Basic Energy Sciences Update

BES Advisory Committee Meeting

July 12, 2018

Harriet Kung
Director, Basic Energy Sciences
Office of Science, U.S. Department of Energy

Outline

- BES Staffing Update
- FY 2018 Appropriation & FY 2019 Budget Status
- FY 2018 Solicitations Update
- Program Highlights

Office of Basic Energy Sciences

Harriet Kung, Director

BES Budget and Planning
- Vacant, Financial Management
- Donetta Herbert, Financial Management
- Thomas Russell, Senior Technical Advisor

BES Operations
- Robin Hayes, Program Manager
- Kerry Hochberger, Program Support Specialist
- Natalia Melcer, Program Manager
- 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
Teresa Crockett, Program Analyst
Vacant, Secretary

Materials Discovery, Design, and Synthesis
Helen Kerch, Acting
Vacant, P.A.
- **Materials Chemistry** – Craig Henderson, Michael Sennett
- **Biomolecular Materials** – Mike Markowitz
- **Synthesis and Processing Science** – Bonnie Gersten
- **Batteries and Energy Storage Hub; Technology Coordination** – Craig Henderson, John Vetrano

Condensed Matter and Materials Physics
Jim Horwitz
Vacant, P.A.
- **Experimental Condensed Matter Physics** – Michael Pechan
- **Theoretical Condensed Matter Physics** – Jim Davenport, Matthias Graf
- **Physical Behavior of Materials** – Refik Kortan
- **Mechanical Behavior and Radiation Effects** – John Vetrano

Scattering and Instrumentation Sciences
Helen Kerch
Vacant, P.A.
- **X-ray Scattering** – Lane Wilson
- **Neutron Scattering** – Thiyaga P. Thiyagarajan
- **Electron and Scanning Probe Microscopies** – Jane Zhu
- **Experimental Program to Stimulate Competitive Research (DOE EPSCoR)** – Tim Fitzsimmons

Scientific User Facilities Division
James Murphy, Director
Vacant, Program Support Specialist
Rocio Meneses, Program Assistant

Operations
- **X-ray and Neutron Scattering Facilities** – Peter Lee, Thiyaga P. Thiyagarajan
- **NSRCs **** – George Maracas
- **Accelerator and Detector Research** – Eliane Lessner
- **Facilities Coordination; Metrics; Assessment** – Van Nguyen

** Nanoscale Science Research Center

Construction
- **Linac Coherent Light Source-II** – Phil Kraushaar
- **Facilities Upgrades and MIE*** Projects** – Phil Kraushaar, Ed Stevens

*** Major Items of Equipment

Chemical Sciences, Geosciences, and Biosciences Division
Bruce Garrett, Director
Vacant, Program Assistant

Fundamental Interactions
Jeff Krause
Vacant, P.A.
- **Atomic, Molecular, and Optical Sciences** – Tom Settersten
- **Gas Phase Chemical Physics** – Wade Sisk
- **Condensed Phase and Interfacial Molecular Science** – Gregory Fiechtner
- **Computational and Theoretical Chemistry** – Mark Pederson

Photochemistry and Biochemistry
Gail McLean
Vacant, P.A
- **Solar Photochemistry** – Christopher Fecko, Vacant
- **Photosynthetic Systems** – Stephen Herbert
- **Physical Biosciences** – Robert Stack
- **Fuels from Sunlight Energy Innovation Hub** – Christopher Fecko

Chemical Transformations
Raul Miranda
Vacant, P.A.
- **Catalysis Science** – Chris Bradley, Viviane Schwartz
- **Separation Science** – ~~Philip Wilk~~, △ Stefan Vajda, Vacant
- **Heavy Element Chemistry** – Philip Wilk
- **Geosciences** – James Rustad

New
Vacancy

LEGEND
△ Detailee from ANL

FY 2017 – FY 2019 BES Budget

FY 2017 Enacted: $1.871B

FY 2018 Enacted: $2.09B (Request: $1.554B)

FY 2019 President's Request: $1.85B (HEWD: $2.129B; SEWD: $2.193B)

Priorities:

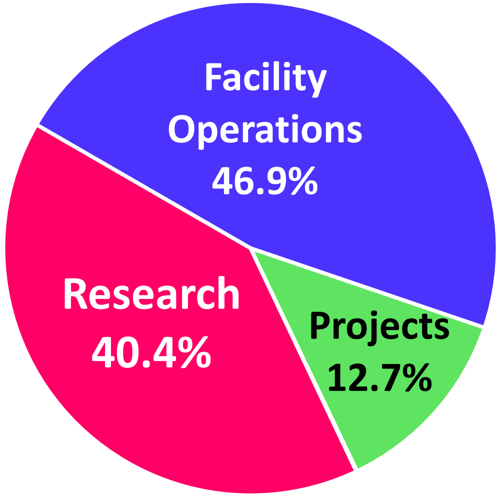
- **Continue support of all Core Research Areas, EFRCs, Hubs, and CMS/CCS**
- **Continue support of all 12 scientific user facilities at near optimal operation level**
- **Expand quantum information science (an SC-wide QIS initiative) and other research priorities following strategic planning reports**
- **Support facility upgrades per 2016 BESAC prioritization study**

BES Budget by Budget Element: 2017 - 2019

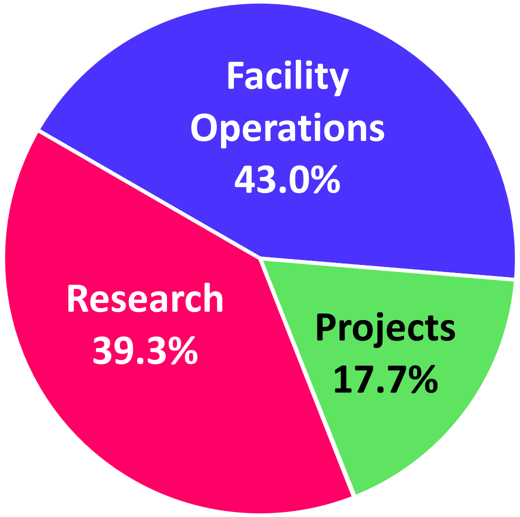
	FY 2017		FY 2018		FY 2019			
	Enacted	% of Total	Enacted	% of Total	President's Request	% of Total	vs. FY18 $ Change	vs. FY18 % Change
Research	755,669	40.4%	821,403	39.3%	746,269	40.3%	-75,134	-9.1%
Facility Operations	877,331	46.9%	898,597	43.0%	878,331	47.5%	-20,266	-2.3%
Projects (Const/MIE)	237,500	12.7%	369,000	17.7%	224,400	12.1%	-144,600	-39.2%
Other	1,000	0.1%	1,000	0.0%	1,000	0.1%	0	0.0%
Total	**1,871,500**	100.0%	**2,090,000**	100.0%	**1,850,000**	100.0%	-240,000	-11.5%

*Other Includes GPP.

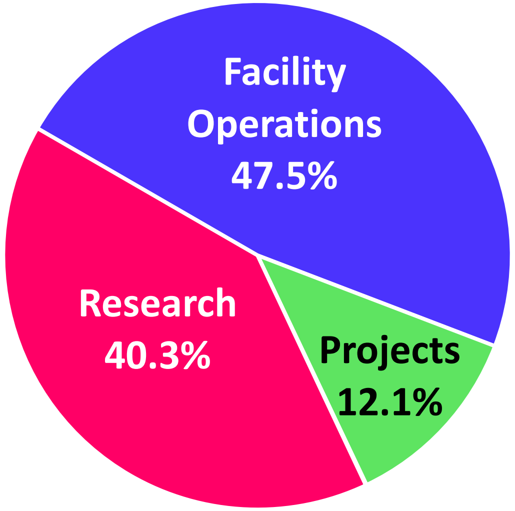
FY 2017



FY 2018



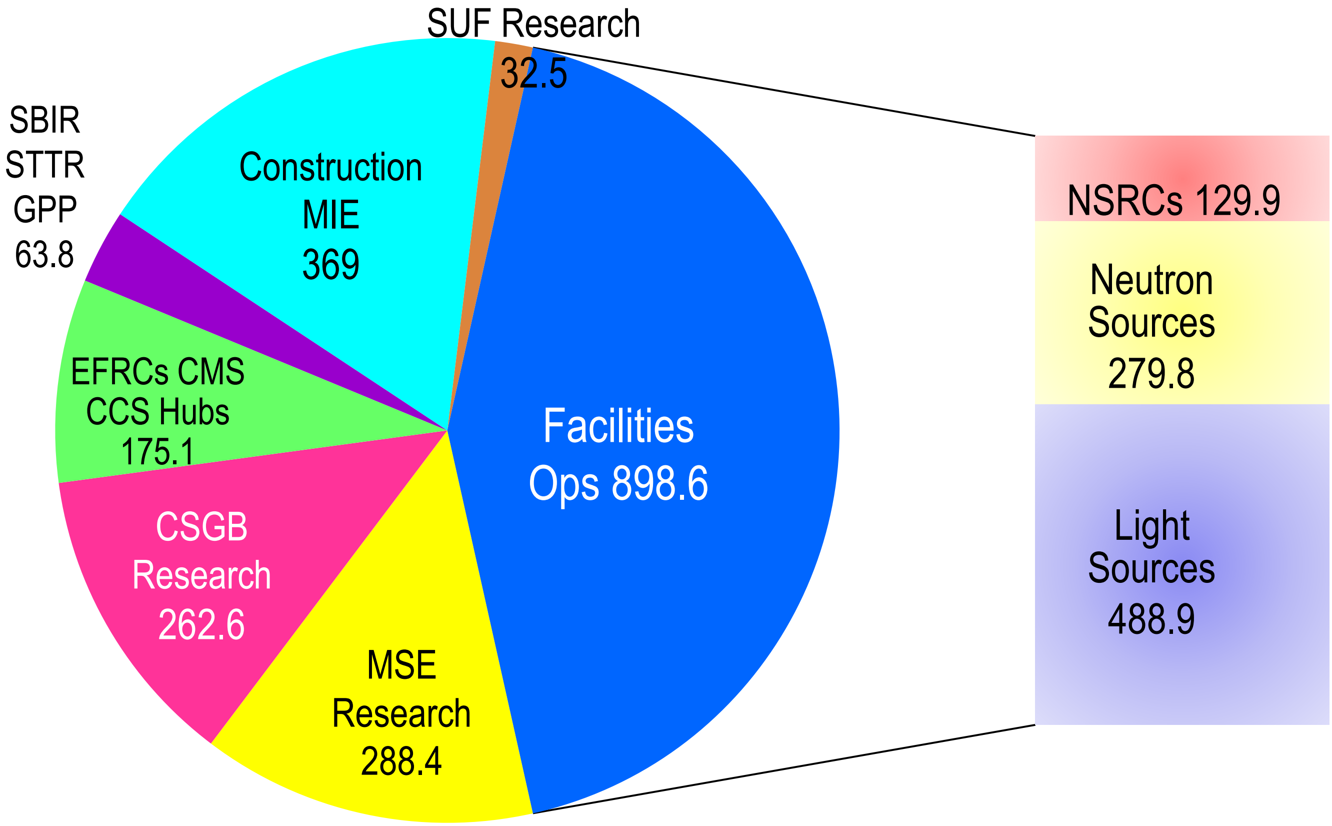
FY 2019 Request



FY 2018 BES Budget:
$2090.0M (+$218.5M or +11.7% from FY 2017)

Research programs

- Core Research ($551M; **Δ=+$62.9M**);
  - New and supplemental awards in key priority areas
  - Early Career Research Awards
  - New Solicitations in QIS, Ultrafast Science
- Computational Materials and Chemical Sciences continue ($26M)
- Energy Frontier Research Centers continue ($110M)
- Funding continues for Energy Innovation Hubs (JCAP & JCESR) ($39M).



