U.S. DEPARTMENT OF ENERGY | Office of Science

Basic Energy Sciences Update

Linda Horton

Associate Director

Office of Basic Energy Sciences

BESAC Meeting

July 30, 2020

Exciting Times for BES

- Welcome to BESAC and the Subcommittees
- Reorganization, Retirements and New Hires
- Continued Impact of the Program
- FY 2020 and FY 2021 Budget Status
- New Research Opportunities and Coordination Activities

Congratulations to Harriet Kung !
Promotion to SC Deputy Director on April 12, 2020

- Associate Director, Basic Energy Sciences for 12 years
- Division Director, Materials Sciences and Engineering for 4 years

Dr. Kung's leadership at BES:

- Successfully launched three new research funding modalities
  - BES DOE Energy Innovation Hubs (JCAP 2010, JCESR 2013)
  - 82 Energy Frontier Research Centers, through 10-year celebration
  - Computational Materials and Chemical Sciences
- Oversaw planning and execution of major facility construction projects
  - Delivered nearly $2 billion of construction projects within designed scope, time, & budget
  - Initiated LCLS-II, LCLS-II-HE, ALS-U, APS-U, SNS-PPU, and SNS-STS, total cost over $4 billion
- Strategic planning of scientific research directions and facility priorities
  - 11 BESAC reports, including Transformative Opportunities (2015), Facilities Prioritization (2013), Future X-ray Light Sources (2013), Facility Upgrades (2016), "BES40" (2018)
  - 10 Basic Research Needs (BRN) reports, 8 roundtable reports, 8 other workshop reports
  - BRN and BES40 have been adopted as models by other SC program offices
- Hired ~80% of the current staff of BES

Farewell to Jim Murphy !
Retirement from BES on March 31, 2020

- Director, Scientific User Facilities Division for ~8 years
- Brookhaven National Laboratory for 29 years

Dr. Murphy's leadership at BES:

- Oversaw operations of 12 scientific user facilities
  - 5 Light Sources (4 rings + FEL); 2 Neutron Sources (spallation + reactor); 5 Nanoscale Science Research Centers
  - Stewardship to deliver effective and reliable operations supporting ~16,000 scientists and engineers annually
  - Advanced the achievement of SNS 1.4 MW operations
  - Supported development of a novel MeV Ultrafast Electron Diffraction tool for Ultrafast Science research
- Led planning and execution of facility construction projects
  - Successful completion of NSLS-II, NEXT, and SING-II
  - Oversaw 9 on-going projects: LCLS-II, LCLS-II-HE, ALS-U, APS-U, PPU, STS, NEXT II, Nano Recap, and CRMF
- Guided 4 workshops/roundtables to define the future of facilities

New Hire – Computational and Theoretical Chemistry Program

Dr. Aaron Holder

Program Manager, Computational & Theoretical Chemistry
Chemical Sciences, Geosciences and Biosciences Division

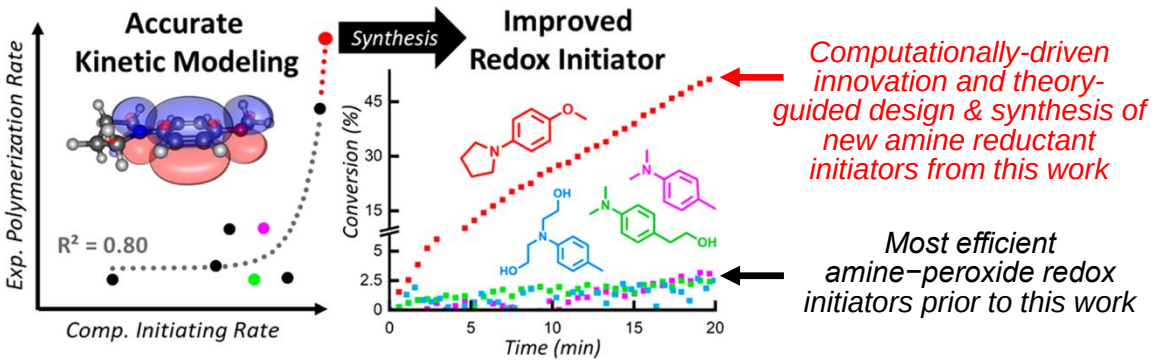
Expertise

- Theoretical and computational chemistry
- Development, application, and integration of scalable and hierarchal electronic structure, molecular dynamics, and data science methods
- Use of leadership-class and emergent computing technologies

Experience

- Materials and Chemical Science and Technology, National Renewable Energy Laboratory
- EFRC Thrust Lead
- Joint Appointment at University of Colorado, Boulder
- University of Colorado, Ph.D. in Chemical Physics

Rational Design of Efficient Amine Reductant Initiators for Amine–Peroxide Redox Polymerization



Holder & co-workers, JACS 2019 141 (15), 6279-6291

Office of Basic Energy Sciences

Associate Director
Linda Horton

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

BES Operations
- Teresa Crockett, Program Analyst
- Robin Hayes, Program Manager
- Kerry Hochberger, Program Support Specialist
- Vacant, Program Analyst / BESAC*
- Andy Schwartz, Senior Technical Advisor for EFRCs**

* Basic Energy Sciences Advisory Committee
** Energy Frontier Research Centers

Materials Sciences and Engineering Division
Andy Schwartz, Acting Director
(Vacant)

Materials Discovery, Design, and Synthesis
Mike Markowitz
- **Materials Chemistry** — Craig Henderson, Michael Sennett
- **Biomolecular Materials** — Mike Markowitz, (Vacant)
- **Synthesis and Processing Science** — Bonnie Gersten
- **Batteries and Energy Storage Hub; Technology Coordination** — Craig Henderson, John Vetrano

Condensed Matter and Materials Physics
Jim Horwitz
- **Experimental Condensed Matter Physics** — Michael Pechan
- **Theoretical Condensed Matter Physics** — Matthias Graf, Vacant
- **Physical Behavior of Materials** — Refik Kortan, (QIS Vacant)
- **Mechanical Behavior and Radiation Effects** — John Vetrano

Scattering and Instrumentation Sciences
Helen Kerch
- **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
Linda Horton, Acting Director
(Vacant)
Rocio Meneses, Program Support Specialist

Operations
- **X-ray and Neutron Scattering Facilities** — Peter Lee, Thiyaga P. Thiyagarajan, (Vacant), ▲ Yiping Feng
- **NSRCs **** — George Maracas
- **Accelerator and Detector Research** — Eliane Lessner, ■ Nicholas Sereno
- **Facilities Coordination; Metrics; Assessment** — Van Nguyen

** Nanoscale Science Research Centers

Construction
- **Linac Coherent Light Source-II** — Phil Kraushaar
- **Advanced Photon Source Upgrade** — Ed Stevens
- **Facilities Upgrades and MIE*** Projects** — Phil Kraushaar, Ed Stevens

*** Major Items of Equipment

Chemical Sciences, Geosciences, and Biosciences Division
Bruce Garrett, Director
Emily Smith, AAAS Fellow

Fundamental Interactions
Jeff Krause
- **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** — Aaron Holder, ● William Kuo

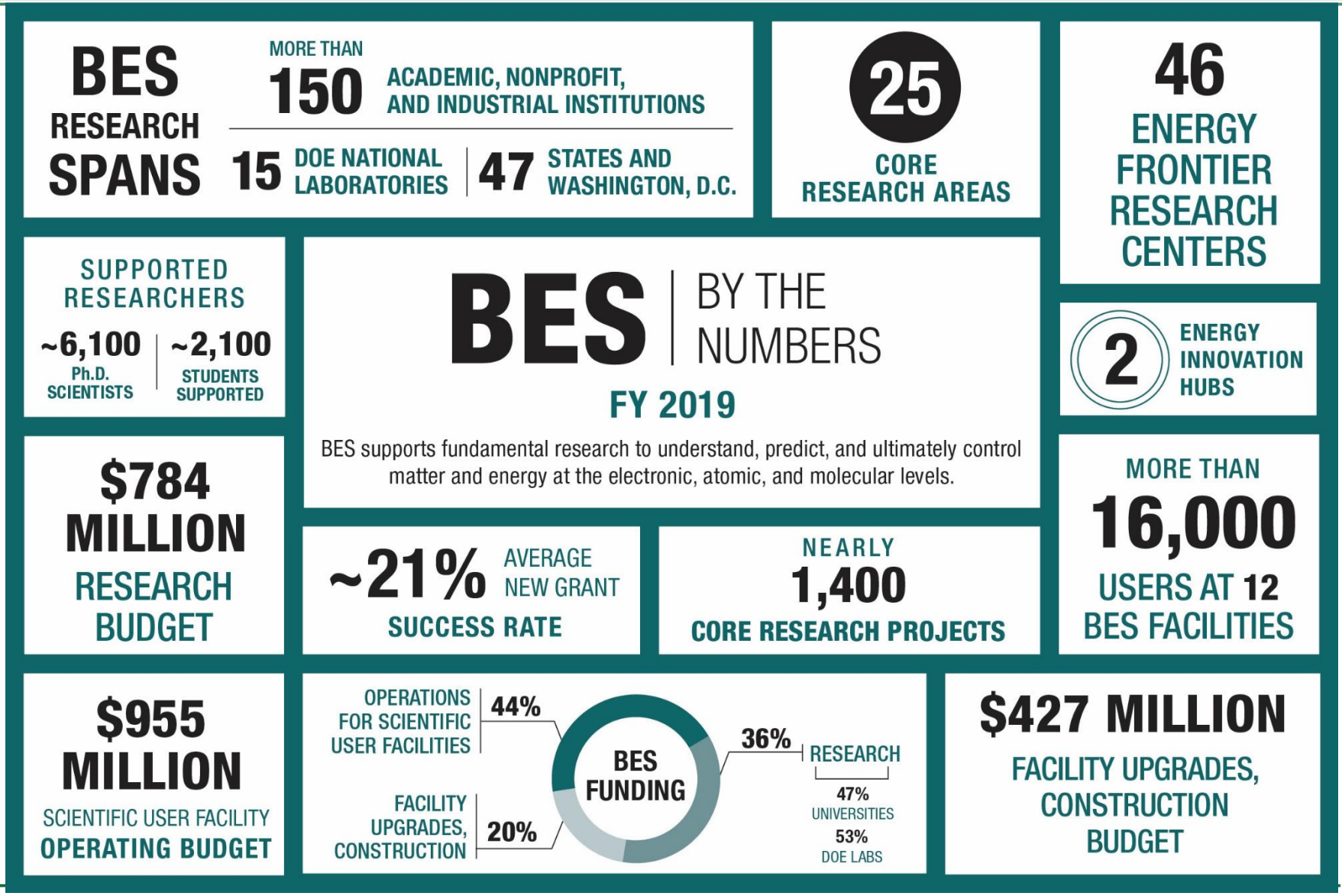
Photochemistry and Biochemistry
Gail McLean
- **Solar Photochemistry** — Christopher Fecko, Vacant
- **Photosynthetic Systems** — Stephen Herbert
- **Physical Biosciences** — Robert Stack
- **Fuels from Sunlight Energy Innovation Hub** — Christopher Fecko

