Basic Energy Sciences Update

Board on Physics and Astronomy

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Associate Director of Science
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

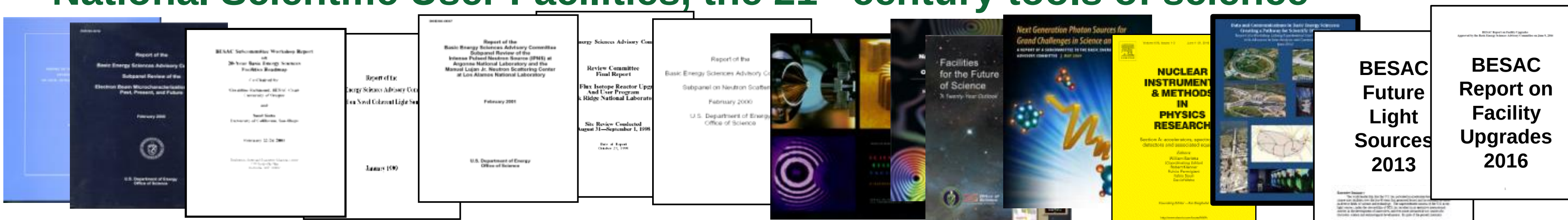
BES strategic planning activities provide the foundation for program strategy

2016 - 2018

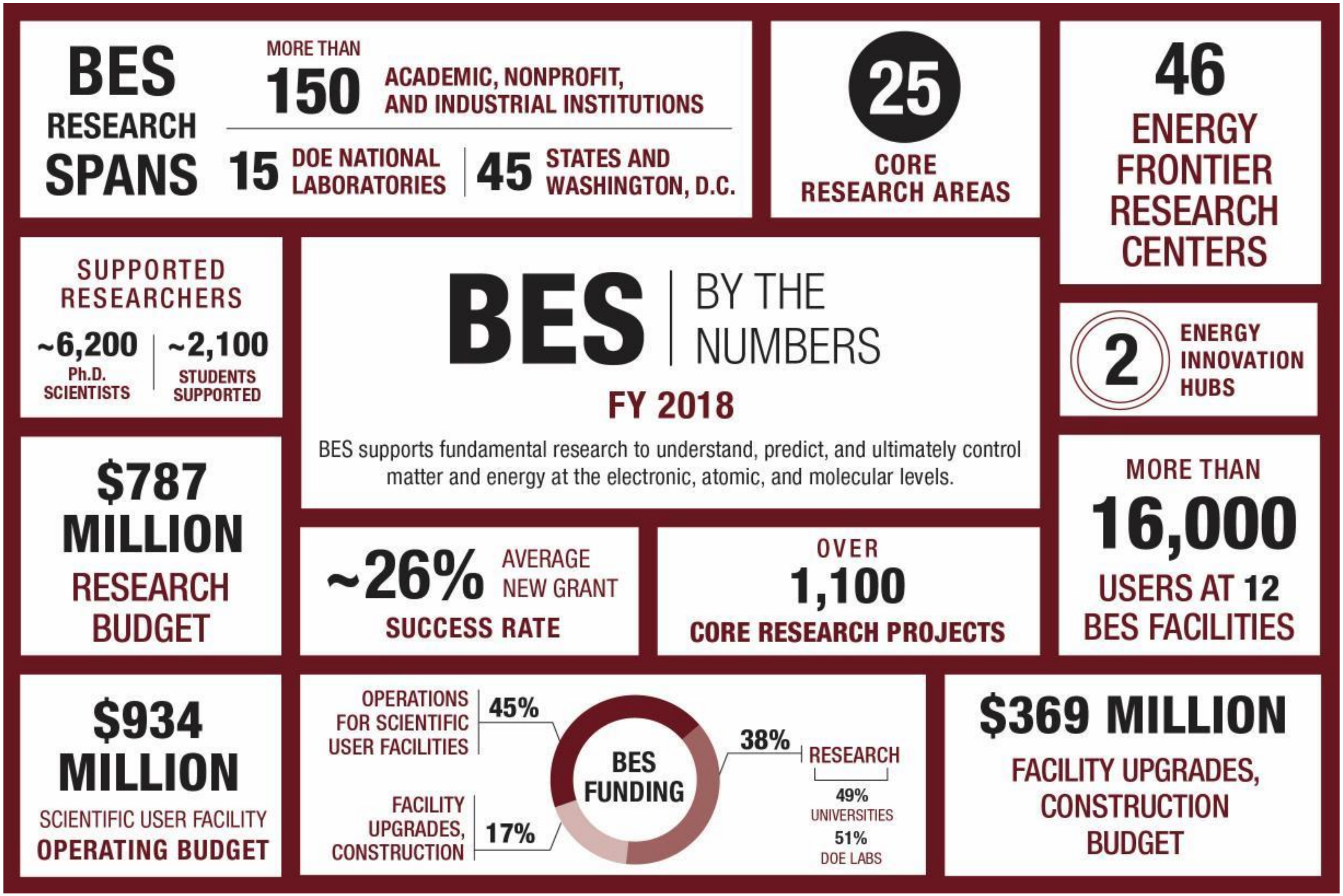
- **Science for Discovery**

- **Science for National Needs**

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



Basic Energy Sciences At a Glance (2018)



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.

National Quantum Initiative Act

H.R. 6227 passed by Congress on 12/13/2018 and signed into law on 12/21/2018

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.