Scientific user facilities

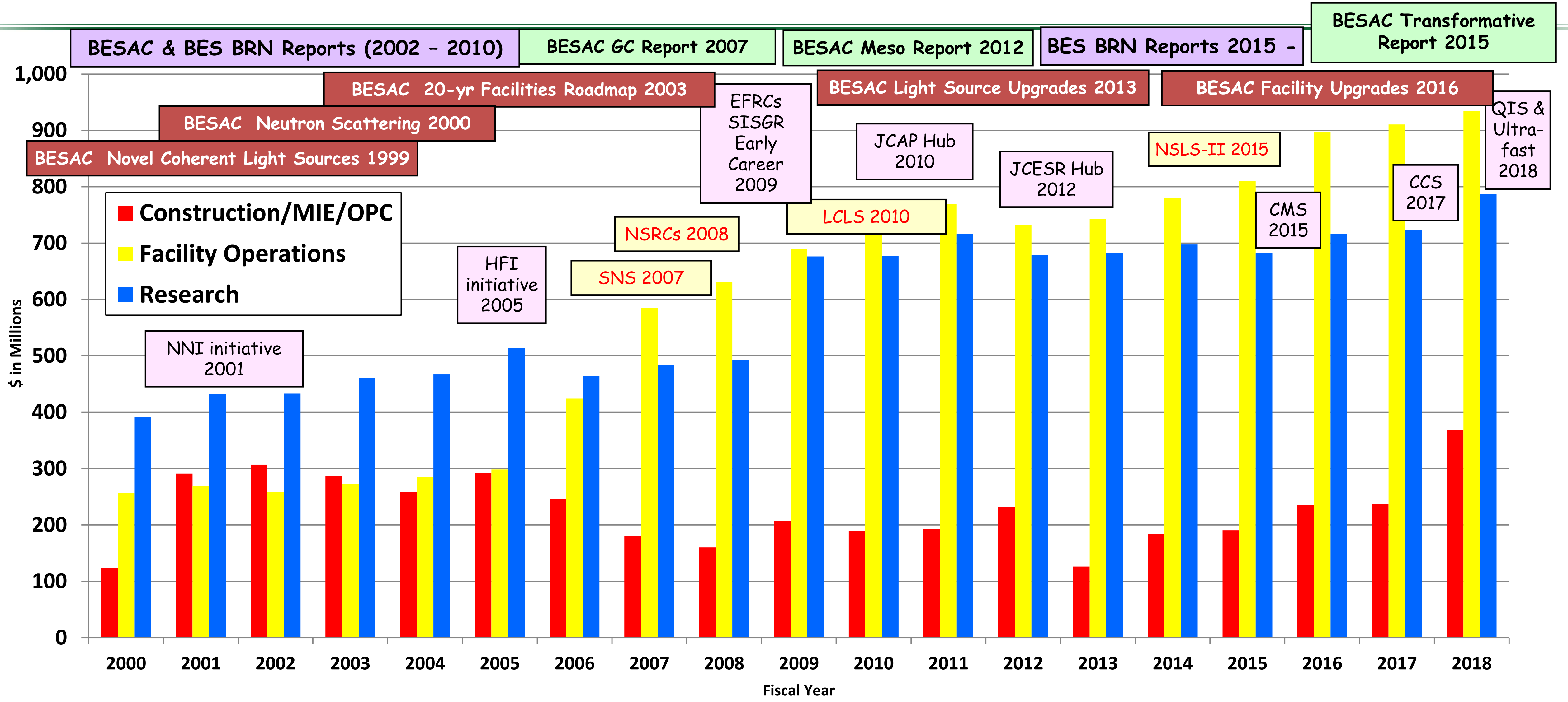
- Operations of 12 facilities at ≥ 95% optimal level ($898.6M; **Δ=+$21.3M**)
- $1M Lujan equipment disposition; $8.5M Long Term Surveillance and Maintenance

Construction/MIE* **Δ=+$131.5M**

- LCLS-II ($200M)
- Advanced Photon Source Upgrade($93M)
- Three new starts: LCLS-II-HE ($10M) and ALS-U ($30M); PPU ($36M)

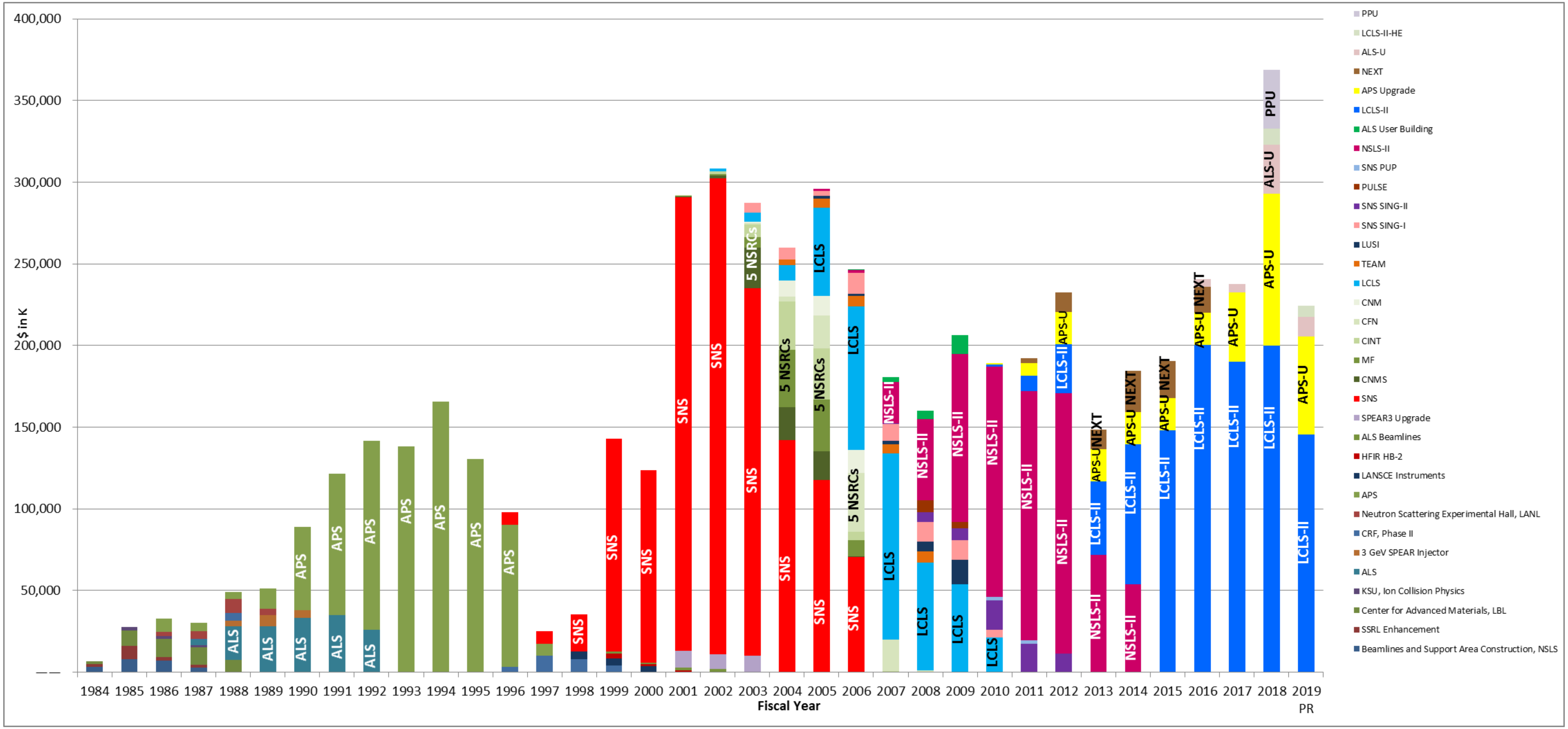
*includes OPC

BES Budget: 2000 - 2018



BES strives to maintain a balanced portfolio of research, facility operations, and construction.

BES Construction/MIE Funding Profile 1984 – 2019

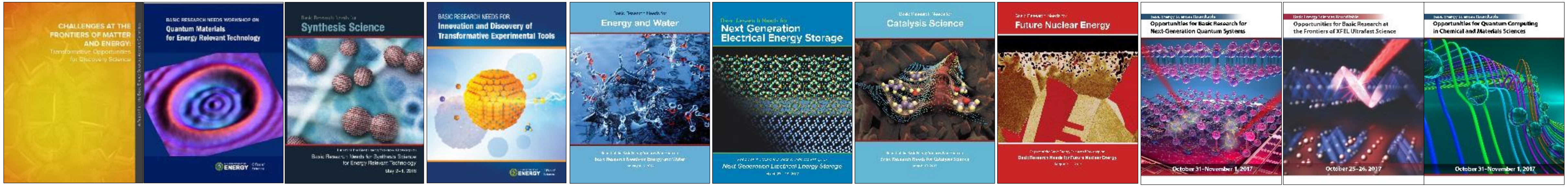


BES Scientific User Facility Upgrade Project Status

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 2.5 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**
Status Q2/18	**CD-3b**	**CD-0**	**CD-1**	**CD-0**	**CD-3**	**CD-0**
FY18 Approp	✓	✓	✓		✓	✓

FY 2018 – FY 2019 BES Research Priorities*

- **Quantum Information Science (QIS) – FY18 = $20M; FY19 = $32M**
  – By exploiting the intricate quantum mechanical phenomena, QIS will create fundamentally new ways of obtaining and processing information and open new vistas of science discovery and technology innovation. Research priorities were identified in two QIS roundtables held in October 2017.
- **Ultrafast Science FY18 = $10M; FY19 = $10M**
  – Ultrafast science remains a priority in both research divisions to position the U.S. leadership in this critical field of science and in anticipation of the completion of the LCLS-II construction project. Research priorities were identified in a roundtable held October 2017.
- **Computational Materials and Chemical Sciences - FY18 = $26M; FY19 = $26M**
  – Computational Materials Sciences (CMS) and Computational Chemical Sciences (CCS) are maintained in support of the Exascale Computing Initiative. CCS was funded in FY 2017 and is moved to a new budget line in the FY 2019 Request.
- **Materials and Chemical Sciences for Future Nuclear Energy**
  – Research will be supported to achieve a multi-scale spatial and temporal understanding of fundamental physical and chemical processes that govern the properties and performance of novel material systems and fuels required for advanced reactors.
- **Priorities identified by BES Advisory Committee and Basic Research Needs Reports**
  – Both the core research and EFRCs will emphasize emerging high priorities identified by the Basic Energy Sciences Advisory Committee and recent Basic Research Needs workshop reports.



*FY19 funding at President's request levels, including SBIR/STTR

Scientific User Facilities Operations
FY 2018 Enacted* & FY 2019 Request

- **In the FY 2018 Enacted budget, LCLS was increased by 1.3% or $1.7M over FY 2017 Enacted in preparation for completion of the LCLS-II construction project.**
- **The remaining light sources were decreased by 0.5% or $1.9M.**
- **Neutron facilities were increased by 5.2% or $13.8M.**
  - SNS increased by 2% or $4.1M; HFIR increased by 14.9% or $9.7M
- **NSRCs were increased by 6.3% or $7.7M, supporting optimal operations.**

<table>
<tr><th>% Optimal Operations</th><th>FY 2017 Enacted</th><th>FY 2018 Enacted</th><th>FY 2019 President’s Request</th></tr>
<tr><td>Linac Coherent Light Source</td><td rowspan="4">97%</td><td>97%</td><td rowspan="4">95%</td></tr>
<tr><td>All Other Light Sources</td><td>95%</td></tr>
<tr><td>Spallation Neutron Source</td><td>99%</td></tr>
<tr><td>High Flux Isotope Reactor</td><td>>100%</td></tr>
</table>

* After applicable reductions due to SBIR/STTR.

