRC Impact on science, technology, and the energy workforce
 - Center Overview Poster Session & Reception
- **Day 2 (July 30): Scientific PI Meeting**
 - Parallel technical sessions with 2-3 technical talks per center
 - Lunchtime panel (organized by Early Career Network)
 - Technical poster sessions

Fuels from Sunlight Energy Innovation Hub

FY 2020 Request \$20M

Multiple ‘abundant resources’ provide promising targets for solar fuels production research to be integrated under the Energy Innovation Hub model:

- Hydrogen from water splitting
- Hydrocarbons and oxygenates from carbon dioxide reduction
- Ammonia and hydrazine from nitrogen reduction



FY 2020 Funding Opportunity Announcement (up to \$20M, pending appropriation)

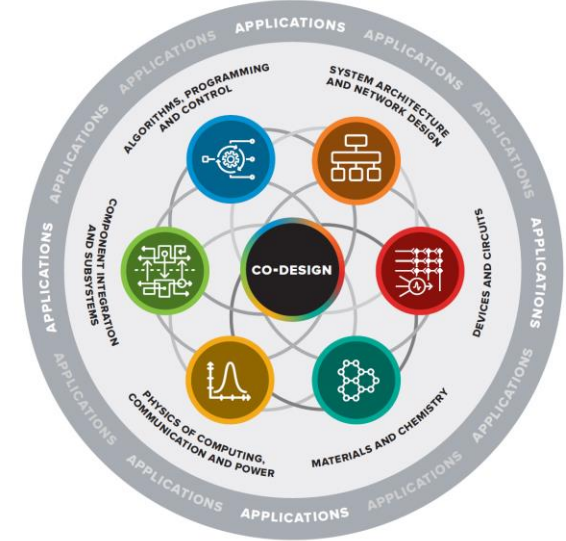
- Solicitation for new proposals aligned with priority research directions identified in a roundtable workshop (August 2019)
 - Initiate multi-PI, multi-disciplinary project(s) based on peer review
 - Engage JCAP capabilities in projects when appropriate
 - Begin funding in late FY 2020, pending appropriation



BES Microelectronics Research

Basic Research Needs for Microelectronics Workshop

- Co-sponsored by ASCR, BES, HEP; October 23–25, 2018
- Workshop identified 5 Priority Research Directions:
 - Flip the current paradigm: Define innovative materials, device, and architecture requirements driven by applications, algorithms, and software
 - Revolutionize memory and data storage
 - Reimagine information flow unconstrained by interconnects
 - Redefine computing by leveraging unexploited physical phenomena
 - Reinvent the electricity grid through new materials, devices, and architectures



The workshop identified a critical need to move from traditional sequential design to an integrated Co-Design framework where each scientific discipline informs and engages the others, with multi-directional information flow .

FY 2020 Plan (up to \$25M, pending appropriation)

- BES will expand core research and the EFRCs in 2020, placing an emphasis on materials and chemical science challenges that are relevant to advanced microelectronics as identified in the BRN workshop.



LCLS-II and APS-U Construction Projects

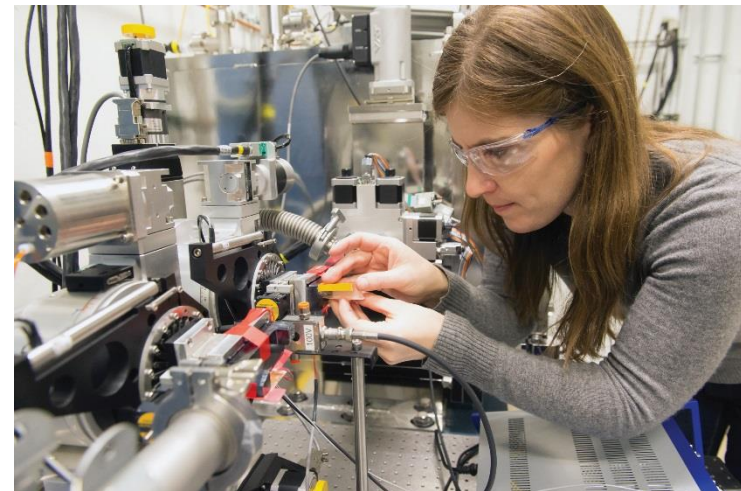
Linac Coherent Light Source-II (LCLS-II)