National Quantum Initiative Act

H.R. 6227 passed by Congress on 12/13/2018 and signed into law on 12/21/2018

Department of Energy

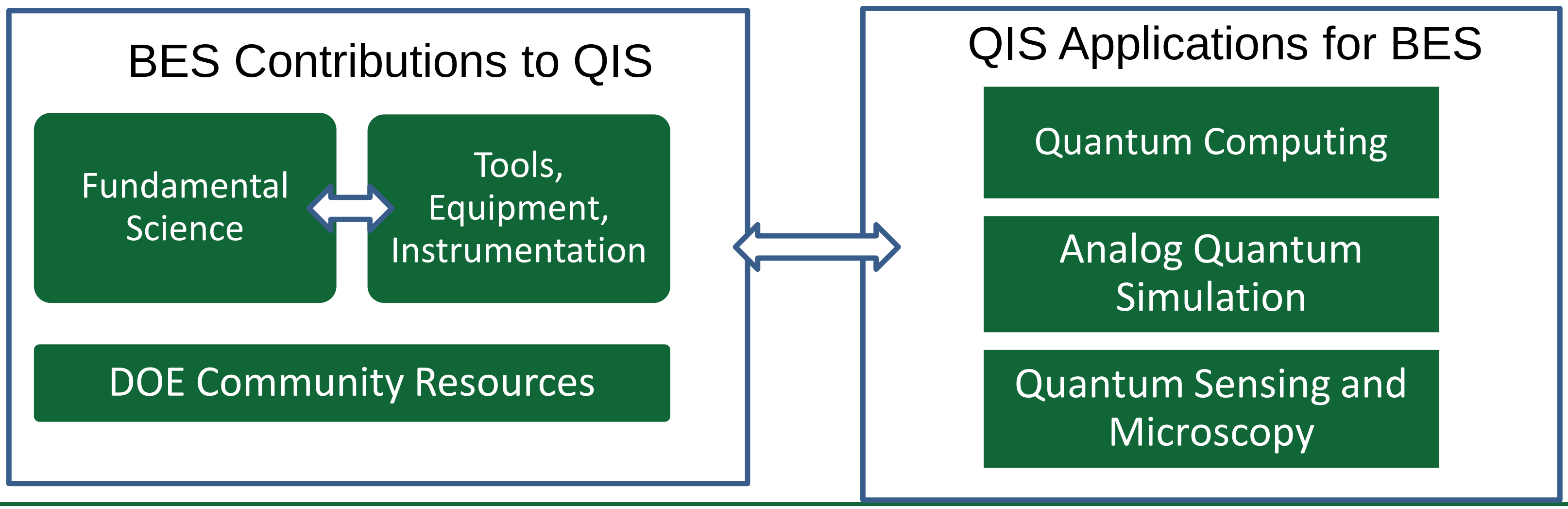
The Committee recognizes **DOE's capabilities, research infrastructure, and expertise in materials science, physics, applied mathematics, and computer science provide a foundation** for significant advances in QIS research and technological development. In particular, the **DOE National Laboratories,** 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.

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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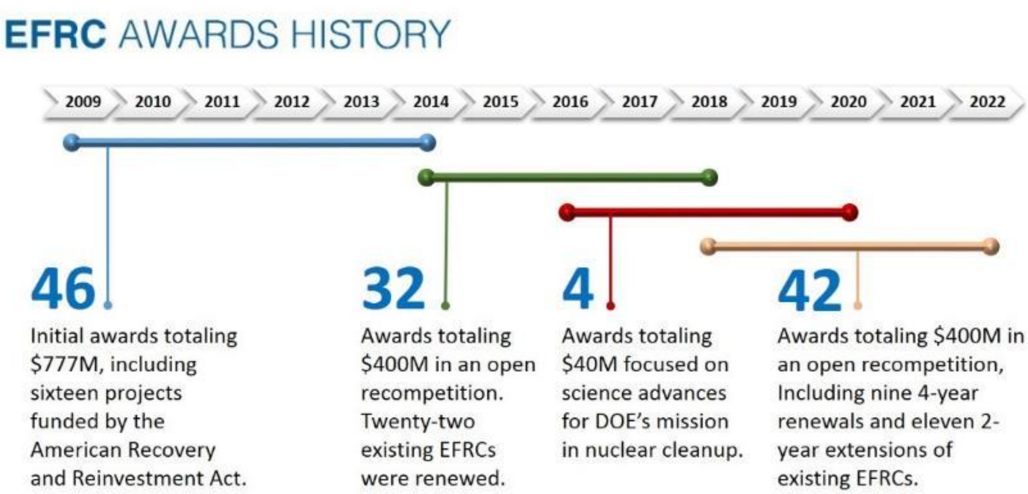
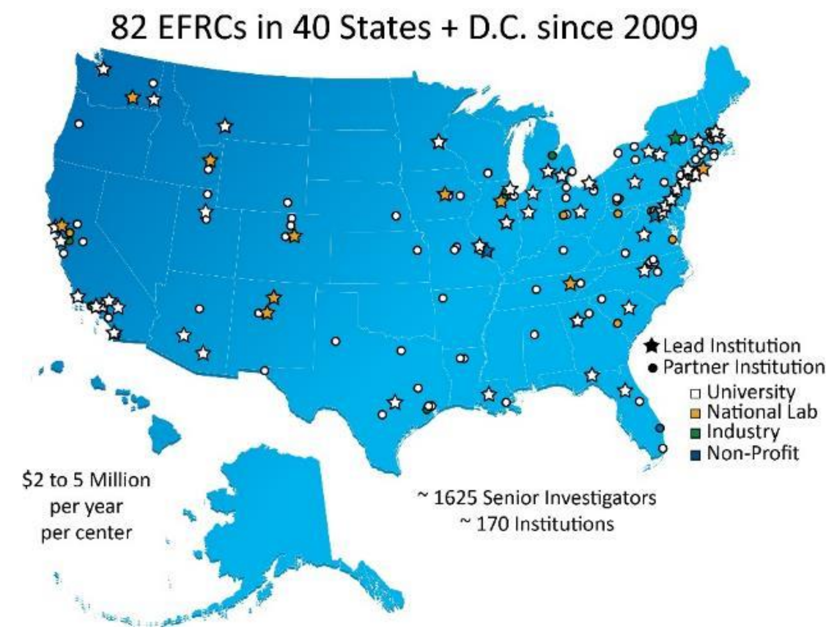
Energy Frontier Research Centers