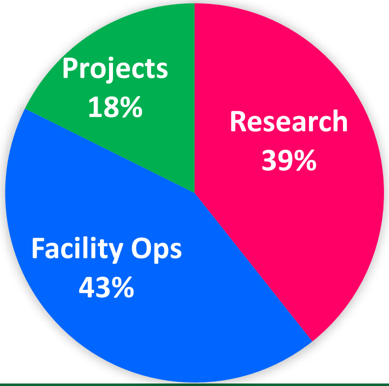
FY 2019 House and Senate Appropriation Language

FY 2019 House Mark	FY 2019 Senate Mark
EFRCs, Hubs flat funded; Batteries Hub encouraged to focus on grid storage applications, particularly on chemistries with low cost reagents.	EFRCs, Hubs, CMS, CCS flat funded; submit a 10-year solar fuels research initiative strategic plan within 120 days of enactment.
Funding levels for NSRCs, light sources, neutron sources specified (+$12M over FY 2018)	Funding levels for NSRCs, light sources (NSLS-II), neutron sources specified (+$45M over FY 2018); submit a plan for beamline buildout at NSLS-II as part of the FY 2020 budget
$20M for EPSCoR; annual or biennial Implementation Grant solicitations encouraged with a report due on BES's plan within 90 days of enactment.	$20M for EPSCoR; annual or biennial Implementation Grant solicitations encouraged with a report due on BES's plan within 90 days of enactment.
Construction (including OPC): LCLS-II $135.4M, APS-U $130M, SNS PPU $20M, ALS-U $52M, LCLS-II-HE $42M	Construction (including OPC): LCLS-II $145.4M, APS-U $140M, SNS PPU $70M, ALS-U $52M, LCLS-II-HE $34M, SNS STS $15M
Encourages support for basic research in polymers and polymer-based materials for energy applications, and implementation of neutron research efforts for polymeric materials.	Supports funding for emergent polymer optoelectronic technologies
$10M for research of artificial light harvesting systems that promise to significantly increase computational processing power and speed.	

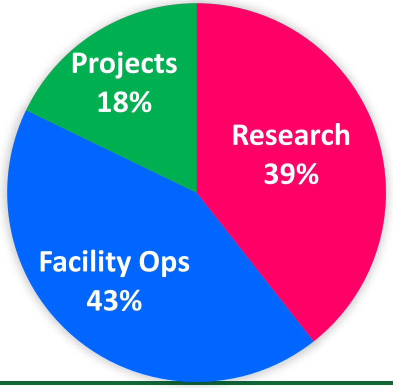
Status of BES FY 2019 Appropriation – HEWD & SEWD vs. FY 2018 Enacted

	FY 2018	FY 2019					
	Enacted	House Mark	Senate Mark	FY 2019 House Mark vs. FY 2018 Enacted		FY 2019 Senate Mark vs. FY 2018 Enacted	
Core Research	555,768	581,068	535,051	25,300	4.6%	-20,717	-3.7%
EPSCoR	19,270	19,270	19,270	…	0.0%	…	0.0%
EFRCs/Hubs/CMS/CCS/GPP	176,088	176,088	176,088	…	0.0%	…	0.0%
Facility Operations	898,597	910,500	944,009	11,903	1.3%	45,412	5.1%
MIEs/Construction/OPC	369,000	379,400	456,400	10,400	2.8%	87,400	23.7%
LTSM	8,500	…	…	-8,500	…	-8,500	…
SBIR/STTR	62,777	62,907	62,582	130	0.2%	-195	-0.3%
	2,090,000	2,129,233	2,193,400	39,233	1.9%	103,400	4.9%

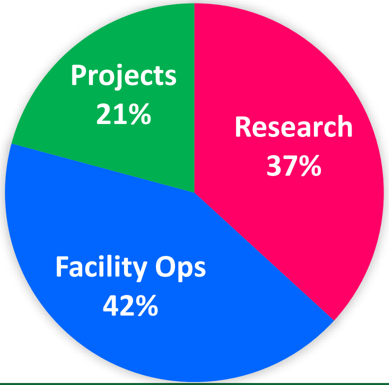
FY 2018 ENACTED



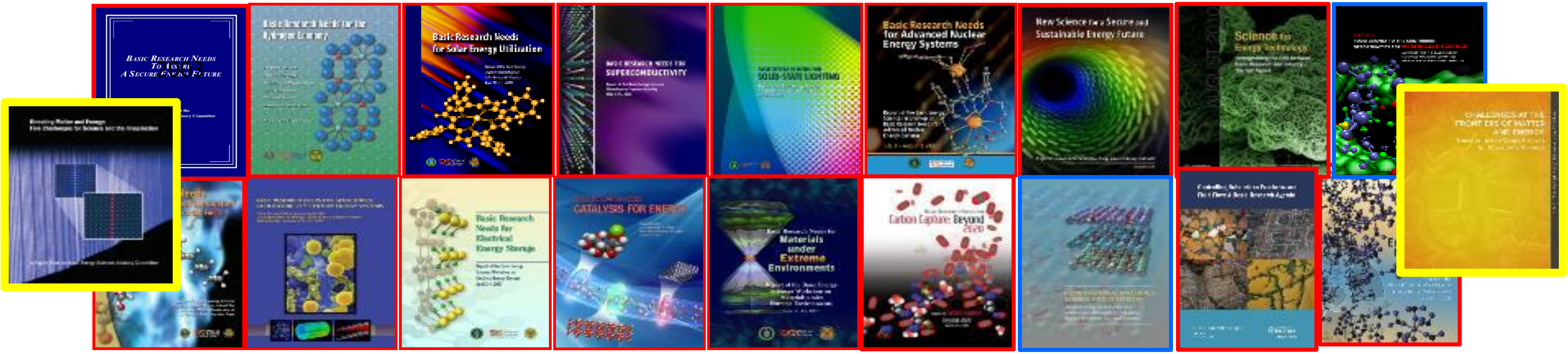
FY 2019 HEWD



FY 2019 SEWD



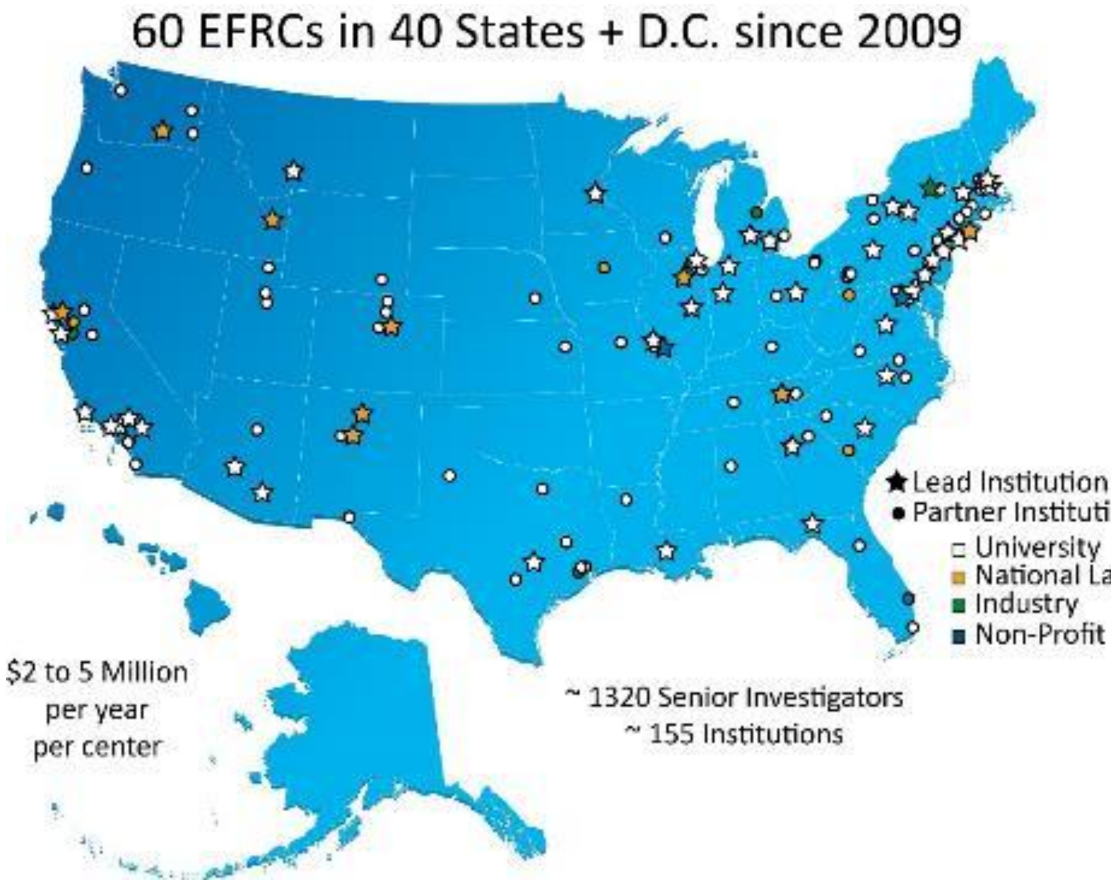
Energy Frontier Research Centers (EFRCs) – History



- History: 20+ community workshops since early-2000s with over 2,000 participants describing “basic research needs” for energy applications and “grand-challenge science”
- Establishment of EFRCs in 2009
  - 46 awards: 30 funded at $100M/year; 16 fully funded by ARRA at $277M; $2-5M/year each for a 5-year term
- Recompetition in 2014
  - 32 awards funded at $100M/year (22 renewal, 10 new); $2-4M/year each for a 4-year term, with competitions now every 2 years
- Targeted FOA in 2016 – Emphasizing science related to environmental management
  - 4 new awards funded at $10M/year ; $2-4M/year each for a 4-year term;
  - Solicitation informed by *Basic Research Needs for Environmental Management* report (2016)
- Recompetition in 2018

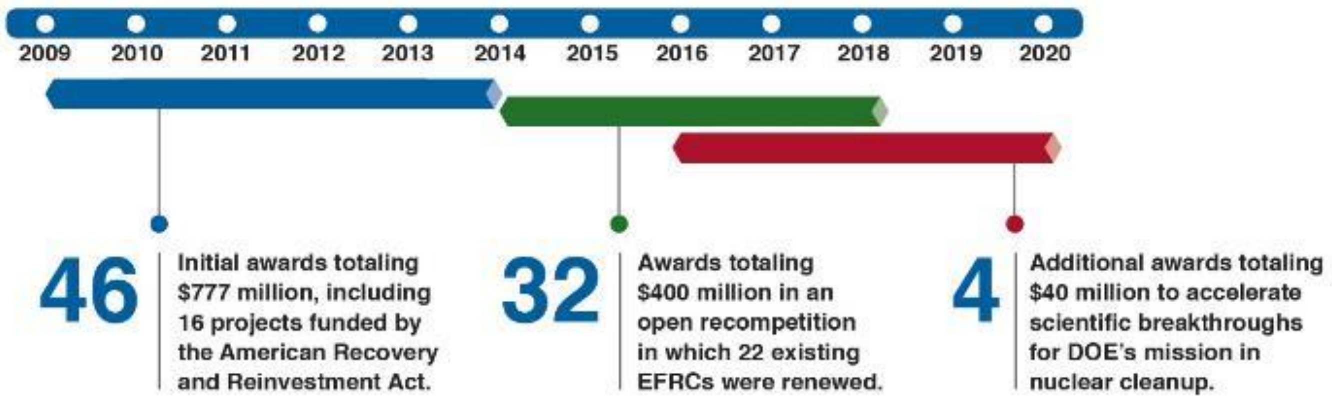
EFRC History (2009-2018)

Cumulative



Current EFRCs

- Over 115 participating institutions, located in 34 states and DC
- 610 senior investigators and more than 1,600 postdocs, grad students, undergrads, and technical staff
- >240 scientific advisory board members from 12 countries and 40 companies



Initial Awards

Re-competition

EM-Related

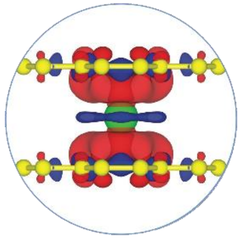
EFRC Communications

Summary Booklet

The 2016 EFRC booklet describes the history and outcomes from the first seven years of the EFRC program, including representative scientific highlights, academic publications, intellectual property, and science commercialization.