- No funding is requested for FY 2020 per the project plan. The project will continue towards an early completion in FY 2021 - 2022.
- LCLS-II will provide high-repetition-rate, ultra-bright, transform-limited femtosecond x-ray pulses with polarization control and pulse length control.
- LCLS has started a year-long operations shutdown to allow the project to install new undulators, reconfigure the Near Experimental Hall (NEH), and install the LCLS-II linac, cryo distribution, and other technical systems. The NEH and undulators work must complete before LCLS can resume operations.



Advanced Photon Source Upgrade (APS-U)

- FY 2019 = \$130M; FY 2020 request = \$150M; FY 2020 House mark = \$170M for R&D, design, prototyping, testing, fabrication, site preparation, installation, long lead and advanced procurements.
- Construction activities and procurements will begin after CD-3 approval for the superconducting undulators, beamline optics, remaining storage ring magnets and civil construction associated with the long beamlines.
- APS-U will provide a hard x-ray source with world-leading transverse coherence and extreme brightness.



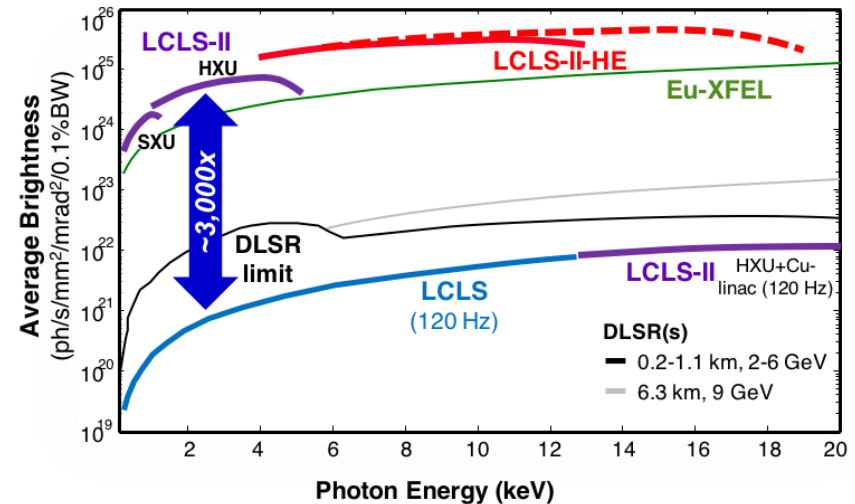
Dr. Mary Upton using RIXS beamline



LCLS-II-HE and ALS-U Construction Projects

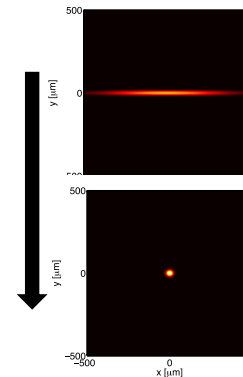
LCLS-II High Energy Upgrade (LCLS-II-HE)

- FY 2019 = \$34M; FY 2020 request = \$18M; FY 2020 House mark = \$54M for planning, engineering, design, R&D prototyping, and long lead procurements.
- LCLS-II-HE will increase the repetition rate of LCLS-II to 1 MHz at higher energy range (12 keV and beyond).
- LCLS-II-HE will increase the energy of the superconducting linac from 4 to 8 GeV and deliver ~1,000-fold higher average brightness hard x-rays at higher energy range.