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)

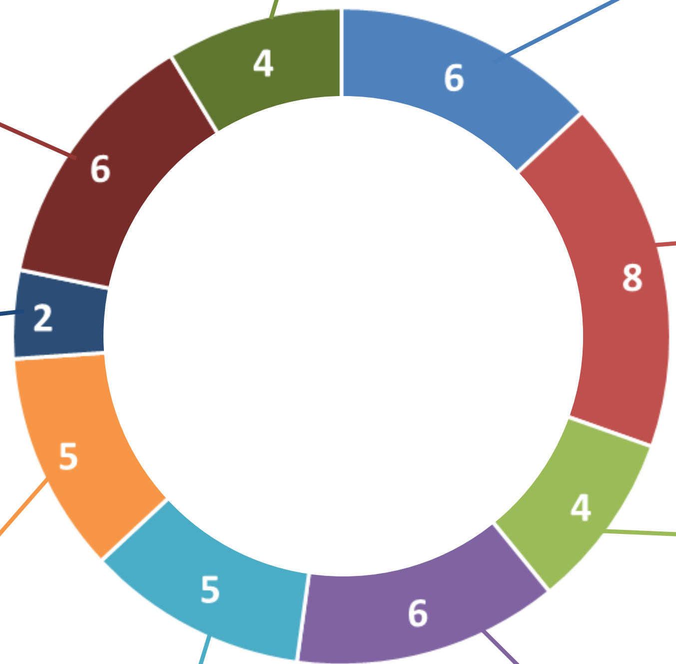
- ❑ Recompetition of four-year EFRC awards made in FY2016, which focused on science relevant to DOE's environmental management mission.
- ❑ Solicitation of proposals for new EFRCs that are responsive to recent BES workshop reports, including use-inspired science relevant to advanced microelectronics 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.

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

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



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

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

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

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

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

- 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

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)

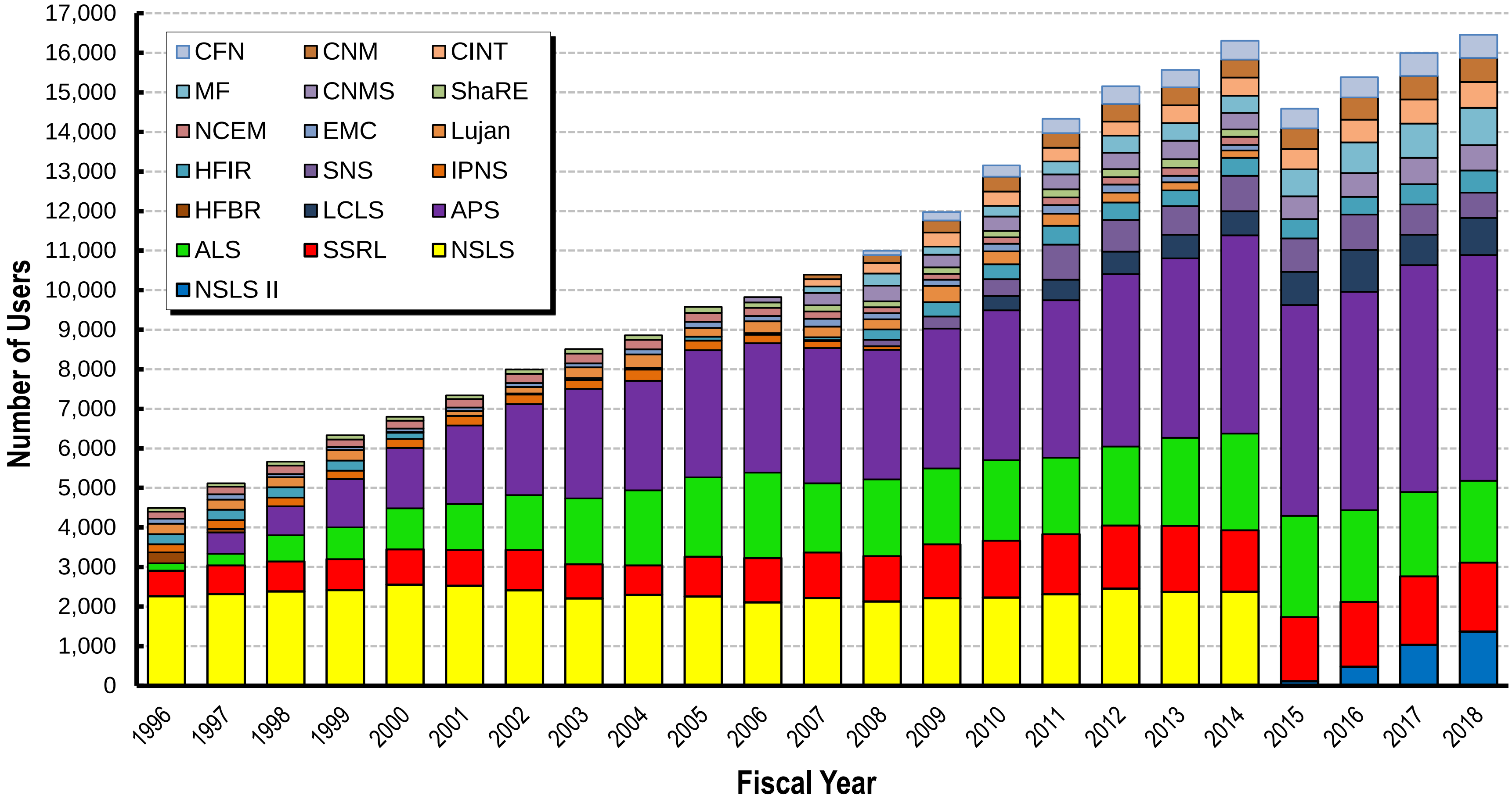
Neutron Sources

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

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 >16,000 Users in FY 2018



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

Movie of summed 11 microsecond frames showing accumulation of single electron hits at 91kHz