Chemical Transformations
Raul Miranda
- **Catalysis Science** — Chris Bradley, Viviane Schwartz
- **Separation Science** — Daniel Matuszak
- **Heavy Element Chemistry** — Philip Wilk
- **Geosciences** — James Rustad

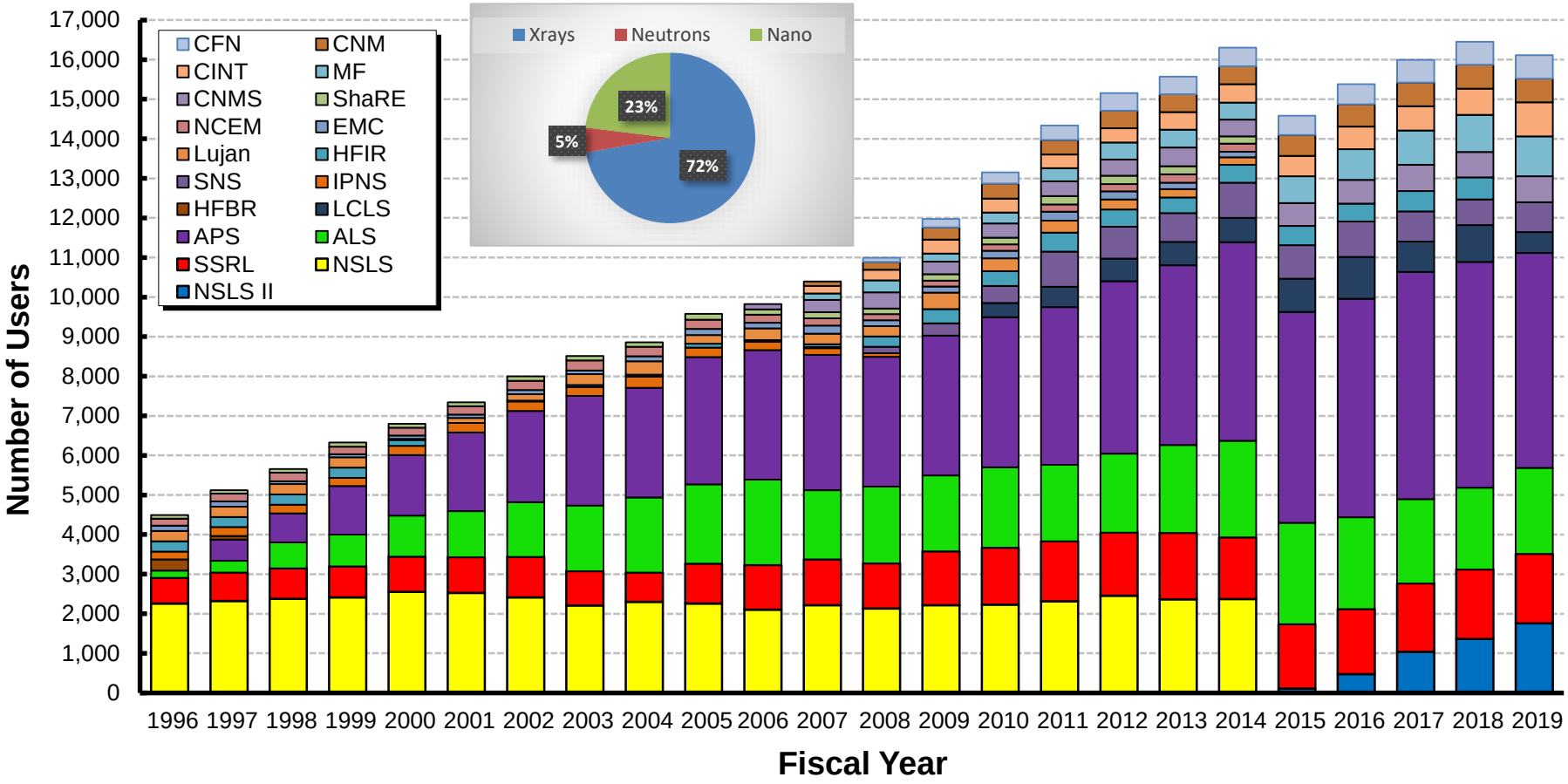
LEGEND
- ■ Detailee (50%) from ANL
- ● Detailee (50%) from LLNL
- ▲ Detailee (70%) from SLAC

July 2020
Posted July 10, 2020

Basic Energy Sciences At a Glance (2019)



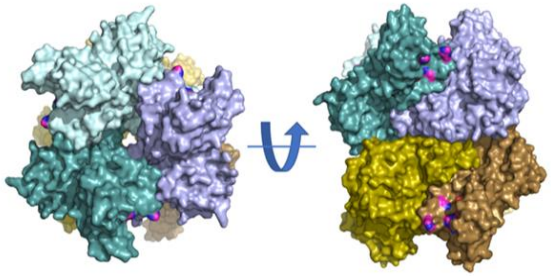
BES User Facilities Hosted Over 16,000 Users in FY 2019



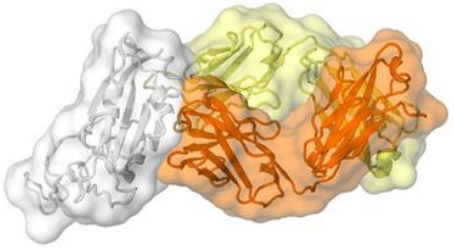
- NSLS-II started early operations in FY 2015
- Electron beam microcharacterization centers merged with site NSRCs in FY 2015

COVID-19 Related Research at BES Scientific User Facilities

- Light sources provide critical support to the development of potential therapeutic drugs and vaccines through structural studies of the proteins of the SARS CoV-2 virus, which causes COVID-19.
  - To date, a total of 70 structures of those proteins and their complexes have been determined based on data measured at BES light sources.
  - At APS, there were 55 unique user groups using 18 beamlines for an accumulated total of over 5500 hours of beamtime since late January at the start of the pandemic. Many important results have been published (e.g., the two figures on the right).
- Neutron facilities research includes high resolution structure analysis of the SARS-CoV-2 main protease enzyme, neutron reflectivity of viral protein interactions with cell membranes, and combined experiment-computational studies of potential therapeutic candidates.
- The NSRCs conduct studies to improve the effectiveness of personal protective equipment (masks, nanoparticle-based antiviral coatings), develop novel methods for virus detection (quantum dot-based, 3D printed platforms for high-throughput screening) and microfluidic devices nanoparticle synthesis for vaccine encapsulation and delivery.



Structure of the Nsp15 protein, a potential drug target: The Nsp15 protein of SARS CoV (the virus that causes SARS) and SARS CoV-2 are 89% identical so drugs that had previously been in development to treat the SARS outbreak could be developed as effective drugs against COVID-19.