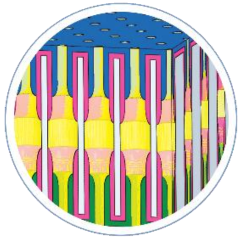
Solar concentrators based on quantum dots

Core-shell quantum dots were rationally designed for efficient light collection and transmission



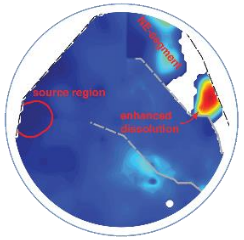
Accurately modeling materials for energy applications

Optimal method identified for multiscale simulations of carbon nanostructures



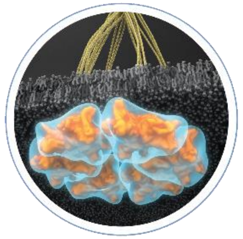
Building precision nanobatteries by the billions

Batteries constructed in nanopores promise to deliver energy at much higher power and longer life



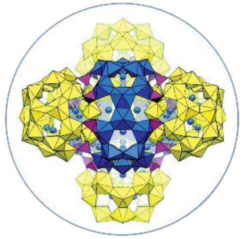
Viability of long-term carbon sequestration in the subsurface

The Bravo Dome gas field was used to estimate CO_2 dissolution rates over milennia



Examining the enzyme complex that makes cellulose fibrils

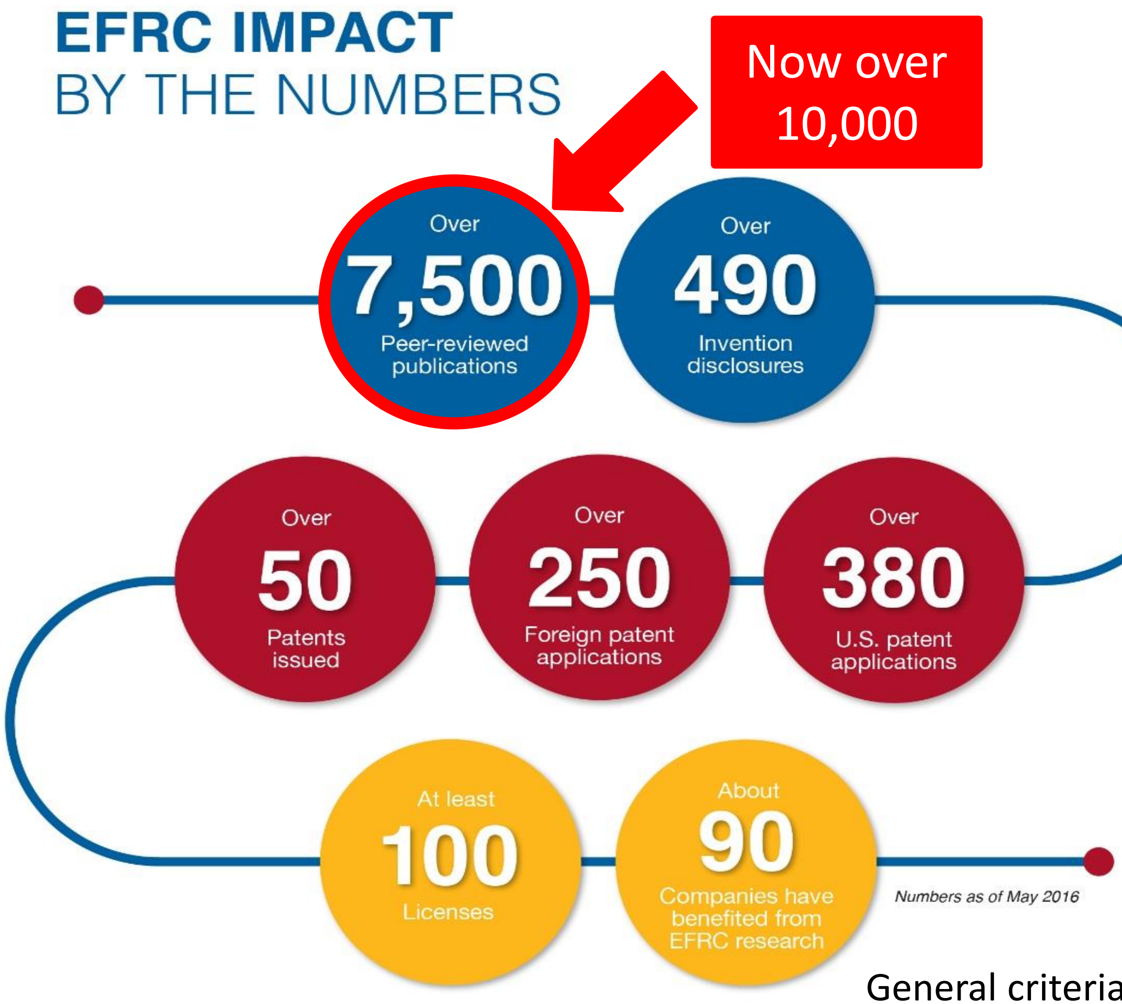
Imaging and computational modeling revealed new structural insights

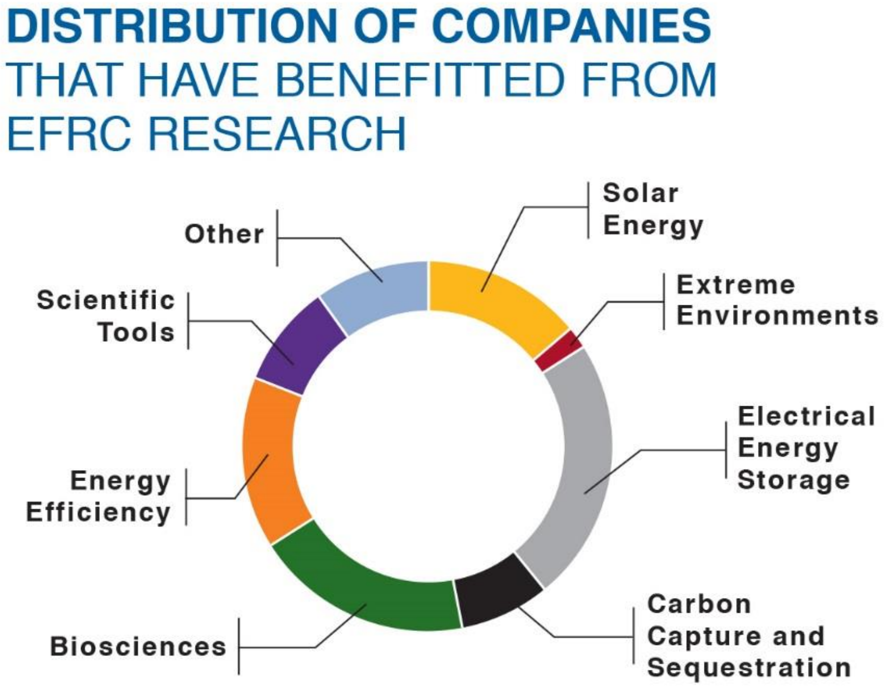


Nanoscale control of uranium for solvent-free recovery

Water-soluble uranium-oxygen clusters are large enough to be filtered using commercial membranes

EFRC Impact – IP and Company Interactions (May 2016)





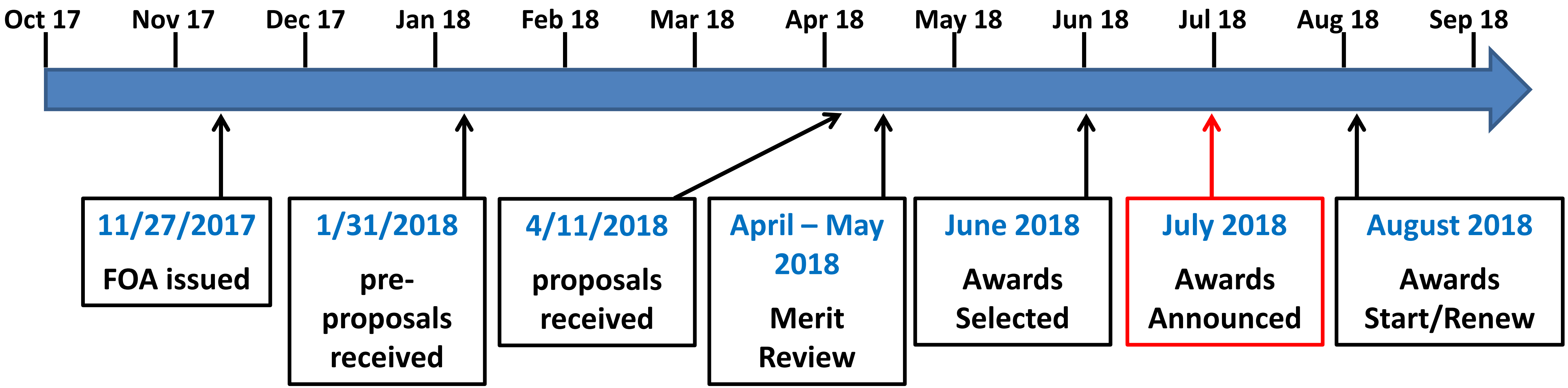
~33% Start-ups
~23% Mid-sized companies
~44% Large companies

General criteria for claiming company's benefits from EFRCs:
Licensed EFRC IP; Established CRADA; Used EFRC ideas in their business; Provided follow-on funding; Substantial interactions, involving personnel or sample exchange

Companies that Benefit from EFRC Research

ALTA DEVICES
Anellotech
BLUE CURRENT
chromation
mc10
activated research company™
UbiQD
UNITE TO LIGHT
SYNOPSYS®
ASYLUM RESEARCH an Oxford Instruments company
Fulcrum BIOENERGY
AMERICAN LITHIUM ENERGY
Washington Diamonds Quality Diamonds, Genuine Value
American Aerogel® Revolutionary materials. Superior products.
amsc®
SAMSUNG
UNIVERSAL DISPLAY CORPORATION™
DIOXIDE MATERIALS™
electroninks
Global Thermostat
ubiquitous energy
TRINITY INDUSTRIES, INC.
UNIFI
AstraZeneca
PHILIPS LUMILEDS
framergy™
P&G
APPLIED MATERIALS®
Schlumberger
mosaic materials
Photon Spot
Milliken
SuperPower Inc. A Furukawa Company
SINTEF
AIR LIQUIDE
SIGMA-ALDRICH
iBeam Materials
WATT FUEL CELL
SOLID POWER
saft
ConocoPhillips
EVIDENT THERMOELECTRICS
intel
DUPONT®
GE
GM
EXXON
Mobil
Reliance Industries Limited
LIONANO
VOXEL8
NANOFLEX POWER CORPORATION
REG Renewable Energy Group®
PIONEER.
DOW®
IBM
TORAY Innovation by Chemistry
QUESTEK® INNOVATIONS LLC
Millifluidica
thermaura
uraniumone™ investing in our energy
Ford
TOYOTA
DELPHI
Spero Pioneering A Greener Future
XERION ADVANCED BATTERY CORP
ADA Technologies, Inc.
CORNING
IHI
BRIDGESTONE
storaenso
GENTHERM
PEC POINT ENGINEERING
MICROMIDAS
XCeleprint
NanoIntegris
muRata INNOVATOR IN ELECTRONICS
KONICA MINOLTA
SHARP
Oorja
INVISTA™
SIRONIX RENEWABLES
PROTON ON SITE
Flexterra
alpha-En pure lithium metal - clean technology
LanzaTech
NuMat TECHNOLOGIES
SiNode SYSTEMS
QuantumScape™
SOFT ROBOTICS
PRIMET PRECISION MATERIALS
ORTHOGONAL
LiOx
nOHms TECHNOLOGIES
NEXT
REMYLOP Structured Materials™