4D = Dynamic Diffraction Direct Detector

- ***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.***

Contributors: Jim Ciston, Ian J. Johnson, Brent R. Draney, Peter Ercius, Erin Fong, Azriel Goldschmidt, John M. Joseph, Jason R. Lee, Alexander Mueller, Colin Ophus, Ashwin Selvarajan, David E. Skinner, Thorsten Stezelberger, Craig S. Tindall, Andrew M. Minor, and Peter Denes

Light Sources: Global Race to the Top

60+ Facilities Worldwide and Growing

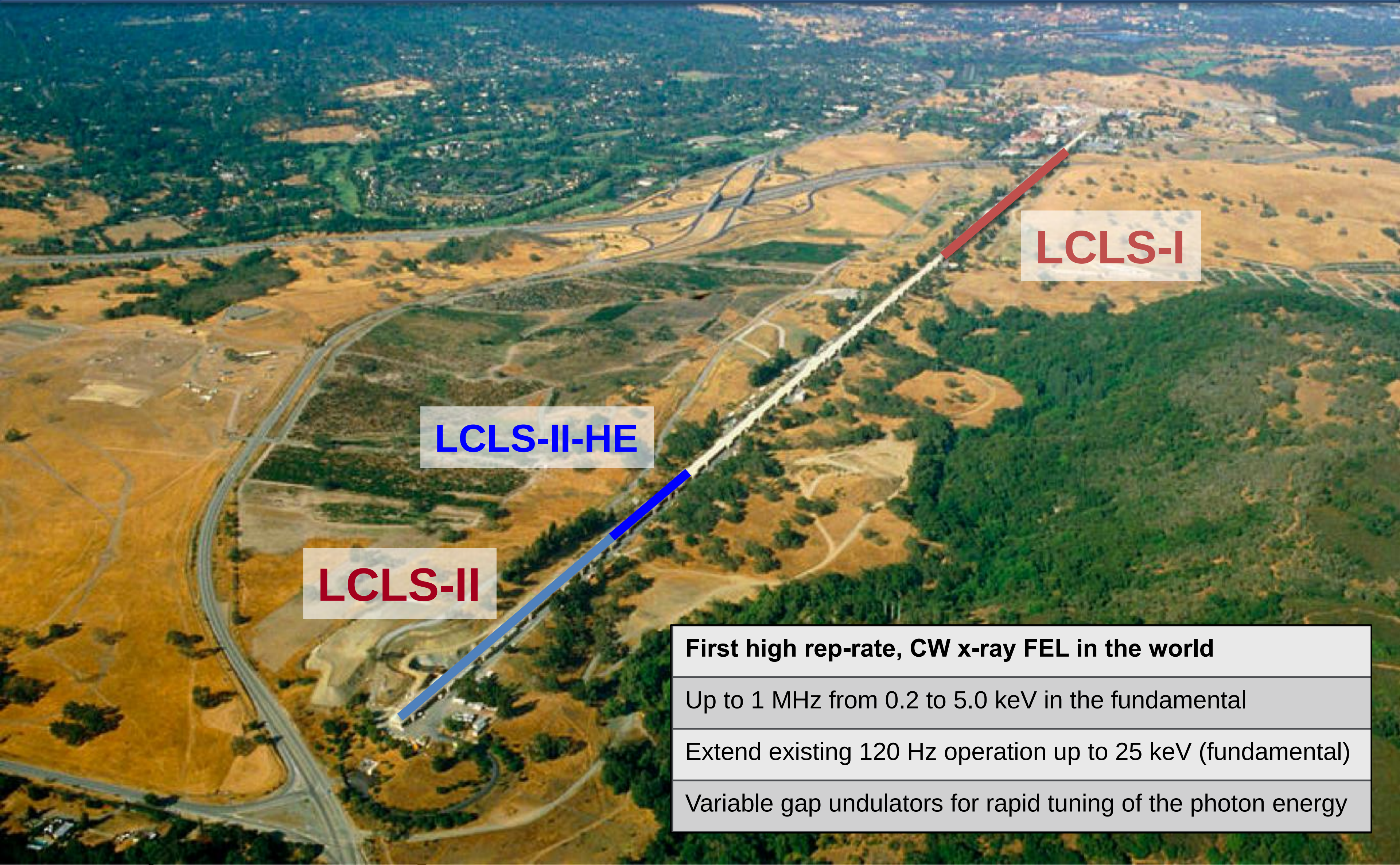
BES Light Sources | Ring Upgrades | *New Rings* | Upgraded & New FELs

ENERGY | Office of Science

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



First high rep-rate, CW x-ray FEL in the world
Up to 1 MHz from 0.2 to 5.0 keV in the fundamental
Extend existing 120 Hz operation up to 25 keV (fundamental)
Variable gap undulators for rapid tuning of the photon energy

BESAC Report on Facility Upgrades (June 2016)