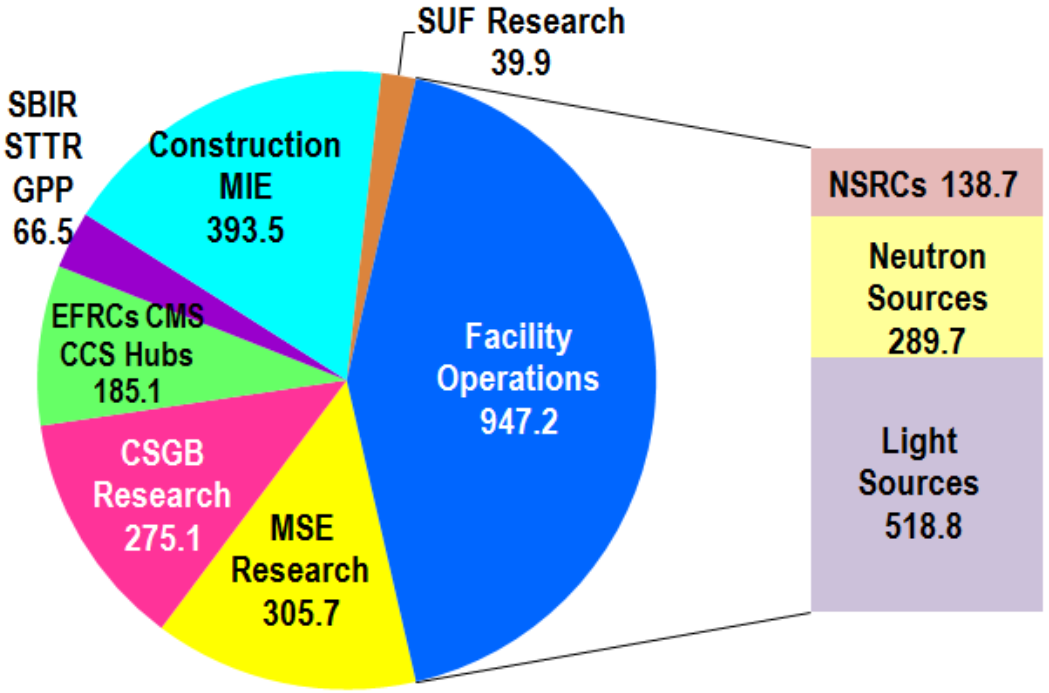


An antibody called CR3022, produced by a patient in response to the SARS, also binds to the SARS CoV-2. (Image courtesy of Meng Yuan and Nicholas Wu of the Wilson lab.)

FY 2020 Appropriation:
$2,213.0M (+$47M or +2.2% from FY 2019)

Research programs Δ = +$39.8M

- Core Research ($581M) includes new investments ($35M) in quantum information science (centers), critical materials, and carbon capture.
- Computational Materials and Chemical Sciences continue ($26M).
- Energy Frontier Research Centers continue Δ = +$5M ($115M).
- Energy Innovation Hubs continue Δ = +$5M ($44.1M).



Scientific user facilities Δ = +$35.6M

- Operations of 12 facilities at 100% optimal level ($947.2M).
- Facilities research increases for AI/ML Δ = +$10M ($39.9M).

Construction/MIE* Δ = -$33.9M

- Advanced Photon Source Upgrade ($170M)
- LCLS-II-HE ($54M); ALS-U ($62M); PPU ($60M); STS ($37M)
- Two new MIEs: NSRC Recap ($5M); NEXT-II ($5.5M)

*includes OPC

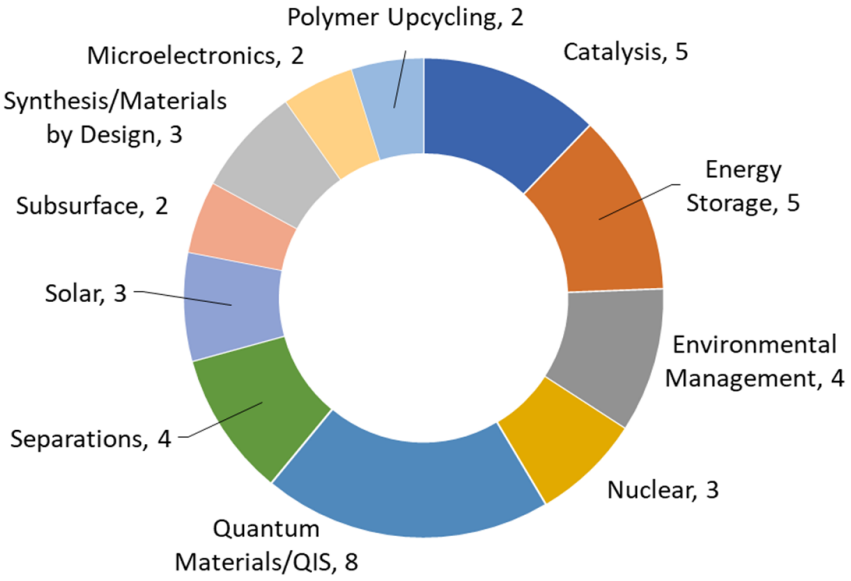
FY 2020 Energy Frontier Research Center Program Awards

FOA Scope:

- Multi-disciplinary, multi-institutional scientific teams.
- Fundamental research focused on one or more grand challenges, transformative opportunities, and basic research needs identified in BRN workshops/roundtables.
- **FY 2020 topical areas**: Environmental Management, Microelectronics, Polymer Upcycling, and Quantum Information Science

Awards:

- 10 Awards (8 University-led; 2 Lab-led)
  - **6 New Awards (4-year)**: Chemical Upcycling of Polymers (2), Microelectronics (2), QIS (2)
  - **2 Renewal Awards (4-year):** Env Mgmt
  - **2 Renewal Extensions (2-year)**: Env Mgmt
- Total funding (4 years): $100M
- 173 Senior Investigators at 55 unique institutions in 24 states and 4 foreign countries



FY 2020 Fuels from Sunlight Hub Program Awards

FOA Scope:

- Recompetition of Fuels from Sunlight Hub Program – new proposals only
- Fundamental research addressing emerging new directions and long-standing challenges in liquid solar fuels generation via artificial photosynthesis.
- Multi-disciplinary, multi-institutional scientific teams
- Must address at least 2 PROs from the BES Liquid Solar Fuels Roundtable
- Must build upon scientific advances and capabilities developed by the field, including efforts funded by BES through core programs, EFRCs, and JCAP

Awards:

- 2 Awards (University-led)
  - Liquid Sunlight Alliance (LiSA), California Institute of Technology
  - Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE), University of North Carolina at Chapel Hill
  - Both partnerships involve universities and DOE national laboratories
- Total funding (5 years): $100M pending appropriations
- Successors to the Joint Center for Artificial Photosynthesis (JCAP, FY 2010-2019)

FY 2020 Early Career Research Program Awards

FOA Scope:

- Support the development of individual research programs of outstanding scientists early in their careers and to stimulate research careers in the areas supported by SC.
- All BES core research areas participate, including SUF (NSRCs, Accelerator/Detector Research, X-ray and Neutron Instrumentation and Technique Development)
- Technical scope developed annually, with topics alternating to maintain reasonable applicant pool, ease reviewer burden, and improve success statistics.

FY 2020 Awards:

- 32 Awards (25 University; 7 Lab) – 20 states
- Total funding (5 years): $36.5M
- Awards span all three BES divisions and most core research areas

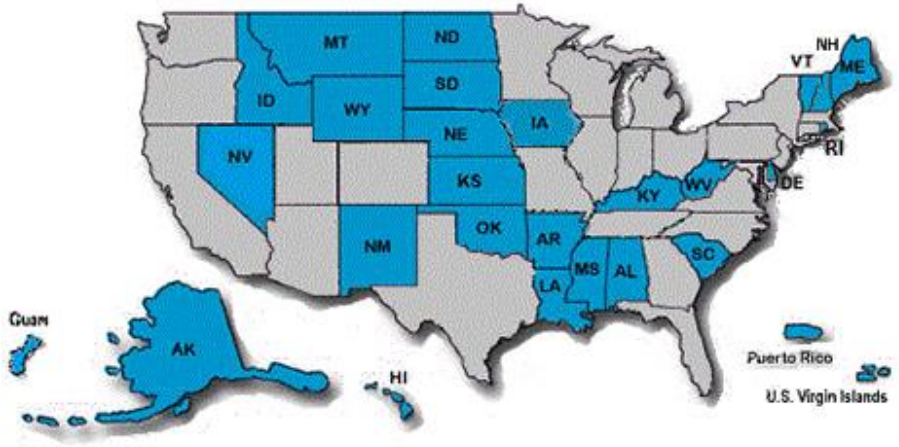
All active early career projects (FY 2016 – 2020):

- 145 awards (113 University; 32 Lab)
- 48 female PIs; 97 male PIs (33% female)
- 34 States (12 EPSCoR)

FY 2020 EPSCoR State-National Lab Partnership Awards

FOA Scope:

- Fundamental/early stage research across a broad range of DOE interests
- Additional areas of interest: Quantum Information Science, Microelectronics, Data Science (AI/ML), Energy Storage, Plastics Recycling
- FOA encouraged junior faculty participation and utilization of DOE user facilities with participation by students/postdocs



Awards:

- 31 Awards (18 states; 12 National Lab Partners)
- Partner programs: EERE (Adv. Mfg., Solar, Water, Vehicles, Bioenergy), FE, OE, SC
- Total funding (3 years): $21.9M (including 10% from partner programs)
- Topics: Advancing Characterization, Advanced Manufacturing, Accelerator Technology, Data Science, Machine Learning, Artificial Intelligence, Energy Conversion, Energy Storage, Grid Stability, Quantum Information Science, Plastic Recycling, Renewable Energy

https://science.osti.gov/-/media/bes/epscor/pdf/files/EPSCoR_DE-FOA-0002215_Selectee_Listing.pdf