Advanced Light Source Upgrade (ALS-U)

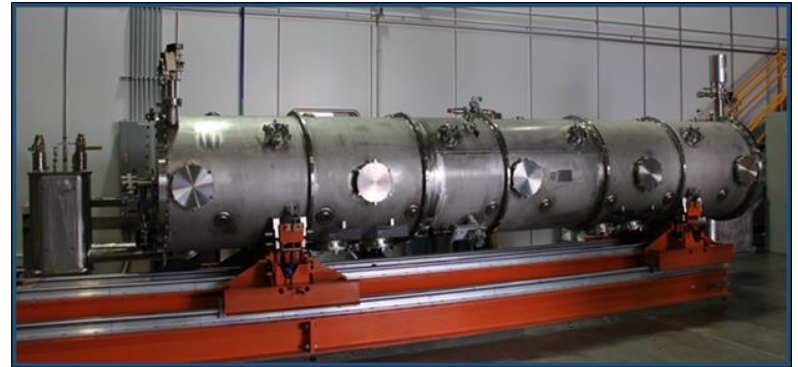
- FY 2019 = \$62M; FY 2020 request = \$15M; FY 2020 House mark = \$55M for planning, engineering, design, R&D prototyping activities, and long lead procurements.
- ALS-U will generate 1,000 times brighter soft x-rays with higher coherence to resolve nanometer-scale features and enable real-time observation of chemical processes and materials as they function.
- ALS-U will install a multi-bend achromat (MBA) lattice to reduce emittance and produce a “round” x-ray beam. The project will also develop new advanced instruments that take advantage of the new beam for cutting-edge experiments.



PPU and STS Construction Projects

Proton Power Upgrade (PPU)

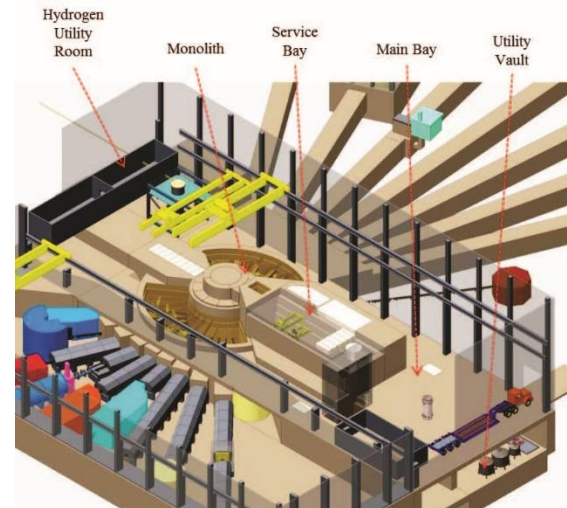
- FY 2019 = \$60M; FY 2020 request = \$5M; FY 2020 House mark = \$50M for R&D, engineering, prototyping, engineering designs, fabrication, testing, and long lead procurements.
- PPU will double the proton beam power capability of the SNS from 1.4 MW to 2.8 MW, upgrade the first target station to accommodate beam power up to 2 MW, and deliver a 2 MW qualified target.
- Additional cryomodules will enable the increased beam power, and a new target gas injection system and redesigned target vessel will improve target performance.



The PPU project will provide 7 new cryomodules to increase the proton beam power at SNS.

Second Target Station (STS)

- FY 2019 = \$6M; FY 2020 request = \$1M; FY 2020 House mark = \$1M for planning, targeted R&D, and engineering design.
- STS will be a complementary pulsed source with a narrow proton beam to produce an order of magnitude higher brightness cold neutrons than were previously achievable. By optimizing the design of the instruments, the detection resolution will be up to two orders of magnitude higher.