Project	ANL APS-U	LBNL ALS-U	ORNL SNS PPU	ORNL SNS STS	SLAC LCLS-II	SLAC LCLS-II-HE
Proposed Project	Hard X-ray ~Diffraction Limited 6 GeV MBA Ring	Soft X-ray ~Diffraction Limited 2 GeV MBA Ring	Proton Power Upgrade to 2.8 MW (W Target) 1.3 GeV SC Linac	High Resolution Neutron Science; Second Target Station	High Rep-Rate, Soft X-ray FEL, 4 GeV SC Linac	High Rep-Rate, Medium Energy X-ray FEL, 8 GeV SC Linac
Current Status of Facility	APS is operational since 1996; ring will be replaced	ALS is operational since 1993; ring will be replaced	SNS Linac is operational since 2006 at 0.94 GeV	SNS is operational since 2006	LCLS is operational since 2010; LCLS-II is under construction	LCLS is operational since 2010; LCLS-II is under construction
Worldwide Competition	EU **ESRF** Germany **PETRA3,4** Japan **SPring-6** China **HEPS**	Sweden **MAX-IV** Brazil **SIRIUS** CH **SLS-II**	EU **ESS** Japan **JPARC** China **CSNS** UK **ISIS**	EU **ESS** Japan **JPARC** China **CSNS** UK **ISIS**	EU **XFEL** Japan **SACLA** Korea **PAL XFEL** CH **Swiss FEL**	EU **XFEL** China **SCLF**
Status Q2/19	CD-2 CD-3B	CD-1	CD-1 CD-3A	CD-0	CD-3	CD-1
FY19 Approp	✓	✓	✓	✓	✓	✓

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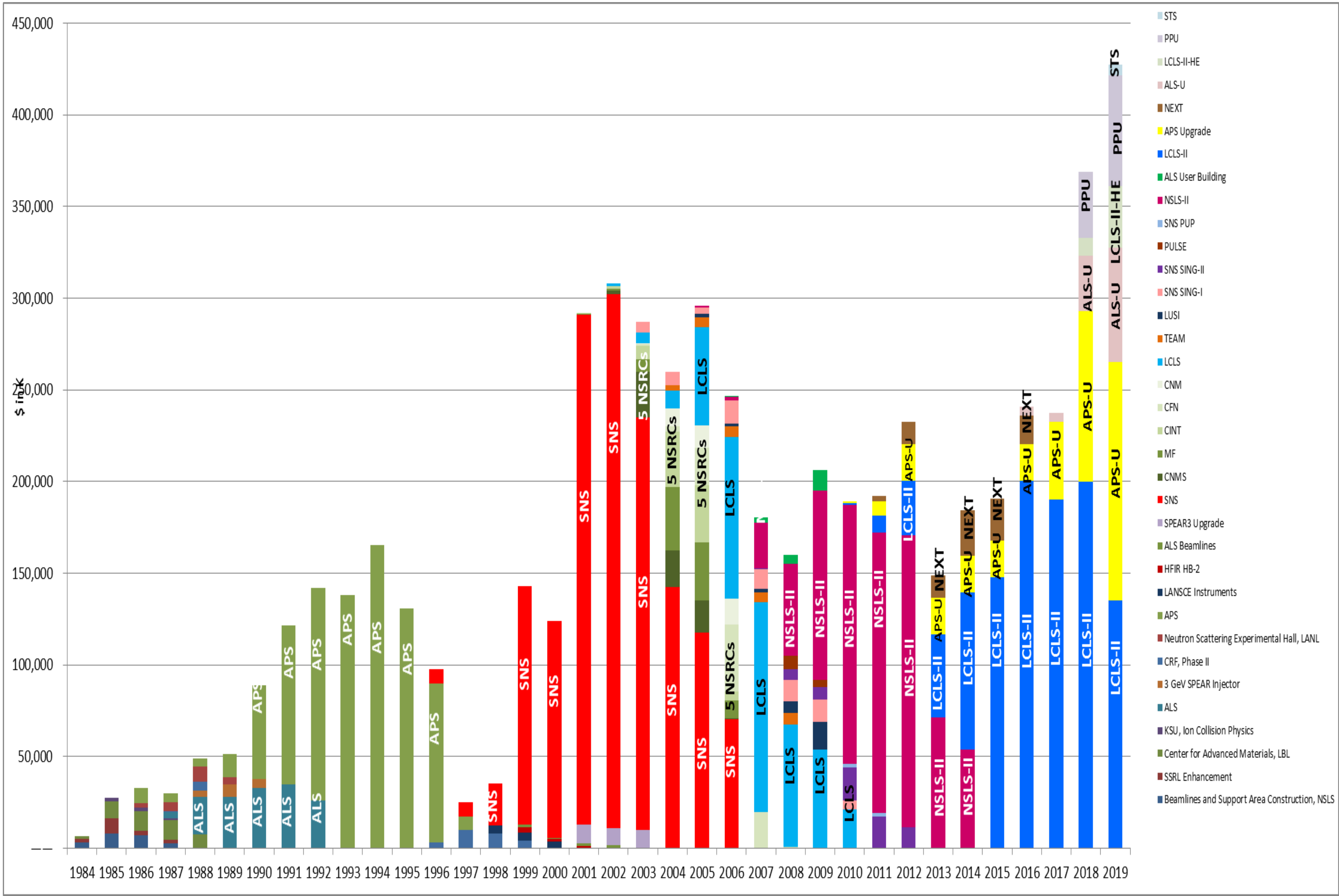
SC Critical Decision Matrix