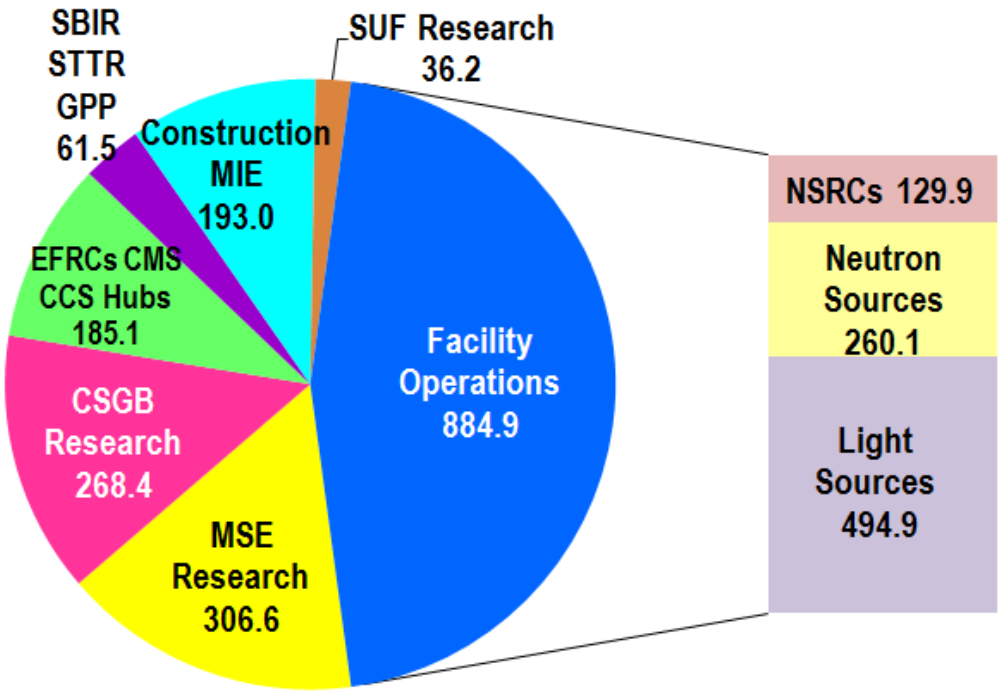
FY 2020 Special FOAs – Awards to be Announced

- QIS Centers: Released Jan.10; full proposals under review (peer review, pre-selection interviews), SC-wide awards to be made by Sept. 30, 2020.
  (2 to 5 five-year awards, up to $25M/year per award, total up to $625M)
  - DOE response to National Quantum Initiative (NQI) Act, enacted Dec. 2018
  - Scope built on extensive community-wide RFI inputs
  - Each Center cuts across multiple SC program offices and technical areas
  - All SC program offices participating; national labs, academia, industry
- AI/ML for User Facilities: Lab announcement with High Energy and Nuclear Physics. Proposals under review. (BES: Total $10M/yr, 3-yr awards).
- Materials and Chemical Sciences Research on Critical Materials:
  Lab announcement. Proposals under review. (Total $6M/yr, 4-8 3-yr awards)
  - Emphasis on Physics/Chemistry of Rare Earths; Novel Materials/Molecular Design and Synthetic Approaches; Advances in Separation Science
- Materials and Chemical Sciences Research for Direct Air Capture of CO_2:
  Lab Announcement. Proposals under review. (Total $4M/yr, 3-5 3-yr awards)
  - Emphasis on Designing High Selectivity, Capacity, and Throughput Separation; Data Science Driven Synthesis and Assembly of Materials for Direct Air Capture; Understanding Temporal Changes that Occur During Separation

FY 2021 President's Request: $1,935.7M (-$277.3M or -12.5% from FY 2020)

Research programs Δ = -$5.9M

- Core Research ($575M) includes new investments ($73M) in critical materials, AI/ML, polymer upcycling, next-generation biology, microelectronics, and accelerator R&D
- Computational Materials and Chemical Sciences continue ($26M)
- Energy Frontier Research Centers continue ($115M)
- Energy Innovation Hubs continue ($44.1M)



Scientific user facilities Δ = -$66M

- Operations of 12 facilities continue at ~91% of optimal. LCLS at 97% of optimal ($884.9M).
- Facilities research continues for AI/ML; increases for accelerator R&D ($36.2M).

Construction/MIE* Δ = -$200.5M

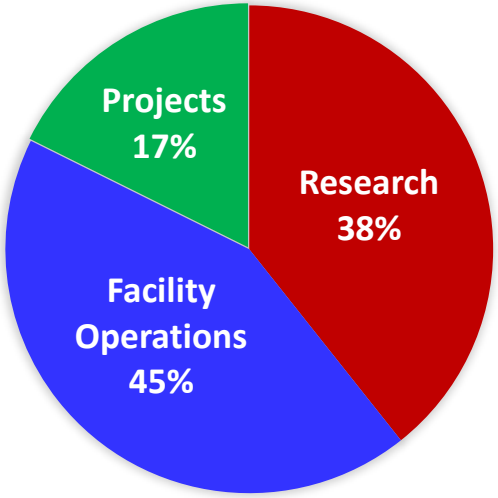
- APS-U ($150M); LCLS-II-HE ($16M); ALS-U ($13M); PPU ($8M); STS ($2M)
- MIEs: NSRC Recap ($1M); NEXT-II ($1M)
- New start: Cryomodule Repair & Maintenance Facility (CRMF) ($2M)

*includes OPC

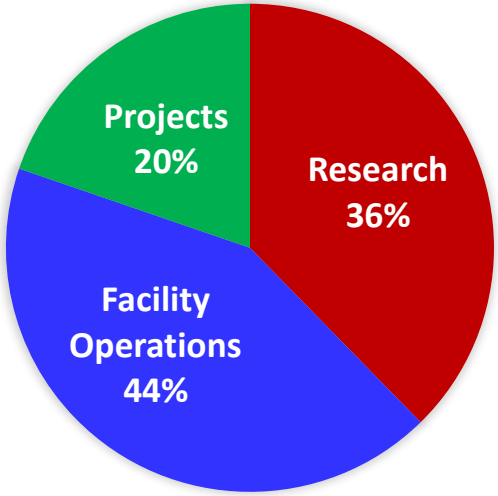
BES Budget by Budget Element: 2018 - 2021

	FY 2018 Enacted	FY 2019 Enacted	FY 2020 Enacted	FY 2021 President's Request	FY 2021 House Mark
Research	821,403	815,600	871,321	856,817	952,912
Facility Operations	898,597	922,000	947,179	884,856	934,088
Projects (Construction + MIE)	369,000	427,400	393,500	193,000	354,000
Other	1,000	1,000	1,000	1,000	1,000
Total	2,090,000	2,166,000	2,213,000	1,935,673	2,242,000

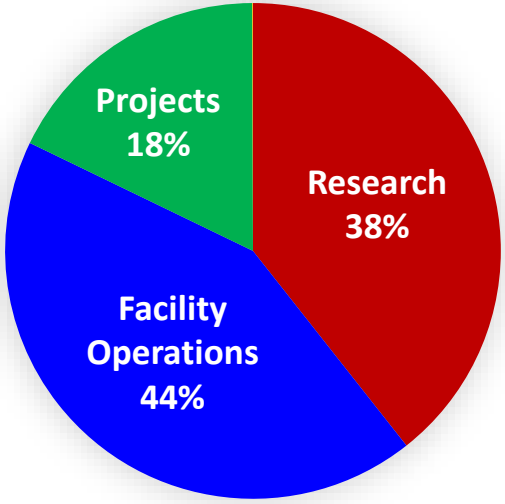
FY 2018



FY 2019



FY 2020



BESAC Report on BES 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, now at 1 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 Q4/FY 2020	CD-3	CD-1	CD-3b	CD-0	CD-3	CD-3a
FY 2020 Approp	✓	✓	✓	✓	**Last Funds in FY 2019**	✓

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All six projects are advancing!

Line Item Construction Projects

Linac Coherent Light Source-II (LCLS-II) – CD-3: LCLS operation with new undulators, August 2020

- Slowly resuming construction and commissioning activities after losing ~5 months of schedule due to COVID-19.
- Performance Baseline Deviation due in part to impact of COVID-19. Projected baseline to increase TPC $85-95M and delay CD-4 date until April to October 2023.

Advanced Photon Source Upgrade (APS-U) – CD-3

- FY 2020 = $170M; FY 2021 request = $150M; House mark = $160M for procurement, integration, and testing of storage ring and experimental equipment and new beamline building construction. OPA status review September 1-3, 2020.
- Some cost and schedule impacts of COVID-19.

Linac Coherent Light Source-II High Energy (LCLS-II-HE) – CD-3a

- FY 2020 = $54M; FY 2021 request = $16M; FY 2021 House mark = $72M for engineering, design, R&D prototyping. LCLS-II-HE received CD-3A approval in May 2020 for long lead procurements.
- Studying long-term COVID-19 impacts. Considering adding a low emittance superconducting electron gun.

Advanced Light Source Upgrade (ALS-U) – CD-1

- FY 2020 = $62M; FY 2021 request = $13M; FY 2021 House mark = $75M for planning, engineering, design, R&D prototyping activities, and long lead procurements. OPA CD-2 review is scheduled for November 2020.
- COVID-19 impacts are being studied and mitigations put in place.