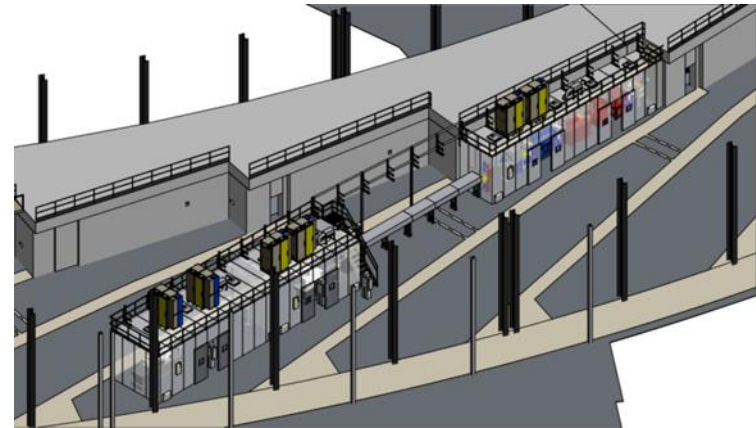


Notional STS Target Layout

FY 2020 New Major Item of Equipment Projects

NSLS-II Experimental Tools-II (NEXT-II)

- NEXT-II is a new major item of equipment (MIE) project to continue the phased build-out of beamlines at the National Synchrotron Light Source-II at Brookhaven National Laboratory. The project will deliver ~3 state-of-the-art beamlines
- The total project cost of \$60M.
- FY 2020 request = \$1M; FY 2020 House mark = \$5M for conceptual designs of new beamlines.



Schematic of the Submicron Resolution X-ray Spectroscopy (SRX) beamline, one of the NSLS-II project beamlines

Nanoscale Science Research Center (NSRC) Recapitalization

- NSRC Recap is a new MIE project to upgrade equipment across all five NSRCs to continue to perform cutting edge science and accelerate advances in the fields of nanoscience, materials, chemistry, and biology.
- The total project cost is \$60M.
- FY 2020 request = \$1M; FY 2020 House mark = \$5M for planning and design activities.



DOE-SC Quantum Information Science Centers

- FY 2020 SC Budget Request includes funds in ASCR, BES, and HEP to establish at least one multi-disciplinary multi-institutional QIS center.
- In May 2019, ASCR, BES, and HEP jointly issued in the Federal Register a combined Notice of Intent (NOI) and Request for Information (RFI).
- NOI indicated that DOE-SC is considering issuing a Funding Opportunity Announcement in FY 2020 for QIS Centers.
- RFI sought community input on the topical areas, organization, requirements, review criteria, and assessment process for prospective QIS Centers.
- Comments were due by 7/5/2019.



Notice of Intent

To issue an FOA for two or more QIS Centers in FY 2020, pending appropriation

- Require highly collaborative research teams, bringing together top talent from the full spectrum of performers—including universities, private industry, non-profits, and national labs.
- Attributes: major, impactful challenge; discovery science to prototypical technology; multi-disciplinary integration of expertise and domains; projectized approach; national resource.
- Complement the existing base research and other activities within individual program offices, and represent coherent efforts beyond the scope of what would normally be supported by those programs individually.
- *Each center addresses mission needs of more than one DOE-SC program office, and integrates elements from multiple technical areas of interest.*
- Technical areas include: Quantum Communication, Materials and Chemistry for QIS Systems and Applications, Qubit Devices and Sensors for QIS and SC Applications, Quantum Emulation and Computing, Quantum Foundries.

Request for Information

Gather input about the topic areas, organization, requirements, review criteria, and assessment process for prospective QIS Centers, in order to inform the DOE-SC formulation of the corresponding FOA.