	TOTAL PROJECT COST (TPC) / DECISION / REQUIREMENTS[1] / APPROVAL[2]	$750M or more	Less than $750M to $400M	Less than $400M to $100M	Less than $100M to $50M*	Less than $50M* to $20M	Less than $20M to $10M** Delegation Allowed
	Prior to CD0, Approve Mission Need Statement	Reviewed by SC-28 (SC-28) Approved by SC-1	Reviewed by SC-28 Approved by SC-1	Reviewed by SC-28 Approved by SC-1	Reviewed by SC-28 Approved by SC-1	Reviewed by SC-28 Approved by SC-1	Reviewed by SC-28 Approved by SC-AD
	PRIOR TO CD-4--PROJECT COMPLETION	Reviewed by SC-28 Approved by SC-1	Reviewed by SC-28 Approved by SC-1	Reviewed by SC-28 Approved by SC-2	Reviewed by SC-28 Approved by SC-AD	Reviewed by SC-28 Approved by SC-AD	Reviewed by SC-28 Approved by SC-AD
CRITICAL DECISIONS	CD-0--APPROVE MISSION NEED	S-2 (CD-1 to 4 delegated, see below)	SC-1	SC-1	SC-AD	SC-AD	SC-AD
CRITICAL DECISIONS	CD-1--APPROVE ALTERNATIVE SELECTION AND COST RANGE	S-4	SC-1	SC-1	SC-AD	SC-AD	SC-AD
CRITICAL DECISIONS	CD-2 --APPROVE PERFORMANCE BASELINE	S-4	SC-1	SC-2	SC-AD	SC-AD	SC-AD
CRITICAL DECISIONS	CD-3--APPROVE START OF CONSTRUCTION	SC-1	SC-1	SC-2	SC-AD	SC-AD	SC-AD
CRITICAL DECISIONS	CD-4--APPROVE START OF OPERATIONS OR PROJECT COMPLETION	SC-1	SC-1	SC-2	SC-AD	SC-AD	SC-AD
BASELINE MANAGEMENT – Changes to TPC	Deviations	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					
BASELINE MANAGEMENT – Changes to TPC	Ne						SC-2
BASELINE MANAGEMENT – Changes to TPC							ies external to the Department.
BASELINE MANAGEMENT – No TPC Change – Routine Project Changes/ Control							SC AD
BASELINE MANAGEMENT – No TPC Change – Routine Project Changes/ Control							Prog. Mgr., SOM or FPD
BASELINE MANAGEMENT – No TPC Change – Routine Project Changes/ Control							Contractor
a	Mission Validation Independe						SC-AD
a	Design Review Prior to CD-1,						Team External to Project
a	Conduct Independent Project Independent Review prior to						Prior to CD-2 & CD-3 Tailored by SC-28
a	SC-AD Request Annual Peer						SC-28 Tailored
a	Performance Baseline Deviat						SC-28
a	EVMS Review--Certification Prior to CD-3 & Bi-annual Surveillance (annual by contractor)	SC-28	SC-28	SC-28	SC-28	SC-28	N/A
a	ORR/RA--Operational Readiness Review/Readiness Assessment Prior to CD-4	Team External to Project	Team External to Project	Team External to Project	Team External to Project	Team External to Project	Team External to Project
a	Technology Readiness Assessment (TRA) prior to CD-2 and 3 by SAE or AE	N/A	N/A	N/A	N/A	N/A	N/A
a	Project Definition Rating Index (PDRI) by APM	N/A	N/A	N/A	N/A	N/A	N/A
a	*Hazard Cat. 1,2,3 Nuclear Facility--Technical IPR Prior to CD-2*	*PSO*	*PSO*	*PSO*	*PSO*	*PSO*	*PSO*
REPORTING	Monthly PARS II Reporting (EVMS for Projects>$20 M)	Project Status After CD-0 and EV After CD-2					Monthly Project Status After CD-0
REPORTING	Monthly or Quarterly Project Reporting (QPR) or Meeting after CD-0	SC-AD Invite SC-1 and SC-28	SC-AD Invite SC-1 and SC-28	SC-AD Invite SC-2 and SC-28	SC-AD to invite SC-28	SC-AD to invite SC-28	SC-AD to invite SC-28

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

BES Construction/MIE Funding Profile 1984 – 2019



New BESAC Charge from Dr. Binkley (Feb. 25, 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?*

BES Roundtable on Chemical Upcycling of Polymers

Workshop Chair: Phillip Britt (ORNL)
Co-Chairs: Geoff Coates (Cornell Univ.)
Karen Winey (Univ. of Penn.)
SC Technical Lead: Bruce Garrett

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

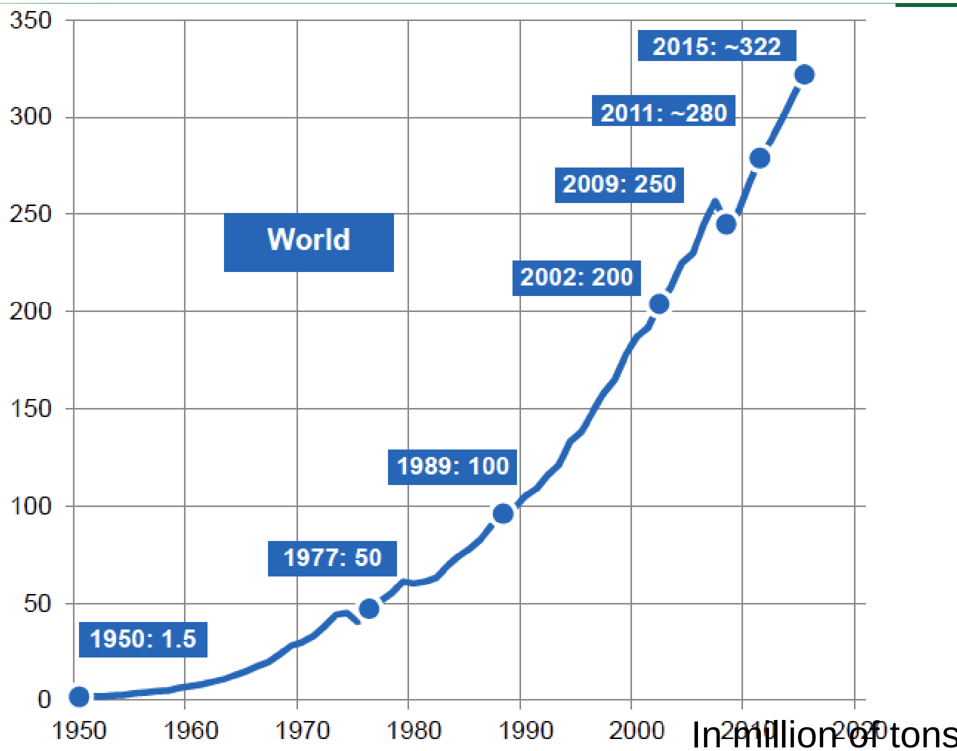
https://science.energy.gov/~/media/bes/besac/pdf/201903/day2/940_Britt_BESAC_Chemical_Upcycling_of_Polymers.pdf