SNS Proton Power Upgrade (PPU) – CD-3b

- FY 2020 = $60M; FY 2021 request = $8M; FY 2021 House mark = $8M for design, engineering, prototyping, fabrication, testing, and long lead procurements. Combined CD-2/3 OPA reviews in July 2020.
- ORNL work for PPU and STS continues onsite and remotely, helping to minimize COVID impacts.

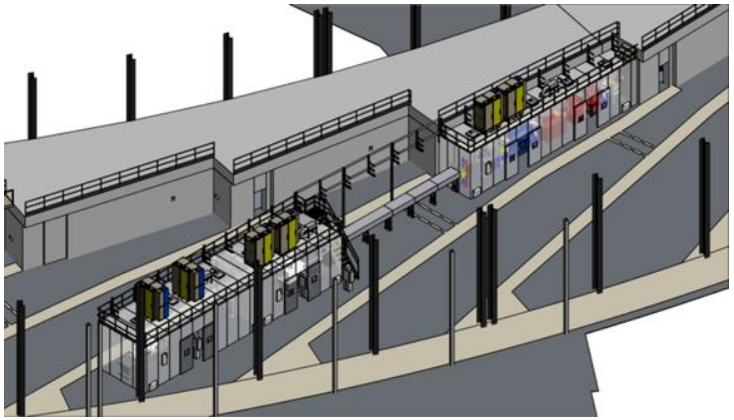
SNS Second Target Station (STS) – CD-0

- FY 2020 = $37M; FY 2021 request = $2M; House mark = $2M for planning, R&D, design and engineering.
- OPA CD-1 review occurred in June 2020.

FY 2020 New Major Item of Equipment Projects (Pre-CD-1)

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

- FY 2020 = $5.5M; FY 2021 request = $1M, House mark = $15M for engineering designs of new beamlines.
- NEXT-II is a 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 project will undergo an SC Independent Project Review in August 2020 for CD-1. The proposed a new cost range is $65M to $95M.



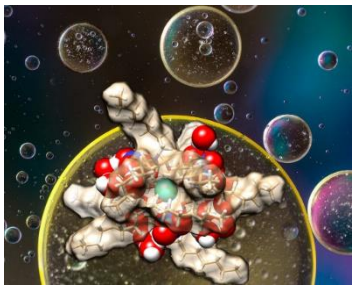
Schematic of the Submicron Resolution X-ray Spectroscopy (SRX) beamline, one of the NSLS-II project beamlines

Nanoscale Science Research Center Recapitalization (NSRC-Recap)

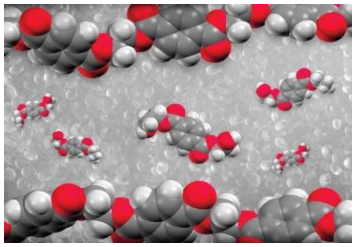
- FY 2020 = $5M; FY 2021 request = $1M; FY 2021 House mark = $15M for planning, R&D, design, engineering and possible procurements.
- NSRC Recap is an MIE project to upgrade equipment across all five NSRCs to continue to perform cutting edge science and accelerate advances in the fields of nanoscience, materials, chemistry, biology and QIS.
- The notional cost range is $50M to $90M.
- The project achieved CD-0 in December 2018. CD-1 OPA review in December 8-10, 2020. Remote work minimizes COVID impacts.

Basic Energy Sciences – FY 2021 Priorities

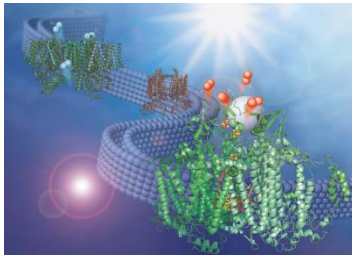
- Critical materials (+$25M) - advance our understanding of fundamental properties of these materials, identify methodologies to reduce their use and to discover substitutes, and enhance chemical processing and separation science for rare earths
- AI/ML (+$10M) - accelerate fundamental research for the discovery of new chemical mechanisms and material systems with exceptional properties and function
- Polymer upcycling (+$8.25M) - provide the foundational knowledge for designing chemical components and processes that enable efficient conversion of plastic waste to high-value chemicals, fuels, and materials; investments informed by BES Roundtable on Chemical Upcycling of Polymers
- Next-generation biology (+$3.75M) - cross-fertilize and leverage discoveries and approaches across the biological, physical, and computational sciences to develop bio-inspired, biohybrid and biomimetic systems; emphasis on neuromorphic computing, programmable biomaterials and biocatalysts, and tools for characterization of chemical, biological, biomaterial, and biohybrid systems



Critical materials: Peculiar outer-sphere water coordination of trivalent lanthanide complexes is shown to correlate with the lanthanide selectivity



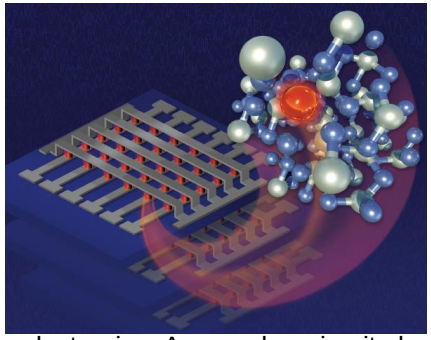
Polymer upcycling: A circular polymer lifecycle would make it easy to recycle polyethylene terephthalate (PET)



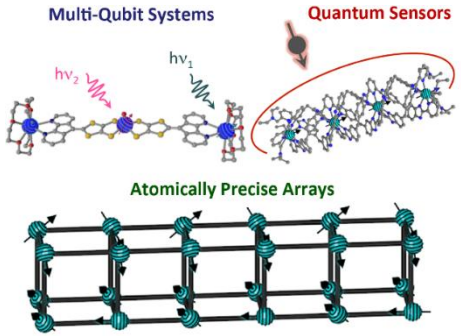
Next-gen biology: Z-scheme solar water splitting via self-assembly of photosystem I-catalyst hybrids in thylakoid membranes

Basic Energy Sciences – FY 2021 Priorities

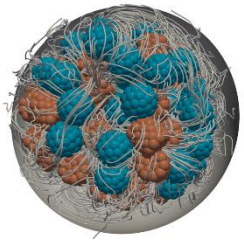
- Microelectronics (+$25M) - focus on materials, chemistry, and fundamental device science; multi-disciplinary research to accelerate the advancement of microelectronic technologies in a co-design innovation ecosystem in which materials, chemistries, devices, systems, architectures, algorithms, and software are developed in a closely integrated fashion
- Quantum information science – investments in core research and the interdisciplinary SC QIS Center(s) started in FY 2020 are maintained at $72M
- Exascale computing – investments in Computational Chemical and Materials Sciences are maintained at $26M



Microelectronics: A cross-bar circuit element designed for future low power, non-volatile memory or neuromorphic computing applications.



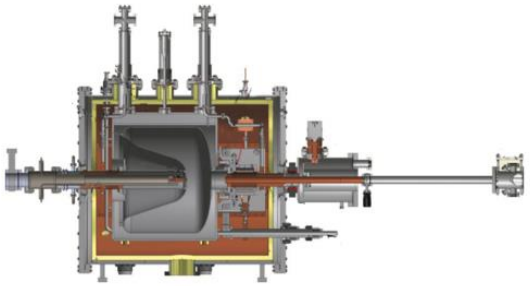
QIS: Coordination compounds as qubits



Preparing for Exascale: Computational modeling of the motion of spherical (blue) and cylindrical (orange) nanoparticles in a solvent

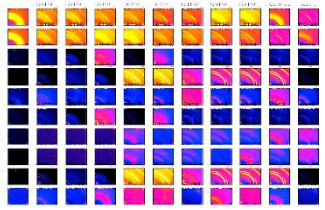
Facilities-related Research

- Strategic accelerator technology (+$6.25M)
  - Strategic investments in high-brightness electron injectors, superconducting undulators with strong focusing, and high gradient superconducting cavities will have the most impactful benefits on existing facilities
  - New materials are needed for future accelerator technologies including magnets, optics, detectors, and sensors



Strategic accelerator technology: Drawing of a superconducting electron gun required to extend X-ray energy towards 20 KeV

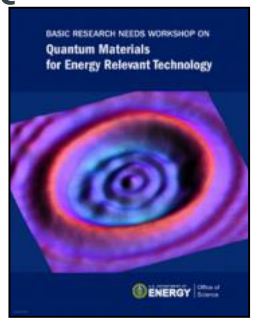
- Data analytics and machine learning for data-driven science – investments in AI/ML to address data and information challenges at the BES user facilities, including accelerator optimization, control, prognostics, and data analysis are maintained at $10M

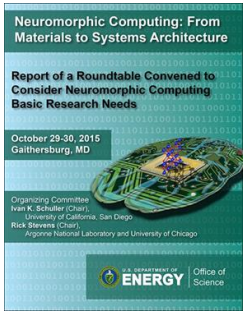


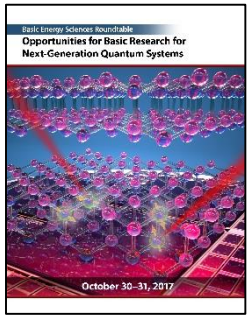
Data analytics and machine learning: Developing a pattern recognition algorithm to retrieve relevant images from a database based on pictorial similarity