1. **Topical Areas and Scope** (e.g., add, delete, prioritize)
2. **Collaboration and Partnerships** (e.g., role of industry)
3. **Management and Organization** (e.g., models, synergy)
4. **Assessment and Criteria for Success** (e.g., metrics)
5. **National Impact and Contribution** (e.g., distinctiveness)
6. **Other** (e.g., obstacles, missing opportunities or issues)

BES/ASCR Collaboration to Address Data Challenges at BES User Facilities

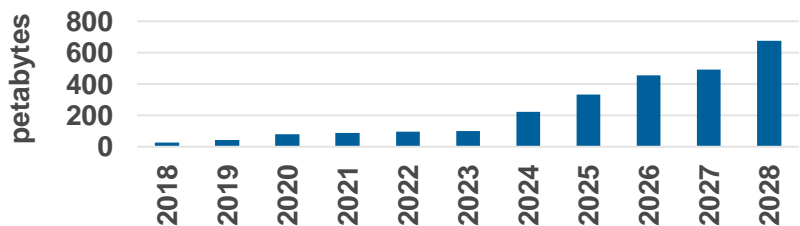
BES/ASCR Joint Data Call to all BES User Facilities (July 2018)

The Light Source Data Working Group, composing of BES facility representatives from the labs, combined the responses from the ALS, APS, LCLS, NSLS-II, SSRL, and summarized high-priority needs as follows (January 2019):

1. **Data management and workflow tools** that integrate beamline instruments with computing and storage resources, for use during experiments, as well as facile user access for post-experiment analysis
2. **Real-time data analysis capabilities** to significantly reduce the data volumes and provide feedback during experiments to improve data quality and to drive the direction of ongoing measurements; the application of advanced machine learning algorithms and the integration of simulations and model-based approaches will allow automated steering of data collection
3. **On-demand utilization of super-computing environments** to enable quasi real-time data processing
4. **Data storage and archival** resources to house the continually increasing amounts of valuable scientific data produced by the BES Light Sources

Estimated cumulative data generation

Total by fiscal year



Estimated peak on-demand computing resources required

FY	Facility / peak petaflops				
	ALS	APS	LCLS/LCLS-II	NSLS-II	SSRL
2021	0.1 PF	4 PF	100 PF	2.5 PF	< 1 PF
2028	30 PF	50 PF	1,000 PF	45 PF	< 1 PF



BES-ASCR Facilities Information Exchange at LBNL, June 12, 2019

The BES and ASCR Facilities Divisions organized a meeting of the BES Light Source and ASCR Facility Directors and data science subject matter experts (including representatives from BES neutron facilities and nano centers, and CAMERA). The goals:

- Foster new connections and build a shared understanding of the strategic landscape for data intensive science challenges, capability and capacity gaps, and opportunities.
- Build momentum towards answering the ultimate questions: How should we close the gaps? What makes sense for the “division of labor” between ASCR-stewarded and BES-stewarded capabilities and infrastructure, and what is realistic?

Outcome: the BES Light Source Directors and ASCR Facility Directors charged a group to provide a short report to sketch their collective views on several strategic questions:

- Requirements for a data management architecture (compute, storage, network, algorithms, middleware, and software)
- Capability gaps, systems integration gaps, sociological gaps, workforce gaps
- Balance of responsibilities between BES and ASCR for the development and stewardship of capabilities and infrastructure