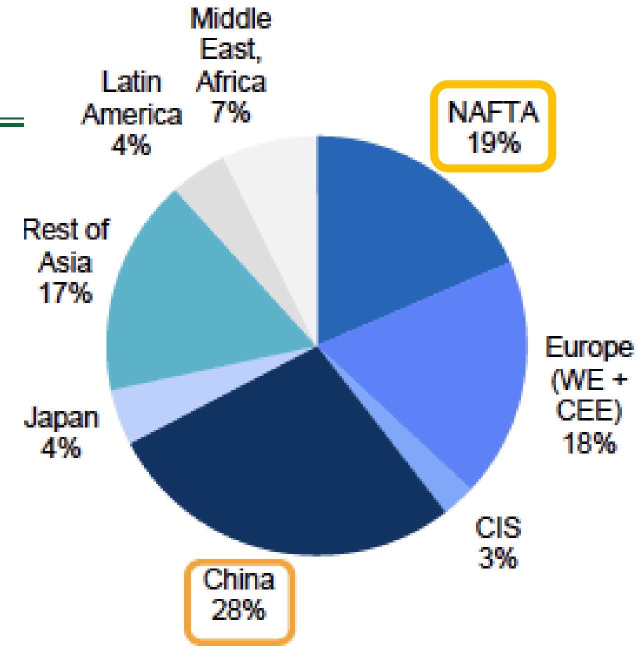
Motivation for Chemical Upcycling of Polymers

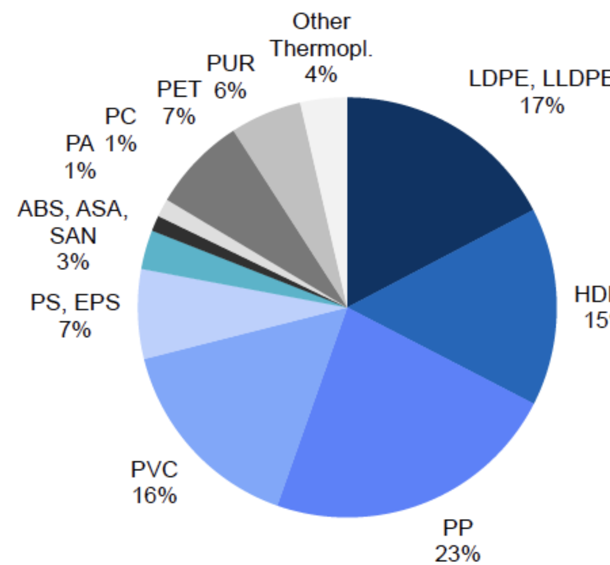
- In the US, plastic materials contribute 13% (34.5M tons) to municipal solid wastes in 2015 with less than 10% recycled, approximately 15% combusted for energy recovery, and the remained sent to the landfill (75%)[1]
- Most recycling of plastic wastes typically involves mechanical processes (primary 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

[1] *Advancing Sustainable Materials Management: 2015 Fact Sheet*; EPA530-F-18-004; UE EPA : Washington, DC, July, 2018.
[2] Rahimi, A.; García, J. M. *Nat. Rev. Chem.* **2017**, *1, Article Number* 0046