EFRC FY2018 Recompetition Timeline



Proposal Statistics (3 preproposals per institution as lead)

- Lead institutions: 76% university, 24% national laboratory
- >150 unique partner institutions in 45 states, DC, Puerto Rico, and 10 foreign countries

Awards

- 31 four-year awards – 22 New and 9 Renewal; 9 led by Labs, 22 by Universities
- Additional 11 two-year extensions to existing centers to support the completion of valuable research

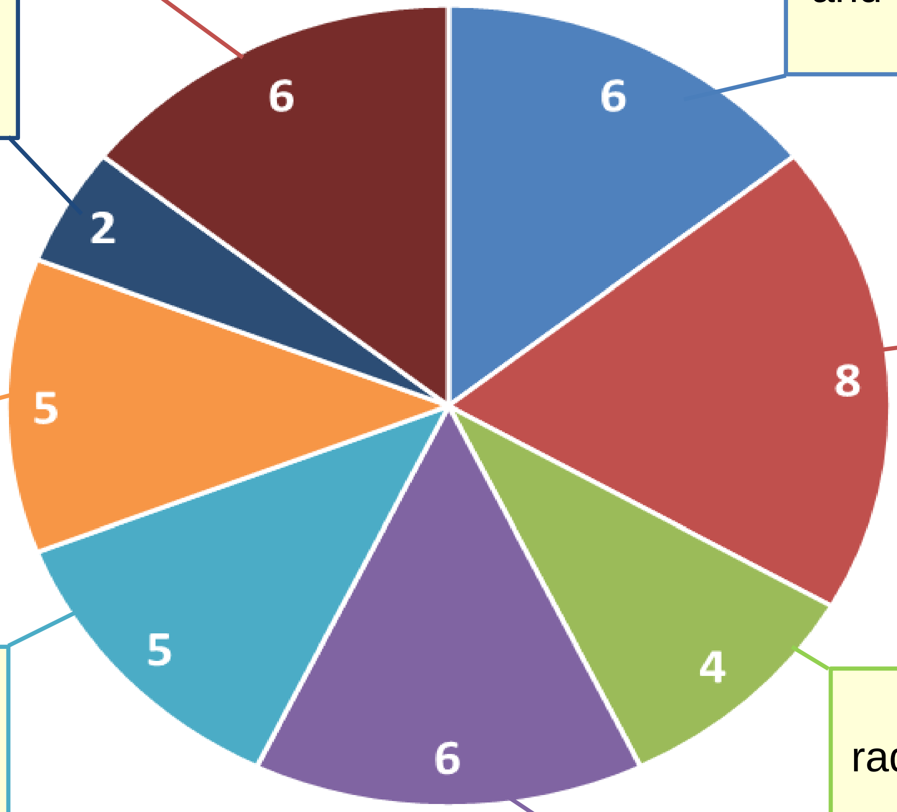
Topical Distribution of 42 EFRCs

4 additional EM-related EFRCs funded 2016-2020

Synthesis/Mat-Chem 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.

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



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

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

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

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

Quantum Materials – Novel materials for innovative electronics, sensors, and communications.

31 Four-Year Awards (1 of 2)

Director	Lead Institution	Center Name	Topical Area
McQueeney	Ames	Center for the Advancement of Topological Semimetals (CATS)	Quantum Materials
Basov	Columbia	Programmable Quantum Materials (Pro-QM)	
Broholm	Johns Hopkins	Institute for Quantum Matter	
Moore	LBNL	Center for Novel Pathways to Quantum Coherence in Materials	
Cheng	Univ of Florida	Center for Molecular Magnetic Quantum Materials	
Schuller	UC San Diego	Quantum Materials for Energy Efficient Neuromorphic Computing (Q-MEEN-C)	
Abruna	Cornell	Center for Alkaline-Based Energy Solutions (CABES)	Energy Storage
Savinell	Case Western Reserve	Breakthrough Electrolytes for Energy Storage (BEES)	
Dai*	ORNL	Fluid Interface Reactions, Structures and Transport (FIRST) Center	
Takeuchi*	SUNY Stony Brook	EFRC: Center for Mesoscale Transport Properties	
Tolbert	UC Los Angeles	EFRC Center for Synthetic Control Across Length-scales for Advancing Rechargeables (SCALAR)	
Uberuaga	LANL	Fundamental Understanding of Transport Under Reactor Extremes (FUTURE)	Nuclear
Hurley	INL	Center for Thermal Energy Transport under Irradiation (TETI)	
Wishart	BNL	Molten Salts in Extreme Environments	

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* Renewal Award

31 Four-Year Awards (2 of 2)

Director	Lead Institution	Center Name	Topical Area
Beard	NREL	Center for Hybrid Organic-Inorganic Semiconductors for Energy (CHOISE)	Solar
Scholes	Princeton	Bioinspired Light-Escalated Chemistry (BioLEC)	
Dionne	Stanford	Photonics at Thermodynamic Limits	
Friend*	Harvard	INTEGRATED MESOSCALE ARCHITECTURES FOR SUSTAINABLE CATALYSIS (IMASC)	Catalysis/Bioscience
Cosgrove*	Penn State	Center for Lignocellulose Structure and Formation (CLSF)	
Vlachos*	Univ of Delaware	Catalysis Center for Energy Innovation (CCEI)	
Gagliardi*	Univ of Minnesota	Inorganometallic Catalyst Design Center	
Bullock*	PNNL	EFRC for Center for Molecular Electrocatalysis	
Strano	MIT	The Center for Enhanced Nanofluidic Transport (CENT)	Separations
Darling	ANL	Advanced Materials for Energy-Water Systems	
Walton*	Georgia Tech	Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy (UNCAGE-ME)	
Freeman	UT Austin	Center for Materials for Water and Energy Systems	
Kovscek	Stanford	Center for Mechanistic Control of Water-Hydrocarbon-Rock Interactions in Unconventional and Tight Oil Formations	Subsurface
Butt	Univ of Utah	Multi-Scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE)	
Stupp*	Northwestern	Center for Bio-Inspired Energy Science (CBES)	Synthesis/Mat-Chem by Design
Parise	SUNY Stony Brook	GENESIS: A Next Generation Synthesis Center	
Baneyx	Univ of Washington	CSSAS: The Center for the Science of Synthesis Across Scales	

* Renewal Award

11 Two-Year Extensions

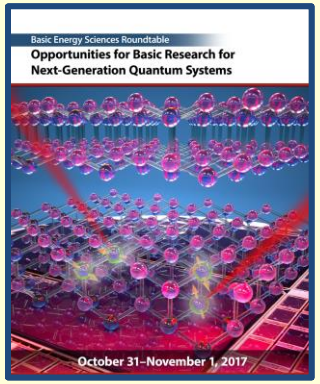
Director	Lead Institution	Proposal Title	Topical Area
Peters	Washington State	Biological Electron Transfer and Catalysis EFRC	Catalysis/Bioscience
Fenter	ANL	CENTER FOR ELECTROLYTE-ELECTRODE INTERFACE SCIENCE	Energy Storage
Whittingham	SUNY Binghamton	NorthEast Center for Chemical Energy Storage (NECCES)	
Rubloff	Univ of Maryland	Precision Ion-electron Control in Solid State Storage (PICS3)	
Zhang	ORNL	Energy Dissipation to Defect Evolution	Nuclear
Long	UC Berkeley	Center for Gas Separations	Separations
Wasielewski	Northwestern	Center for Light Energy Activated Redox Processes (LEAP)	Solar
Meyer	UNC Chapel Hill	Alliance for Molecular PhotoElectrode Design for Solar Fuels (AMPED)	
Perdew	Temple	Center for Complex Materials from First Principles (CCM)	Synthesis/Mat-Chem by Design
Shi	UC Riverside	Spins and Heat in Nanoscale Electronic Systems (SHINES)	
Tumas	NREL	Center for Next Generation of Materials Design	

Quantum Information Science in BES

Two Roundtable Reports (October 2017) defined a BES research agenda for emerging quantum systems and computing research opportunities:

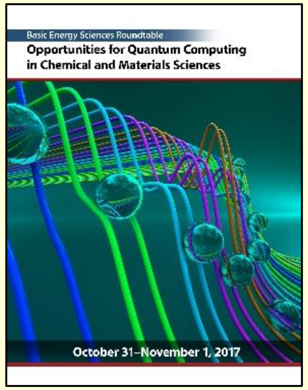
BES Science for Quantum Systems

- Advance artificial quantum-coherent systems
- Enhance creation and control of coherence in quantum systems
- Novel approaches for quantum-to-quantum transduction
- New quantum methods for advanced sensing and process control



Quantum Computing for BES Science

- Control the quantum dynamics
- Unravel the physics and chemistry of strongly correlated electron systems
- Embed quantum hardware in classical frameworks
- Bridge the classical–quantum computing divide



BES QIS Funding Opportunity Announcement (1)

MATERIALS AND CHEMICAL SCIENCES RESEARCH FOR QUANTUM INFORMATION SCIENCE

DE-FOA-0001909 and LAB 18-1909

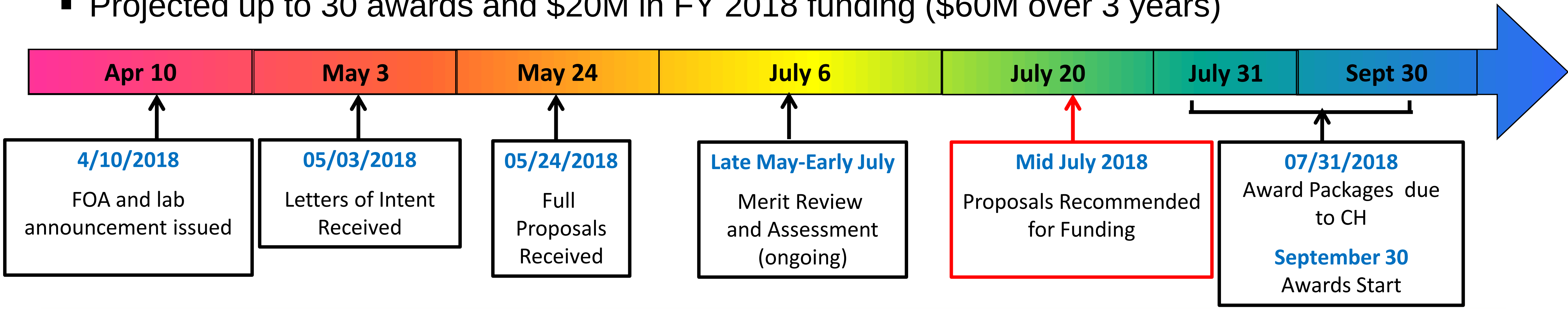
FOA Scope:

Fundamental research in materials and chemical sciences to:

- Advance understanding of quantum phenomena in systems that could be used for QIS
- Use today's quantum computers for chemical and materials sciences research.
- Topics related to BES roundtable reports on QIS.