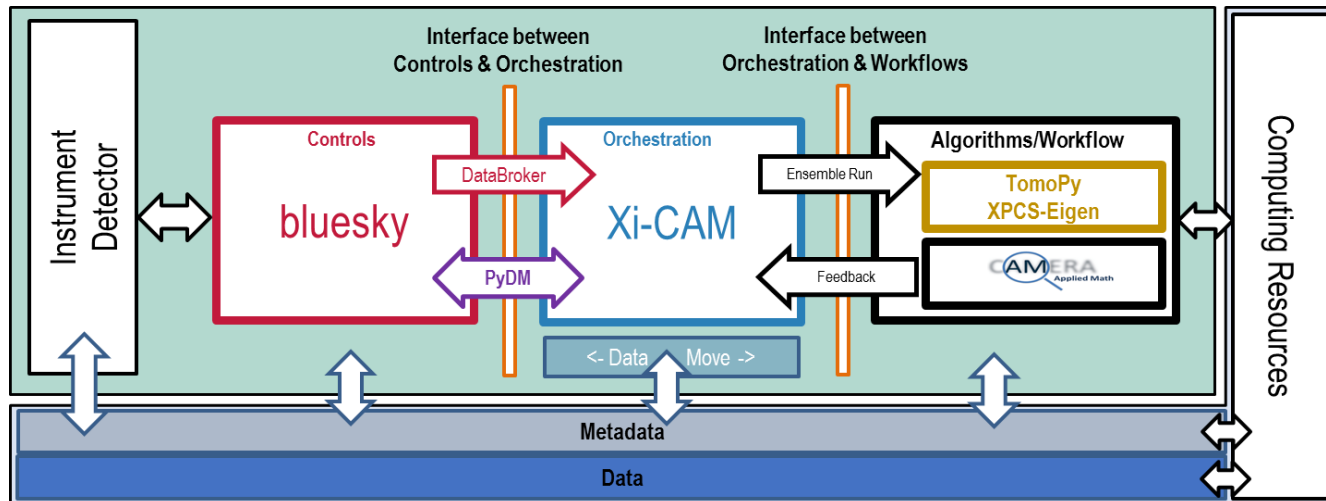


BES Light Source Data Solution Pilot Project

Develop synergistic approach to software solutions and common data science platform among light source facilities

Initial Tasks (2-year pilot; starting July 2019):

- Working closely with CAMERA, build, implement, and demonstrate common software solutions for experimental techniques common across the light sources - initially focusing on XPCS, ptychography, and tomography
- Leverage tools and expertise from all of the BES light sources and CAMERA by integrating complementary components - **Bluesky** (Data Acquisition, NSLS-II), **PyDM** (Control GUI, LCLS), **Xi-CAM** (Software/Data platform, ALS/CAMERA), **XPCS-Eigen** (XPCS software, APS), **TomoPy** (Tomography software, APS), Algorithms and Applications by CAMERA (e.g. SHARP, M-TIP, SMART, MS-D Networks)



LCLS-II progress

86.5% complete as of the end of May



18/35 1.3 GHZ Cryomodules are in place. ~ one arriving per week



13 of 32 hard x-ray undulators were delivered



Undulator hall SXR install July 15 start



2 x 4K Cold box room



Cryo Plant 1 Installation underway



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LCLS-II Leadership Transition



John Galayda



Norbert Holtkamp



- LCLS-II Project Director changed from John Galayda to Norbert Holtkamp as of May 23, 2019
- The project is in its final phase with major components delivered. The transition reflects the change in project focus from design and procurement to integration and installation.
- Dr. Holtkamp will be dual-hatted as Deputy Director and command resources across the lab.

BES thanks John Galayda for 40+ years of leadership

First turn at NSLS VUV (1981)



Always safety first!

LCLS: We have a laser (2009)

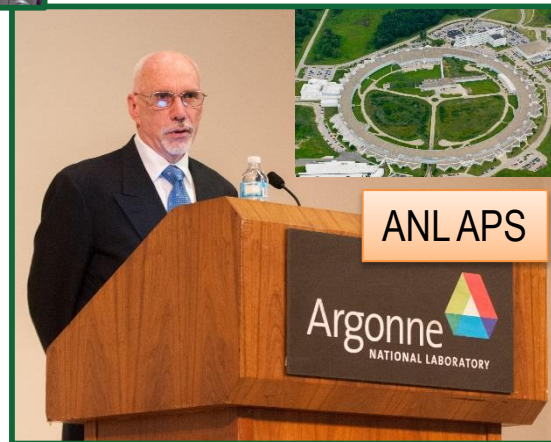


We have a laser: The Launch of LCLS (2009)

1,361 views

8 0 SHARE SAVE ...