Globally Plastics are Growing





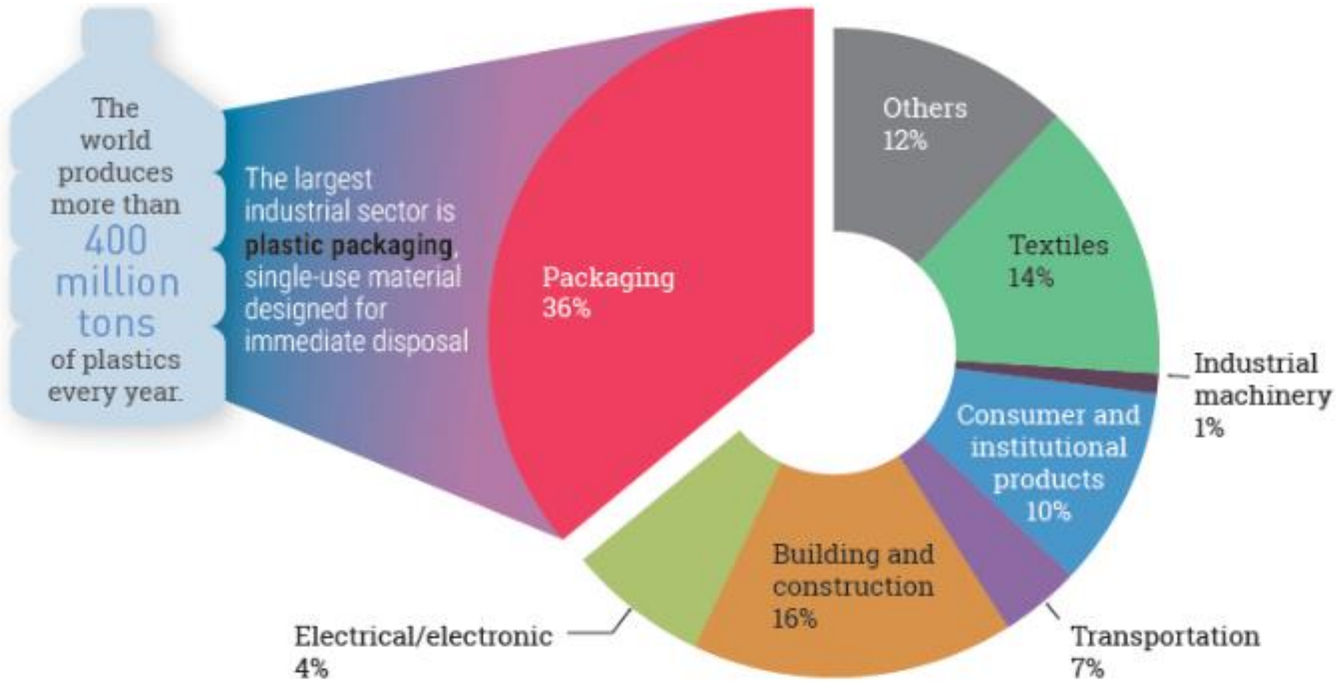


- If plastic production continues its current growth rate, then the plastics industry may account for 20% of the world's total oil consumption
- In 2015, global plastic waste disposal
  - Discard: 55%; Recycle: 19.5 %; Incineration: 25.5%

https://committee.iso.org/files/live/sites/tc61/files/
The%20Plastic%20Industry%20Berlin%20Aug%202016%20-%20Copy.pdf

Global Industrial Use of Plastics

- **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%)



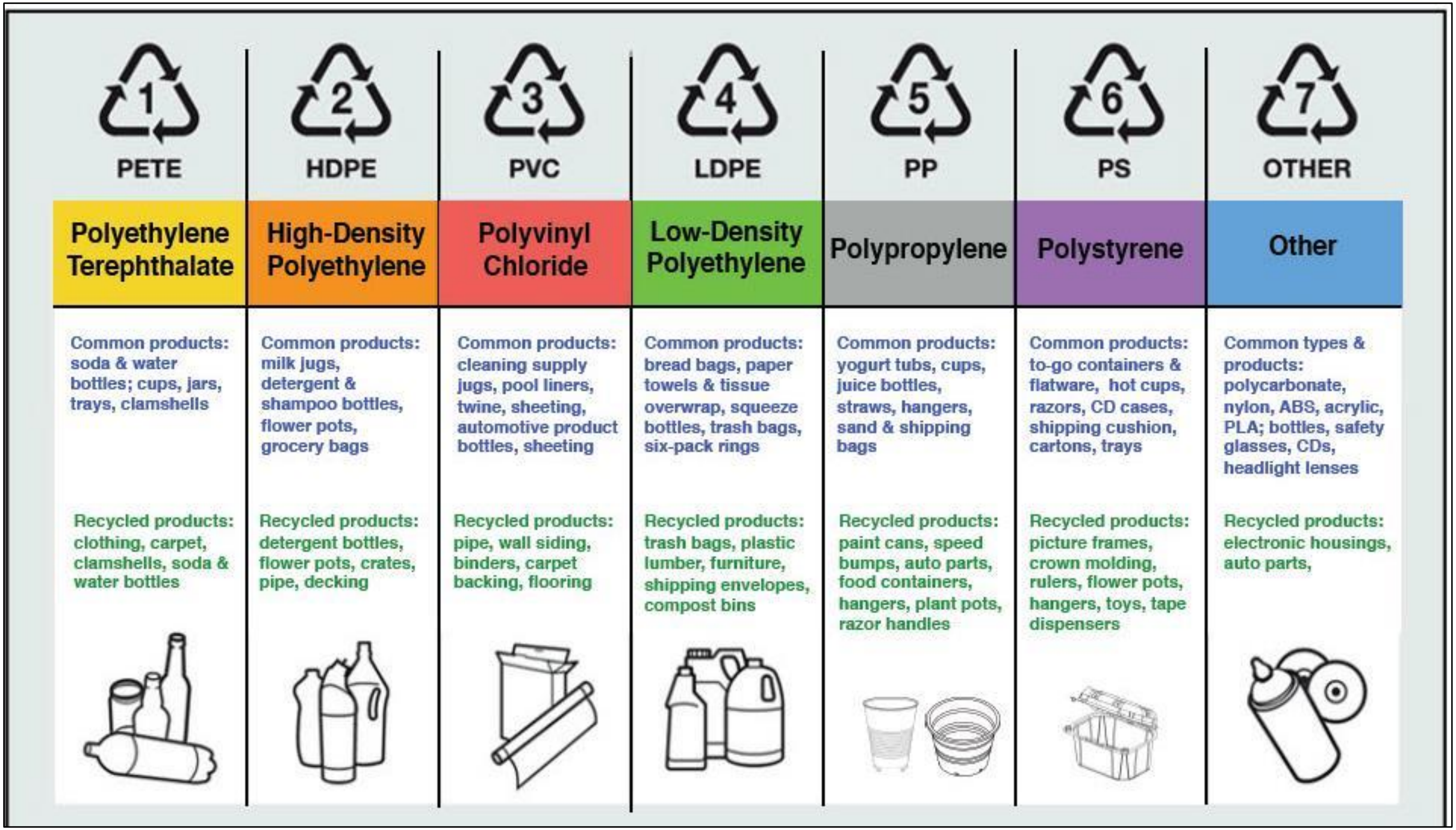
Global Flow of Packaging Waste

40% Landfill
32% Leakage
14% Incinerated
14% Recycled

Adapted from Geyer, R., et al. Sci. Adv. **2017**, *3,* e1700782

- **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*

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



19.5 %	10%	0 %	5 %	1 %	1 %	varies

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https://www.bluelinelabels.com/glossary-of-resins-containers-decorating/
https://science.energy.gov/~/media/bes/besac/pdf/201903/day2/940_Britt_BESAC_Chemical_Upcycling_of_Polymers.pdf

New BESAC Charge from Dr. Binkley (Feb. 5, 2019)

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?*

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