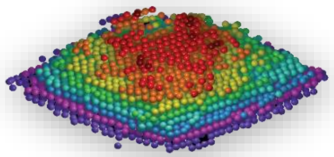
Application requirements:

- A maximum of 2 applications were accepted per institution as lead
- Single investigator/small group and team proposals: $150K to $1.5M per year, up to 3 year awards
- Projected up to 30 awards and $20M in FY 2018 funding ($60M over 3 years)

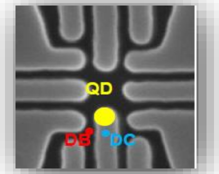


Quantum Integration Across Scales

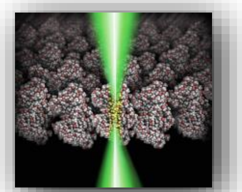
- BES Nanoscale Science Research Centers user facilities are key to the synthesis and characterization of materials and structures from nano-components to prototype-scale quantum systems.
  - Integration and testing couple closely to theory, design, and systems efforts
  - Development and testing of physical models of behavior of quantum devices
  - Co-located with National Lab x-ray, neutron, computing, and microfabrication facilities for understanding and scale-up of quantum structures
  - Next-generation qubits and sensors



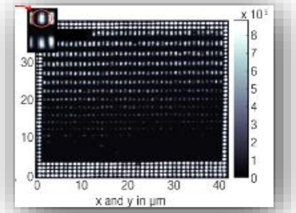
Sub-atomic Spatial Precision



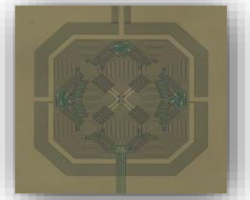
Solid State Artificial Atoms



Single-nm lithography

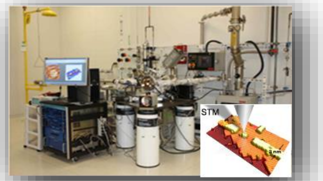


Entangled Qubit Arrays

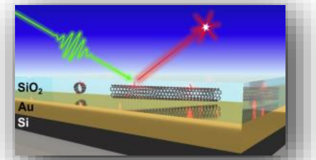


Quantum-Limited Sensors

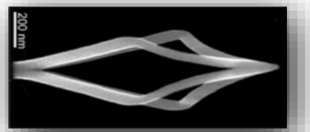
Quantum Chip Testing



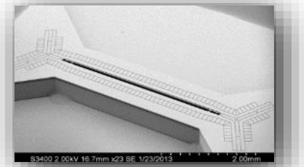
Atomic Precision Fabrication



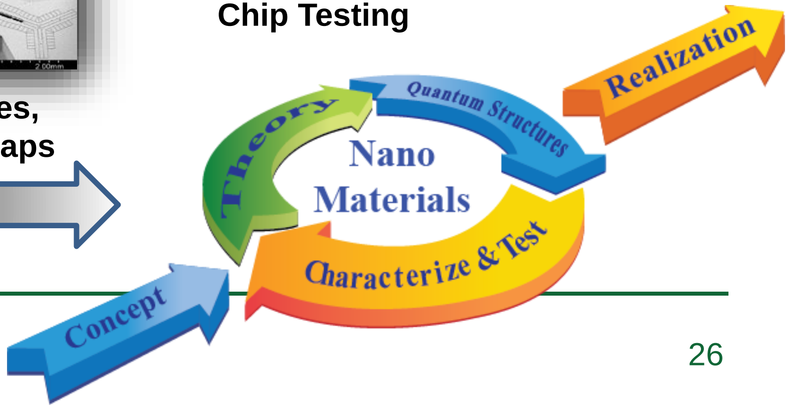
Single Photon Emitters and Detectors



Nanoscale 3D Printing



Waveguides, Cavities, Traps



BES QIS Funding Opportunity Announcement (2)

QUANTUM INFORMATION SCIENCE AND RESEARCH INFRASTRUCTURE (LAB 18-1910)

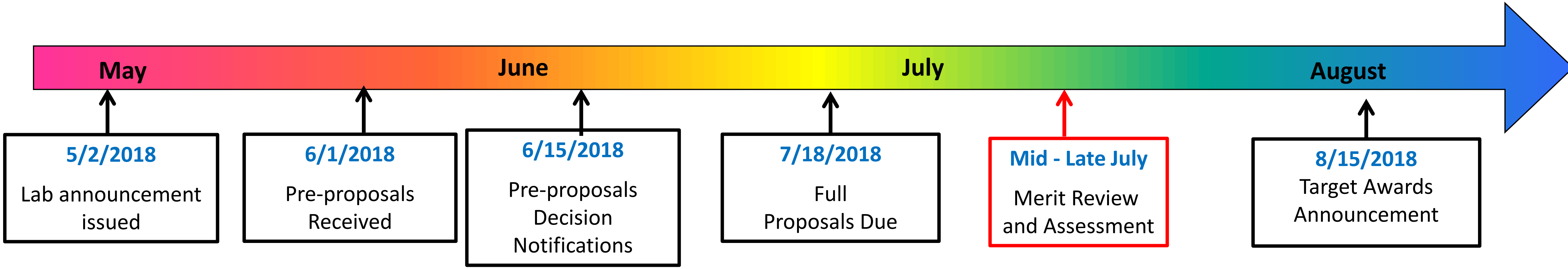
FOA Scope:

Research Infrastructure: includes funding for metrology, fabrication, and prototypes (measurement science instrumentation, modeling and simulation, and shared DOE-lab based user facilities).

Research: Topics related to BES roundtable reports on QIS.

Application requirements

- A maximum of 3 pre-applications were accepted per Nanoscale Science Research Center
- Team proposals: $500K - $2M per year, up to 3 year awards
- Projected up to 8 awards and $10M in FY 2018 funding ($30M over 3 years)



BES Ultrafast Science Funding Opportunity Announcement

Research at the Frontiers of X-ray Free Electron Laser Ultrafast Chemical and Materials Sciences

DE-FOA-0001904 and LAB 18-1904

Fundamental research in materials and chemical sciences enabled by new ultrafast x-ray free electron laser (XFEL) capabilities at LCLS-II and its prospective upgrades:

- Probing and controlling electron motion within a molecule
- Discovering novel quantum phases through coherent light-matter coupling
- Capturing rare events and intermediate states in the transformation of matter

Application requirements:

- A maximum of 2 applications were accepted per institution as lead
- Small groups and team proposals: $300K to $1.5M per year, up to 3 year awards
- Projected up to 15 awards and $10M in FY 2018 funding ($30M over 3 years)

April — **May** — **June** — **July**

- **4/2/2018** FOA & Lab announcement issued
- **4/30/2018** Letters of Intent Received
- **5/21/2018** Full Proposals Received
- **Late May – Early July** Merit Review and Assessment (ongoing)
- **Mid - Late July** Proposals Recommended for Funding
- **7/31/2018** Target Awards Announcement
  9/30/2018 Award Start

BES Leads: Helen Kerch and Jeff Krause

BES Exascale Computing Initiative Funding Opportunity Announcement
Computational Chemical Sciences Research

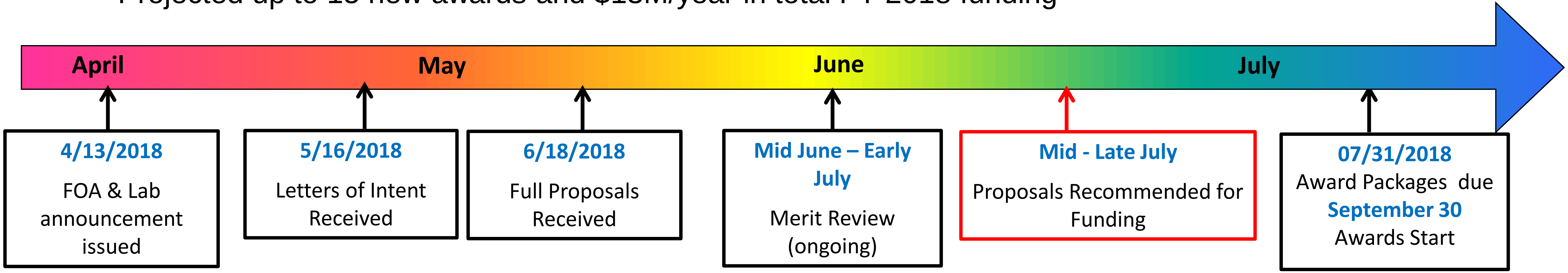
DE-FOA-0001912 and LAB 18-1912

FOA Scope:

Fundamental research to develop validated, public access codes and databases and to advance new approaches to use large complex data sets for deriving fundamental knowledge from calculations and advanced characterization of chemical systems.

Application requirements:

- A maximum of one application was accepted from each institution (as lead)
- Small groups and team proposals: $150K to $2M per year, up to 4 year awards
- Projected up to 15 new awards and $13M/year in total FY 2018 funding



BES Lead: Mark Pederson

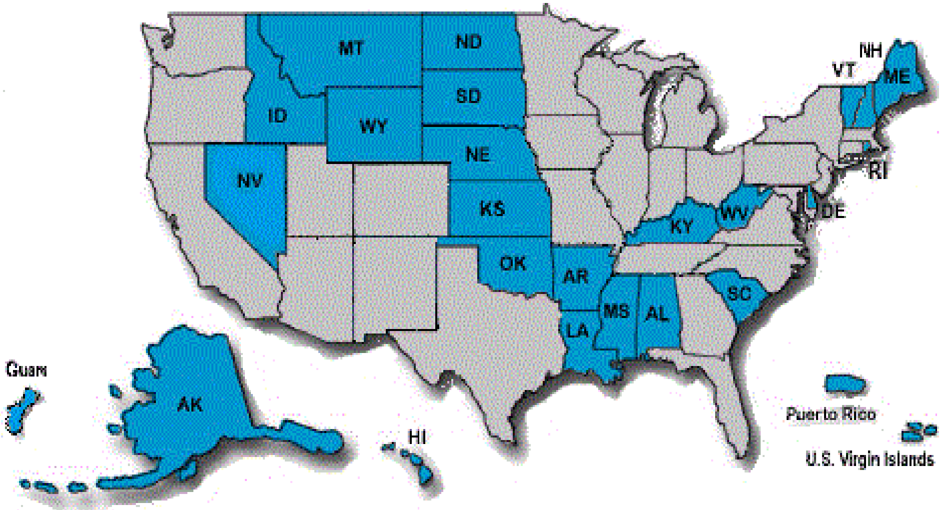
DOE Established Program to Stimulate Competitive Research Funding Opportunity Announcement

BUILDING EPSCOR-STATE/NATIONAL LABORATORY PARTNERSHIPS

DE-FOA-0001897

Partnerships to advance fundamental, early-stage energy research collaborations between the EPSCoR jurisdictions and the DOE national laboratories

- Research must be within DOE's mission-space
  - Office of Science
  - Energy Technology Offices



Application requirements:

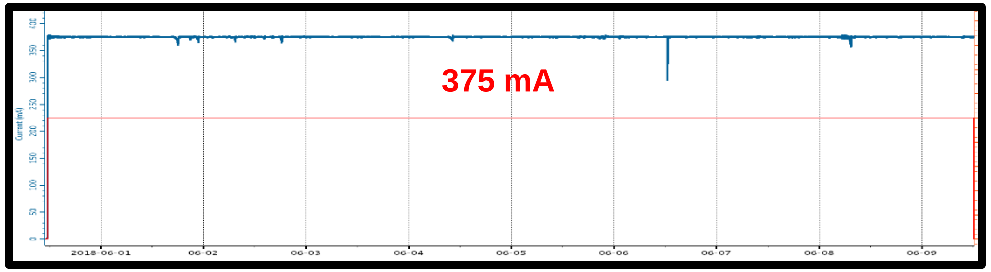
- A maximum of 1 application was accepted per institution
- Requires (unfunded) collaboration with a DOE National Laboratory
- Small team proposals: up to $750,000 over three years
- Up to 20 fully funded awards; up to $15M in FY 2018 funding

March **April** **May** **June** **July** **August**

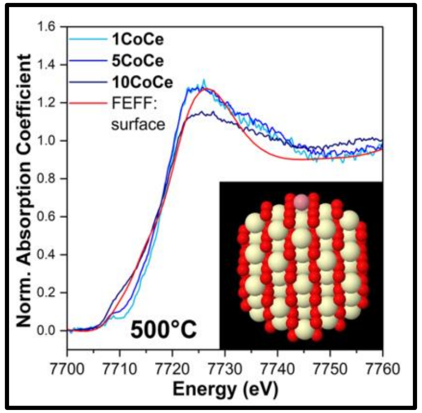
- **03/28/2018** FOA issued
- **4/25/2018** Letters of Intent Received
- **5/16/2018** Full Proposals Received
- **Late May – Early July** Merit Review and Assessment (ongoing)
- **Mid - July** Proposals Recommended for Funding
- **7/31/2018** Target Awards Announcement; **9/30/2018** Award Start

National Synchrotron Light Source-II on a Path to Mature Operations

- **Reliable accelerator operation**
  - ➢ **Operating at 375 mA and will increase to 400 mA by the end of July**
  - ➢ **FY2018 reliability to date is over 97%**
- **Steady increase in both the number of beamlines and the number of users**
  - ➢ **18 beamlines in General User Program and 8 beamlines in commissioning**
  - ➢ **28 beamlines will be in operation by the end of CY2018**
  - ➢ **Over 1,000 unique users for FY2017 and already nearly 1,000 unique users for FY2018 to date**
- **5,000 planned operating hours for users for FY2019**



Mesoporous Catalysts for Hydrogen Production

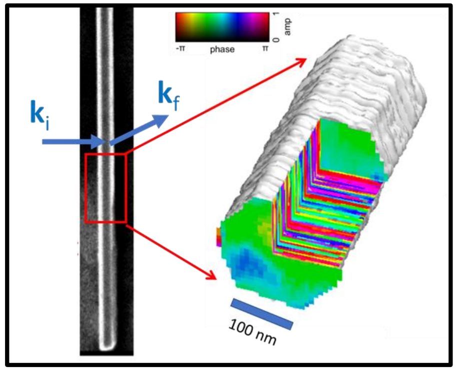


Mesoporous Co/CeO2 catalysts were characterized and found the catalysts to be active for water-gas shift reactions at 300 – 500°C.

Figure: *Co K-edge XANES and FEFF 9 models of Co atom on top of CeO2 particle.*

J. Phys. Chem. C (2018)

3D Nanoscale Imaging of Defects in a Nanowire

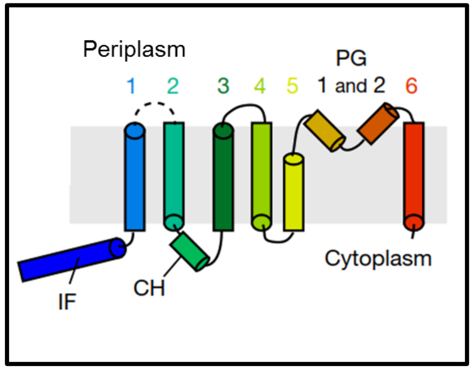


In a single nanowire, the 3D distribution of both strain and stacking defects was measured using coherent x-rays, revealing structural heterogeneity from nano- to micrometer scales.

Figure: *(Left) a SEM image of a nanowire with diffraction geometry and (right) cutouts from 3D images sensitive to stacking defects.*

Nano Letters (2018)

Unexpected Architecture of a Membrane Protein Revealed



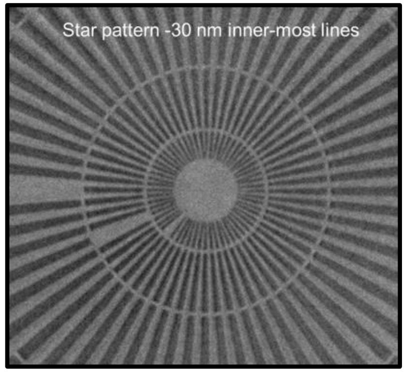
The crystal structure of a channel-forming O-antigen polysaccharide transporter called Wzm-Wzt was revealed and showed an unexpected, non-traditional architecture.

Figure: *Wzm forms six transmembrane helices and the cytoplasmic loop (CH) forms the coupling helix. The periplasmic loop, between helices 5 and 6, generates two periplasmic gate helices (PG1 and PG2). Gray box indicates likely membrane boundaries.*

Nature (2018)

Newly Completed Full Field X-ray Imaging (FXI) Beamline Started Science Commissioning

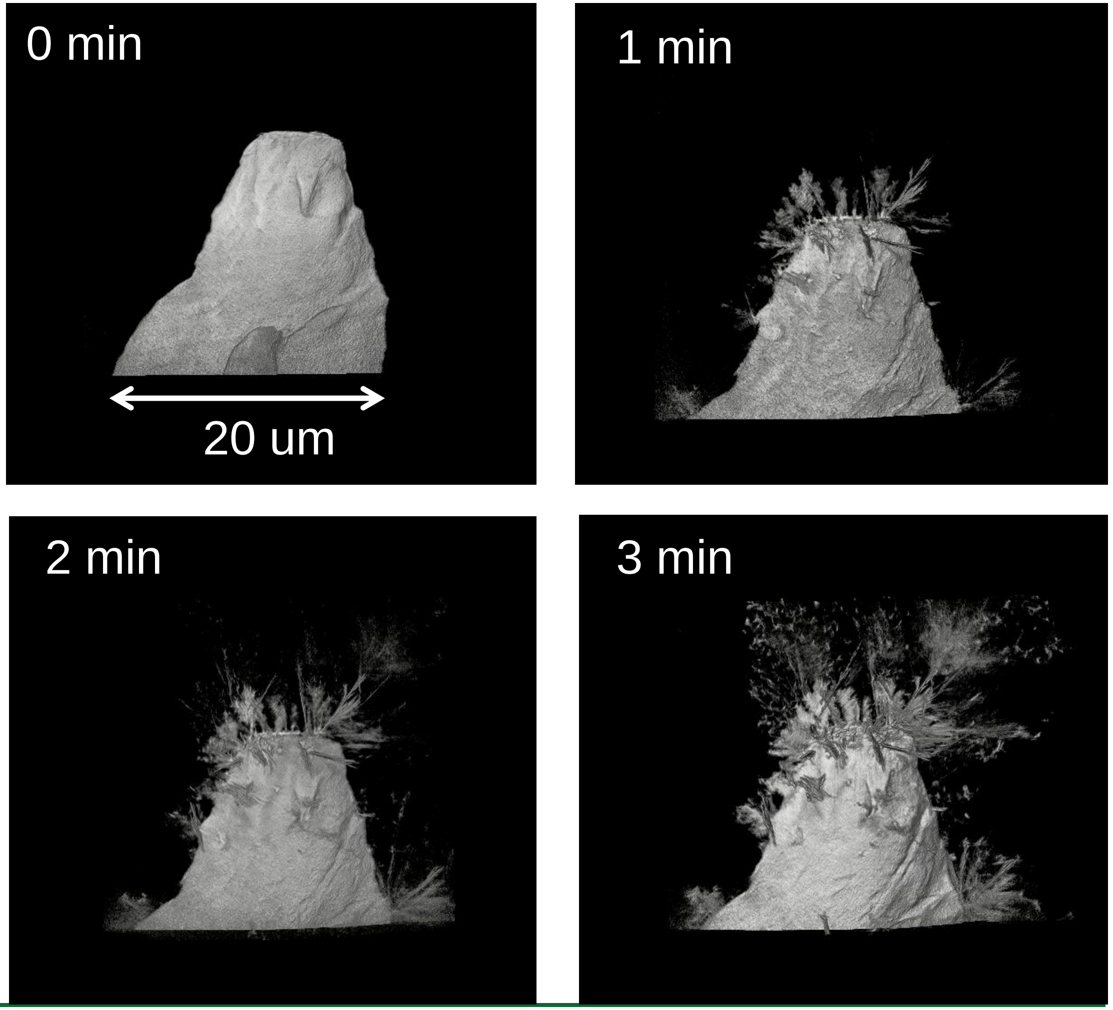
Transmission X-ray Microscope



- TXM achieved a complete 3D nanotomography measurement in 1 min., at ~50 nm resolution
  - ➢ with 20 ms exposures and 3°/s rotation speed

- World-leading capabilities, based on cutting-edge in-house design that leverages NSLS-II nanopositioning capability

Tracking 3D nano-dendritic growth in real time
In-situ reaction: $Cu + AgNO_3 \rightarrow Ag + Cu(NO_3)_2$



Helical Superconducting Undulator:
Sending Electrons on a Rollercoaster Ride

Technical Achievement

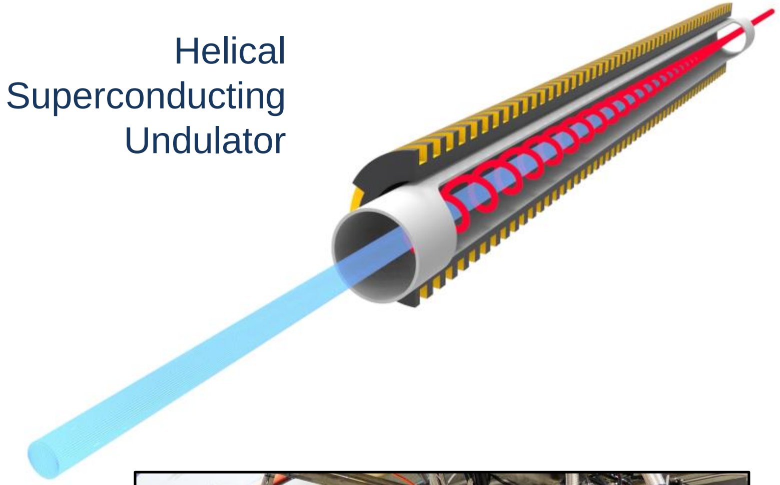
- A first-of-its-kind x-ray source based on superconducting undulator technology has been designed and built at the Advanced Photon Source (APS). The new source -- the Helical Superconducting Undulator (HSCU) -- forces the 7-GeV electron beam into a helical trajectory.

Significance and Impact

- Light produced by electrons moving on a helical trajectory is unlike that from planar undulators. It is circularly polarized and monochromatic (with no harmonics on axis), and still high-brightness. This x-ray beam can be used directly, i.e. without any optics, for experiments.
- The flux from the HSCU surpasses the flux from planar APS undulators with monochromators by several orders of magnitude.

Research details

- The integration of the HSCU into the APS storage ring went flawlessly
- The measured spectrum confirmed the predicted ratio of flux for 1st and 2nd harmonics. (A very weak 2nd harmonic arises from the finite beam emittance; it is not strong enough to affect user experiments.)