Having cut his teeth as a pioneering member of the NSLS team, John went on to lead the construction of three premier BES light source facilities: APS, LCLS & LCLS-II...the BES community is truly grateful for all your many contributions!



ANL APS



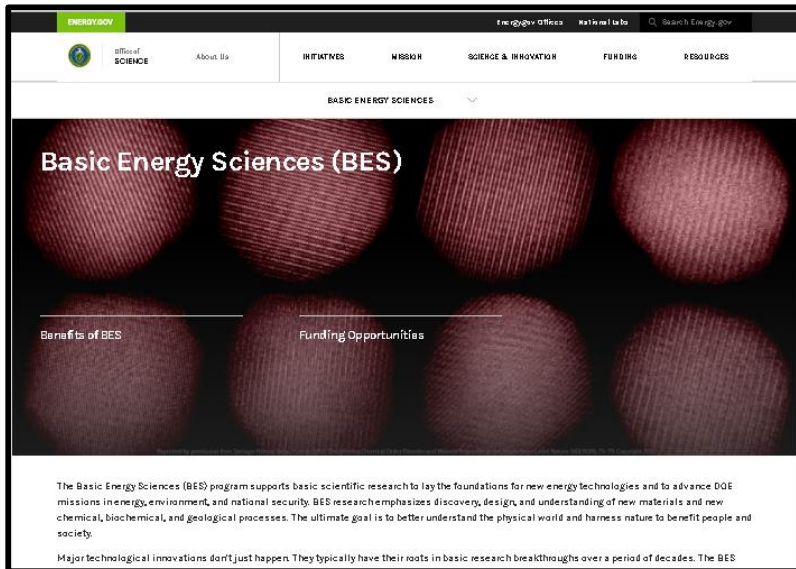
Secretary's Appreciation Award (2010)



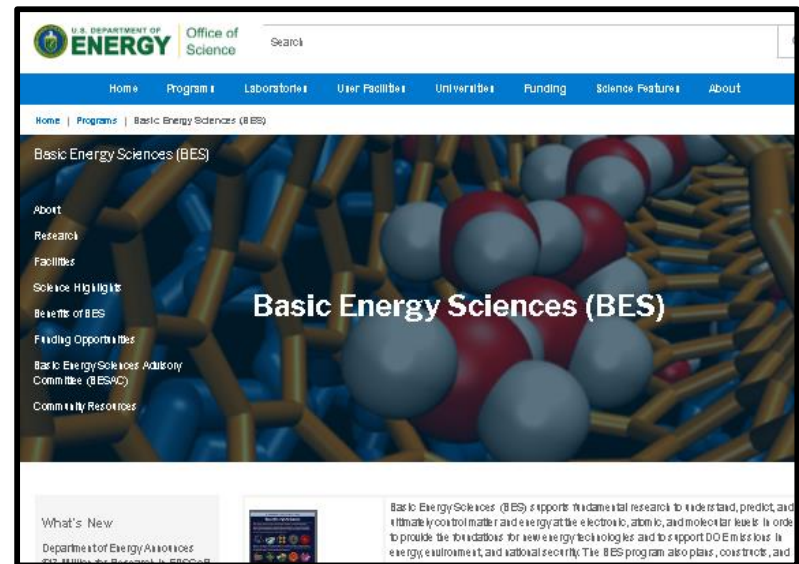
Office of Science Website Transition

- The previous science.energy.gov site has been replaced with two different websites:
 - A public-oriented energy.gov with Science Highlights, Program News, and more
 - A PI-oriented OSTI site (old SC website content) with FOAs, etc.