Strategic Planning Workshops and Roundtables Provide Insights on Priority Research Areas

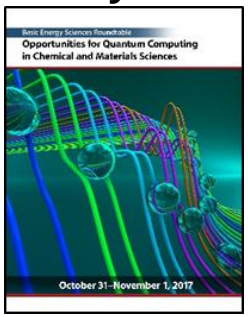
- Quantum Science

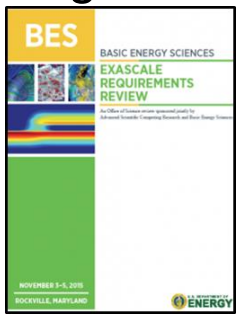


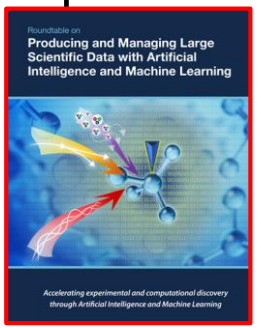




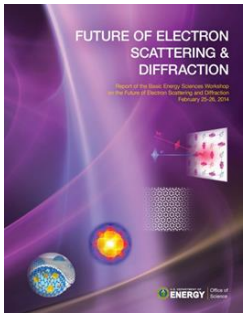
Theory, Modeling and Computation

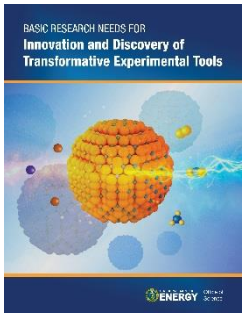




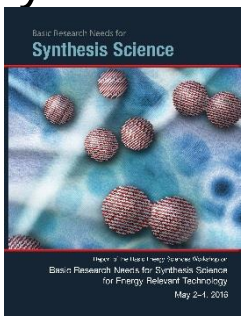


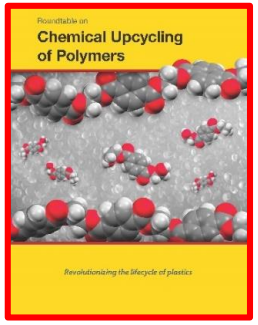
- Characterization



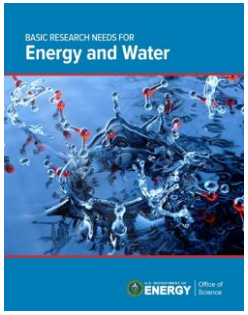


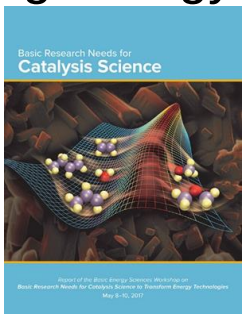
Synthesis

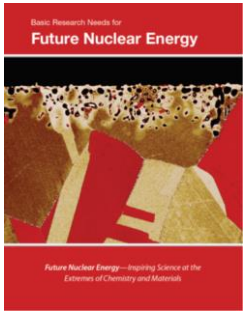


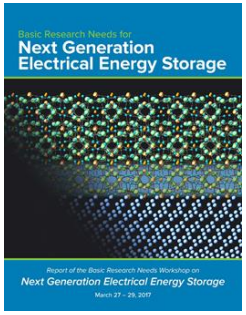


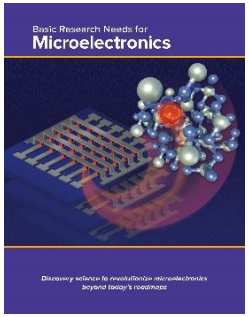
- Cross-Cutting Energy

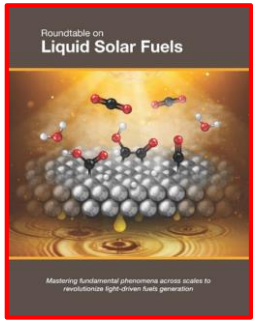








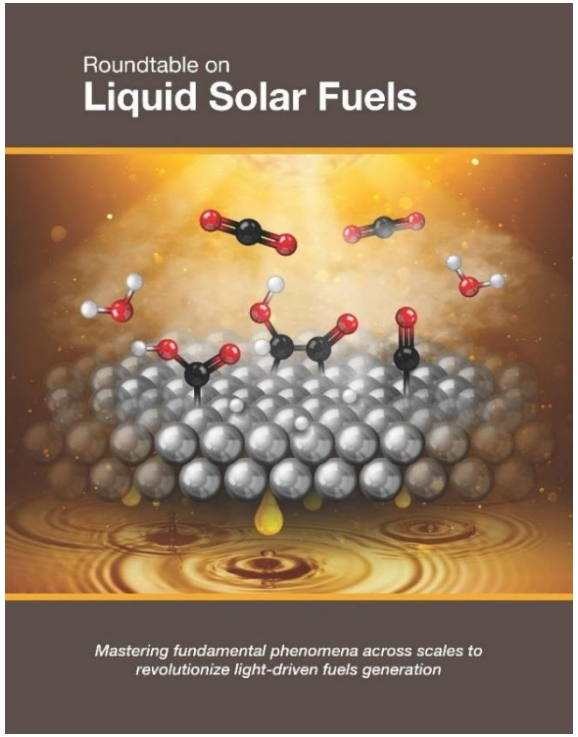




Priority Research Opportunities in Liquid Solar Fuels
Report based on BES Roundtable in August 2019

- Understand the mechanisms that underpin constituent durability and performance
  - *How can molecular-level knowledge of individual processes in solar fuels generation lead to predictive design of components with enhanced lifetime and desired activity?*
- Control the catalyst microenvironment to promote selective and efficient fuel production
  - *How do we probe, understand, and tailor the structure, composition, and dynamics of the local region surrounding catalytic active sites to direct chemical reaction pathways?*
- Bridge the time and length scales of light excitation and chemical transformations
  - *How do we probe, understand, and tailor the structure, composition, and dynamics of the local region surrounding catalytic active sites to direct chemical reaction pathways?*
- Tailor interactions of complex phenomena to achieve integrated multicomponent systems
  - *How can the fundamental science of integration advance the predictive design and control of interfaces and processes to enhance the performance, including durability, of solar fuels systems?*

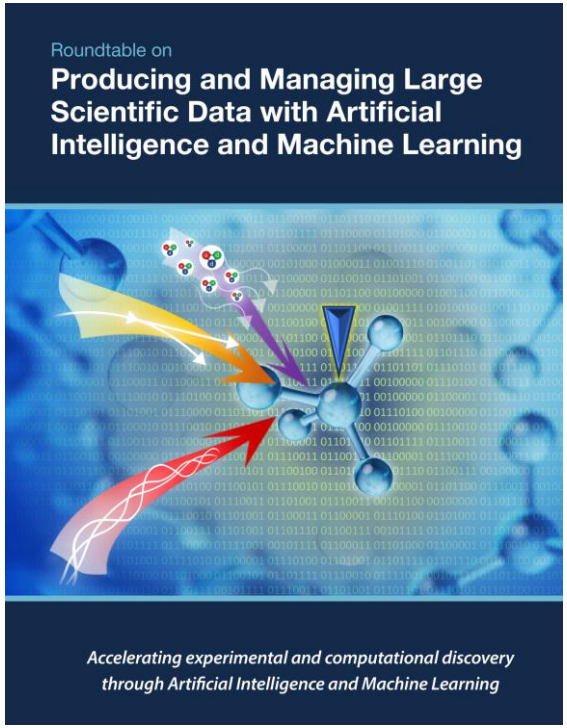
Used as source document for Fuels from Sunlight FOA



Roundtable Chaired by Bill Tumas (NREL) with Co-chairs Jillian Dempsey (UNC-CH) and Tom Mallouk (U Penn)

Producing and Managing Large Scientific Data with Artificial Intelligence and Machine Learning

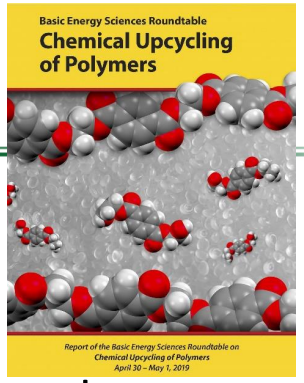
- Efficiently extract critical and strategic information from large, complex data sets
  - *How do we extract robust and meaningful information from the increasingly vast and complex data now being produced at BES' scientific user facilities?*
- Address the challenges of autonomous control of scientific systems
  - *How do we address challenges inherent in real-time operation of large, complex scientific user facilities?*
- Enable offline design and optimization of facilities and experiments
  - *How do we enable virtual laboratories - offline design and optimization of facility operation and experiments – to achieve new scientific goals?*
- Use shared scientific data for machine learning–driven discovery
  - *How can we catalyze scientific discovery by leveraging the wealth of diverse and complementary data recorded across the BES scientific user facilities?*



Roundtable held in October 2019. Chairs: Bobby Sumpter (ORNL), and Daniel Ratner (SLAC)

Used as source document for AI/ML Lab Announcement for Scientific User Facilities