Helical Superconducting Undulator
in Sector 7 of the APS storage ring

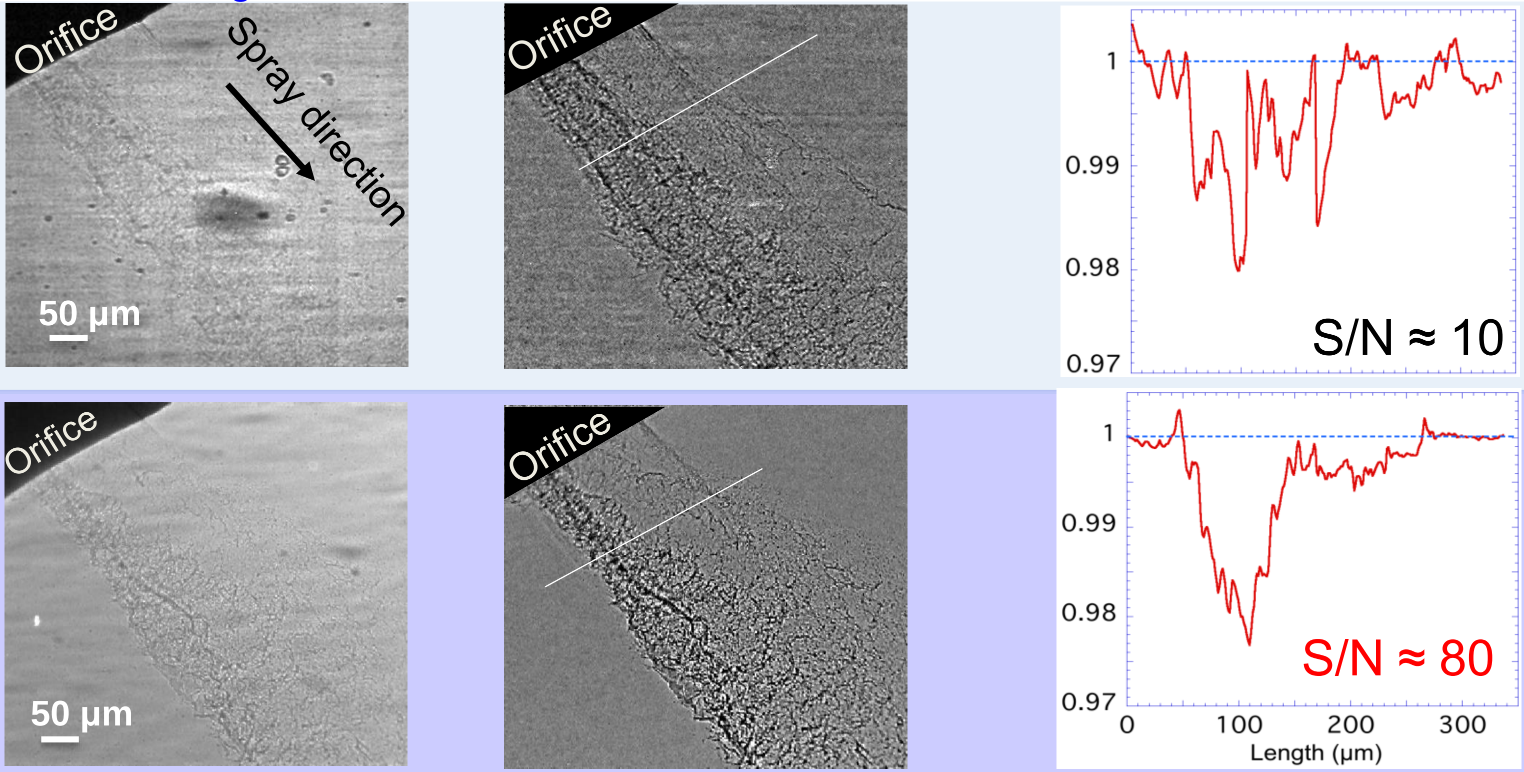
Single-pulse X-ray White-Beam Imaging Using HSCU at the APS 7-ID

- Fuel-spray research requires single-pulse (100 ps) white-beam to image high-speed, transient liquid jets.
- Undulator A at 6 keV: power density > 100 W/mm^2, > 90% is unwanted higher-energy (HE) photons.
  - Requires a mirror to reject HE photons and to reduce power, but it introduces artifacts and additional noise.
- HSCU white beam at 6 keV: low power density < 15 W/mm^2, much lower HE contents, so NO need of a mirror.
  - 5× beam intensity and 8× S/N compared to UA

Raw images | Transmission | Line-scan

UA at 6 keV
≈ 100 W/mm^2 power
> 90% HE photons
Requires mirror
Intensity: 150/pixel

HSCU at 6 keV
≈ 13 W/mm^2 power
Low HE contents
No mirror needed
Intensity: 750/pixel

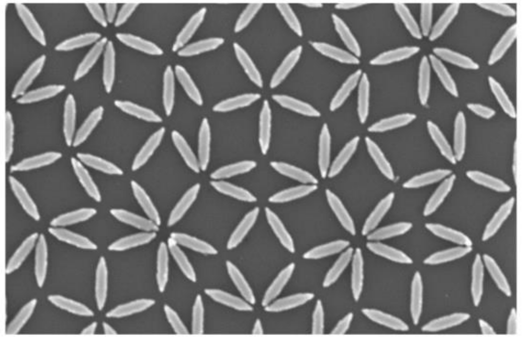


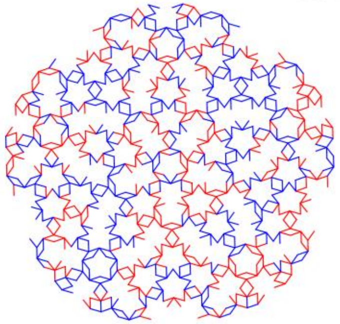
HSCU beam enables quantitative imaging analysis and simulation.

U.S. DEPARTMENT OF ENERGY | Office of Science

Magnetic quasicrystals are both ordered and disordered nanomaterials

CFN User and Staff Highlight





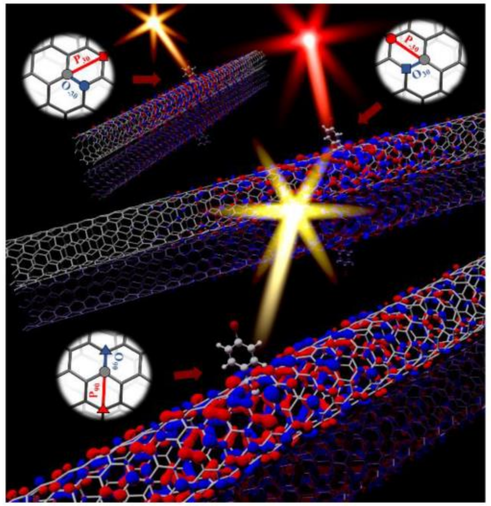
Researchers observed that quasicrystals made of nanomagnets form magnetic states having both an ordered, rigid 'skeleton' spanning the entire network, and smaller domains with configurations that are switchable without energy cost.

(Left) Scanning electron microscope image of nanofabricated Permalloy magnets arranged in a Penrose tiling. (Right) The quasicrystal arrangement leads to thermal ordering of magnetic domains measured by magnetic force microscopy.

D. Shi, Z. Budrikis, A. Stein, S. A. Morley, P. D. Olmsted, G. Burnell, and C. H. Marrows, *Nature Physics*, doi:10.1038/s41567-017-0009-4 (2017).

Tailored Nanotubes for Sensors and Lasers

Category: *Enablers & Cross-cutting*



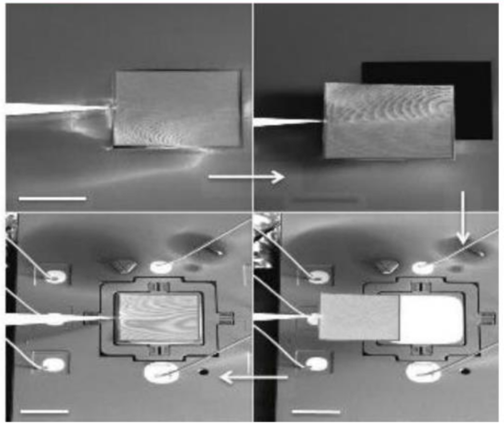
Low temperature single defect photoluminescence spectroscopy and quantum chemistry modeling revealed existence of six distinct chemical binding configurations for sp^3 defects as the source of diverse spectral behavior.

This provides a rational strategy toward controllable creation and manipulation of individual covalent quantum defects with desired optical functionalities.

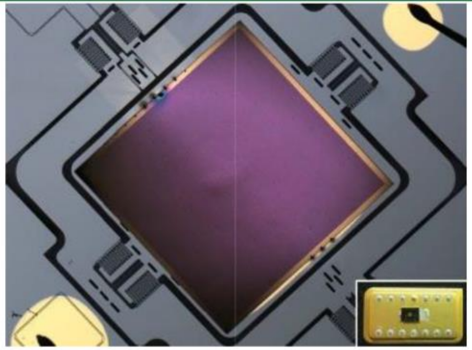
Aryl functional groups (gray dots) can bind to nanotubes (gray lattice) in six distinct configurations (white circles) leading to defect states emitting photons at different energies (red, orange and yellow stars). Wavefunction spread of the lowest energy exciton states are plotted in red and blue.

Xiaowei He, et al., Low-Temperature Single Carbon Nanotube Spectroscopy of sp^3 Quantum Defects. ACS Nano 11 (11), 10785-10796(2017).

Dynamic Lens-on-MEMS Brings New Vision to Optics



Integration process of a metasurface-based flat lens onto a MEMS scanner. Integration process: an FIB probe was used to cut, grab and weld the lens onto the MEMS scanner.



Flat lens mounted on 2-axis MEMS scanner.

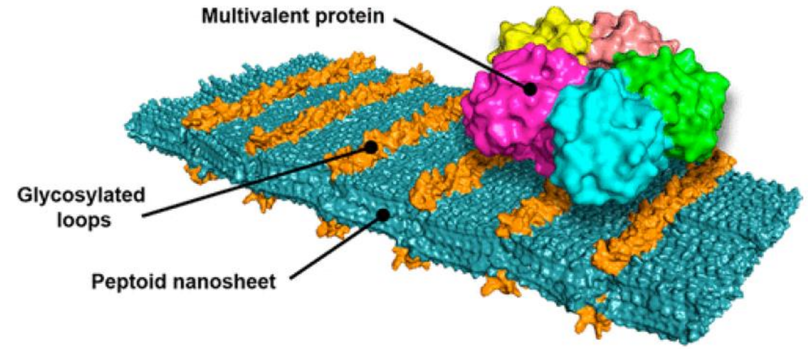
Metasurfaces were dynamically controlled by integrating them onto Micro-Electro-Mechanical Systems (MEMS).

T. Roy, S. Zhang, I.L. Woong Jung, M. Troccoli, F. Capasso, D. Lopez, *Applied Photonics* 3, 021302 **2018**.

Work was performed in part at the Center for Nanoscale Materials.

Sugar-coated Peptoid Nanosheets Selectively Detect Multivalent Proteins

A model of a glycosylated peptoid nanosheet binding a multivalent protein.



A team led by Foundry researchers has developed a method to engineer the surface of peptoid nanosheets, mimicking some of the properties of cell membranes, to interact with multivalent proteins.

This work was performed in part at the Molecular Foundry.

A. Battigelli, J.H. Kim, D.C. Dehigaspitiya, C. Proulx, E.J. Robertson, D.J. Murray, B. Rad, K. Kirshenbaum, R.N. Zuckermann. *ACS Nano.* **Article ASAP** (2018). DOI: 10.1021/acsnano.7b08018