<https://www.energy.gov/science/bes>



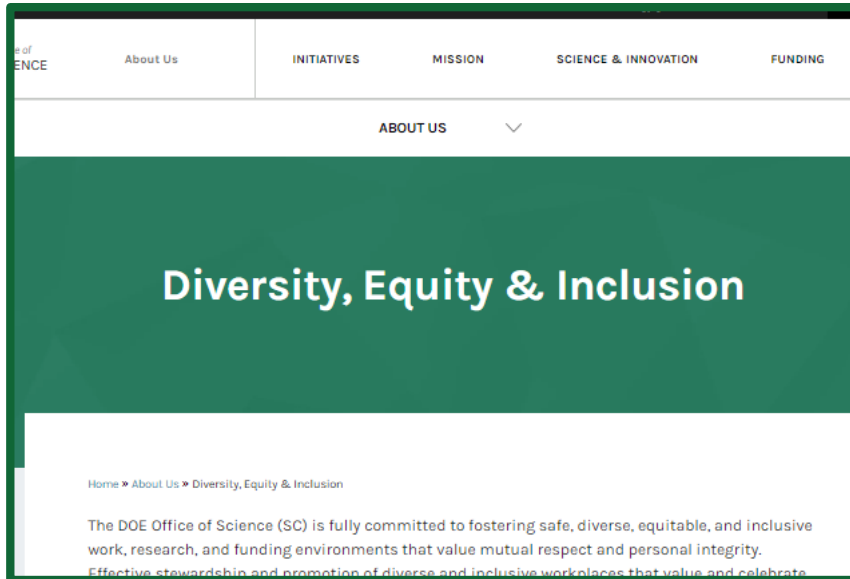
<https://science.osti.gov/bes>



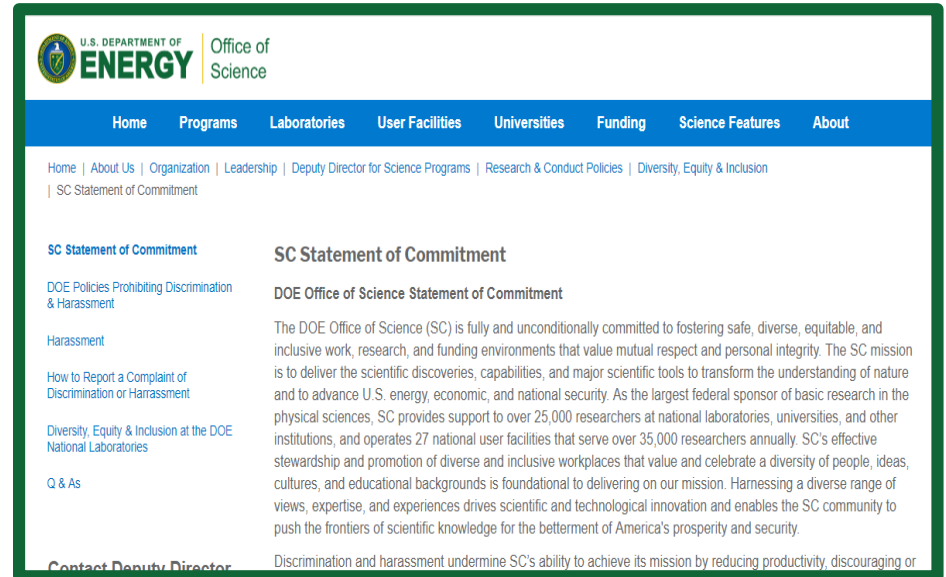
Upcoming BES Strategic Planning

- **Roundtable on Liquid Solar Fuels (August 2019)**
- **Roundtable on Artificial Intelligence Methods and Machine Learning (October 2019)**
- **Basic Research Needs for Transformative Manufacturing (December 2019)**

Office of Science Statements on Diversity, Equity, and Inclusion



<https://www.energy.gov/science/diversity-equity-inclusion>



<https://science.osti.gov/sc-2/Research-and-Conduct-Policies/Diversity-Equity-and-Inclusion/SC-Statement-of-Commitment>

The DOE Office of Science (SC) is fully committed to fostering safe, diverse, equitable, and inclusive work, research, and funding environments that value mutual respect and personal integrity.