Research Coordination Activities



Polymer Upcycling

- SC cross-cutting initiative engages BES, BER, and ASCR
  - Chemical upcycling of polymers aligned with BES Roundtable report
  - Biological upcycling of polymers builds on BER capabilities (Genomic Science and Biosystems Design) and aligns Industrialization of Biology (NAS report) and Genome Engineering for Materials Synthesis (BER report)
  - Development of data science tools to discover and control chemical and biological mechanisms
- DOE Plastics Innovation Challenge engages SC, EERE, and ARPA-E
  - PIC announced in November 2019, includes collection, deconstruction, upcycling, plastic design for circularity, and commercialization
  - SC effort aligns with deconstruction, upcycling, and plastic design for circularity
  - Quarterly coordination meetings, roadmap under development

Research Coordination Activities

Research and Technology Investment Committee (RTIC) – within DOE

- Established in 2019 to implement the Department of Energy Research and Innovation Act (Pub. L. 115-246)
- Identify strategic opportunities for coordination and collaborative research, development, demonstration, and commercial application of innovative science and technologies
- Topical RTIC Subcommittees: Energy Storage, AI/ML, Critical Materials, Electricity Delivery Systems (Grid), STEM/Workforce

Semiconductor Leadership R&D Working Group – Interagency

- Established by OSTP in 2020 to enable interagency coordination around non-classified R&D related to semiconductor technologies
- Co-chaired by DOE and DOD
- Holding a series of Fed-only information sharing meetings
- Plans to engage industry and other stakeholders through roundtables

International Workshops

US – Germany Workshops on Artificial Photosynthesis

- Virtual workshop held June 24-26, 2020
- Sponsored by BES and German Federal Ministry for Science and Education
- Chairs: Frances Houle (LBNL), Thomas Hannappel (TU Ilmenau)
- Objective of workshop series: provide a strong foundation for future U.S.-German collaborations to accelerate progress in Artificial Photosynthesis research

US – UK Catalysis Workshops

- Initial workshop (virtual) planned for October 8, 2020
- Sponsored by BES and the UK Catalysis Hub
- Objective of workshops: identify opportunities for U.S.-U.K. collaborations in catalysis science with a focus on sustainability

Energy Storage Workshops: US-UK and US-Japan

- In planning

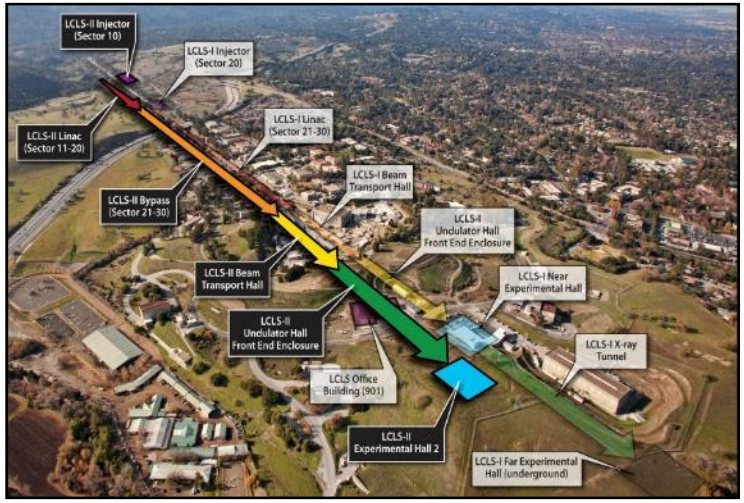
Questions

Back-Up

LCLS-II and APS-U Construction Projects

Linac Coherent Light Source-II (LCLS-II)

- LCLS-II will provide high-repetition-rate, ultra-bright, transform-limited femtosecond x-ray pulses with polarization control and pulse length control.
- LCLS-II project is slowly resuming construction and commissioning activities after losing ~5 months of schedule due to the Shelter in Place orders. COVID-19 mitigations are impacting work durations and costs. Travel restrictions are preventing foreign vendors from returning to SLAC to complete work.
- The project has experienced a Performance Baseline Deviation due in part to the impact of the COVID-19. The projected new baseline will increase the TPC between $85M to $95M and the new CD-4 date between April 2023 to October 2023. The project will run out of funding by the end of calendar 2020.



Advanced Photon Source Upgrade (APS-U)

- FY 2020 = $170M; FY 2021 request = $150M; FY 2021 House mark = $160M for procurement, integration, and testing of storage ring and experimental equipment and new beamline building construction.
- APS-U will provide a multi-bend achromat lattice hard x-ray source with world leading transverse coherence and extreme brightness.
- The project experienced some cost and schedule impacts. APS-U is maintaining close contacts with vendors to manage COVID-19 delays.
- Upcoming OPA Status Review scheduled for September 1-3, 2020.

Mike Kelly checks & prepares APS-U Super Conducting Cryovessel at ANL.

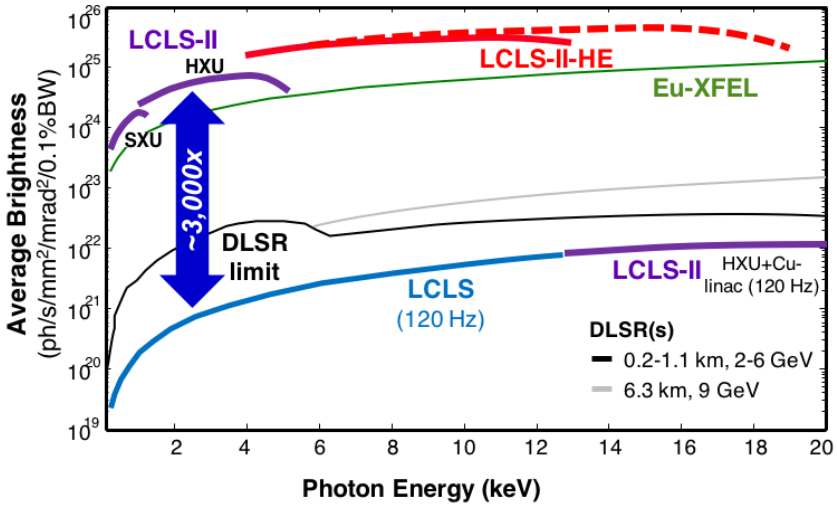
Kris Meitsner tests a quadrupole magnet during COVID using ANL safety protocols.

Tim Grager inspects APS-U monochromater before testing.

LCLS-II-HE and ALS-U Construction Projects (Pre CD-2)

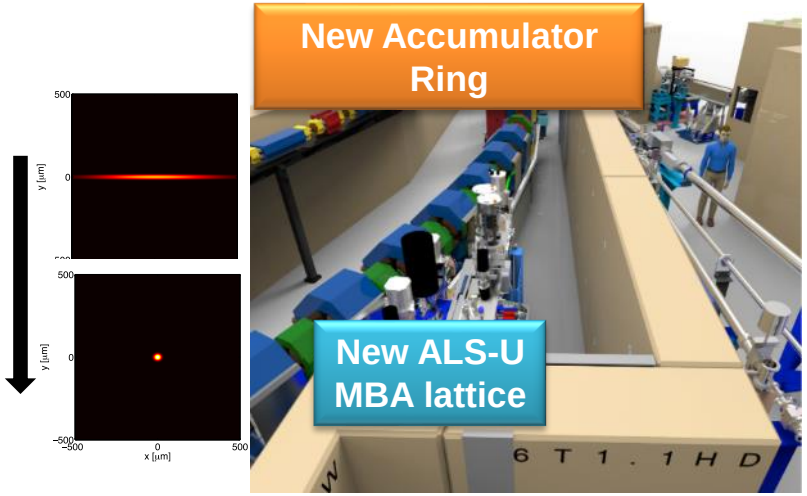
LCLS-II High Energy Upgrade (LCLS-II-HE)

- FY 2020 = $54M; FY 2021 request = $16M; FY 2021 House mark = $70M TEC and $2M OPC for engineering, design, R&D prototyping, and long lead procurements.
- LCLS-II-HE will increase the energy of the LCLS-II linac from 4 to 8 GeV at 1 MHz and deliver ~1,000-fold higher average brightness for hard x-rays up to and beyond 12 keV.
- LCLS-II-HE received CD-3A approval in May 2020. The project is proceeding with 3A procurements while studying the long term COVID-19 impacts. The project is considering adding a low emittance superconducting electron gun to the project.



Advanced Light Source Upgrade (ALS-U)

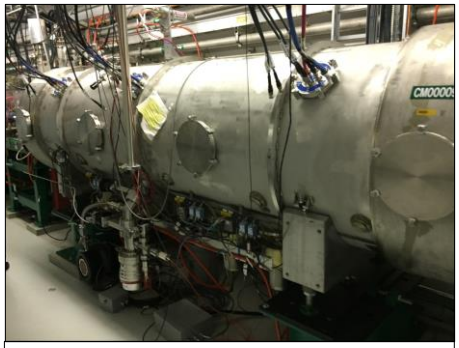
- FY 2020 = $62M; FY 2021 request = $13M; FY 2020 House mark = $75M for planning, engineering, design, R&D prototyping activities, and long lead procurements.
- ALS-U will install a multi-bend achromat lattice to reduce emitance and generate 1,000 times brighter soft x-rays with higher coherence to resolve nanometer-scale features and enable real-time observation of chemical processes and materials as they function.
- ALS-U will seek to baseline the project in FY2021. An SC OPA CD-2 review is scheduled for November 2020. COVID-19 impacts are being studied and mitigations put in place.



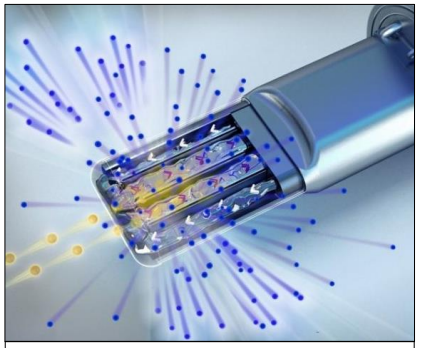
PPU and STS Construction Projects (Pre CD-2)

Proton Power Upgrade (PPU)

- FY 2020 = $60M; FY 2021 request = $8M; FY 2021 House mark = $8M for limited design, engineering, prototyping, fabrication, testing, and long lead procurements.
- PPU will double the beam power capability of the SNS accelerator to 2.8 MW, add gas injection to improve target performance and reliability to 2 MW of beam power.
- PPU held combined OPA reviews for CD-2 project baseline and CD-3 start of construction in July 2020. ORNL work continues onsite and remotely, helping to minimize COVID impacts.



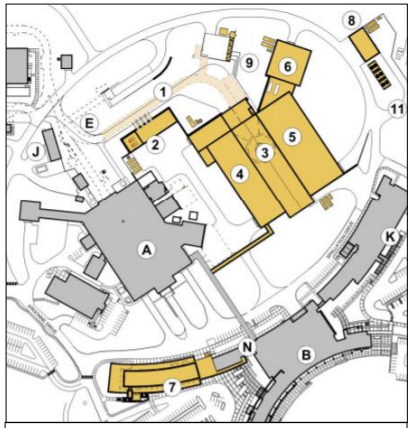
7 new cryomodules increase the proton beam power at available to the target.



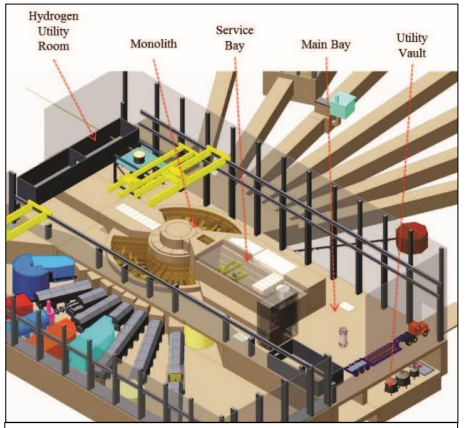
Protons (yellow) strike the liquid Hg target creating neutrons by spallation.

Second Target Station (STS)

- FY 2020 = $37M; FY 2021 request = $2M; FY 2021 House mark = $2M for limited planning, R&D, design and engineering.
- STS will be a complementary pulsed source producing an order of magnitude higher brightness cold neutrons than were previously achievable. By optimizing instruments, the detection resolution increases by up to 100x.
- The OPA review for CD-1 Approve Alternative Selection and Cost Range and Independent Cost Review occurred in June 2020. ORNL work continues onsite and remotely, helping to minimize COVID impacts.



New STS facilities in yellow, existing SNS facilities in gray. Target building top right (numbered 3,4,5,6).



Notional STS target facility layout with target monolith and potential locations for beamlines and service bay.

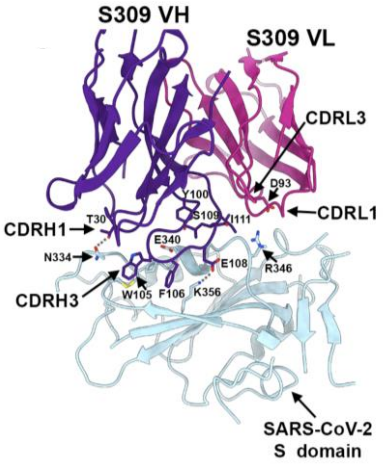
Antibody from SARS Survivor Neutralizes SARS-CoV-2

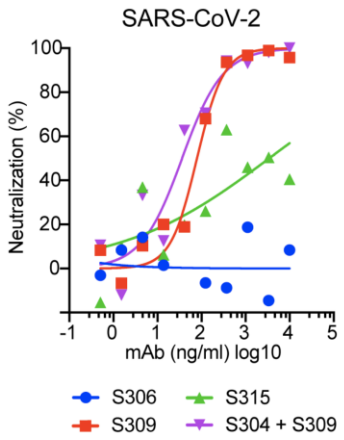
Scientific Achievement

Using structural data from the Advanced Light Source (ALS) and cryo-EM, researchers have characterized how an antibody binds to and neutralizes SARS-CoV-2.

Significance and Impact

This work provides the basis for therapeutic and vaccine development for the SARS-CoV-2 virus, which is responsible for the COVID-19 pandemic.





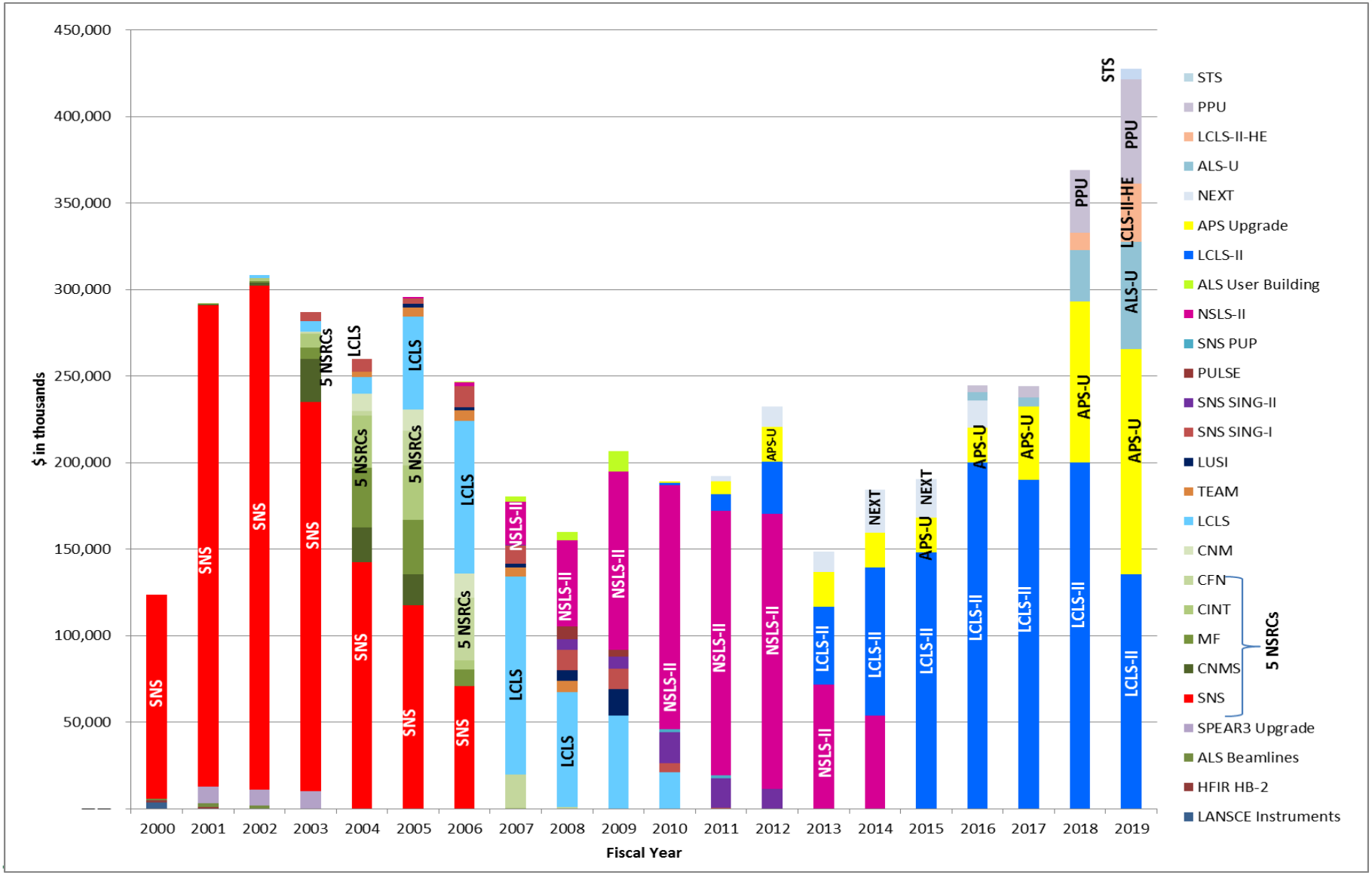
Left: The antibody S309 (purple and pink) makes contact with SARS-CoV-2 (blue) via complementarity-determining regions (CDRs), or loops that attach to residues in the virus's spike protein. Right: S309 and antibody cocktails containing S309 are effective in neutralizing SARS-CoV-2 in Vero E6, a primate cell line.

Research Details

- Antibodies from an individual who survived SARS in 2003 were tested for their ability to neutralize the related virus SARS-CoV-2, currently ravaging the globe.
- The structural data showed that one antibody, S309, has six loops that recognize and attach to the spike protein of SARS-CoV-2, neutralizing the virus and recruiting other antiviral mechanisms.

Publication about this research: D. Pinto, Y.-J. Park, M. Beltramello, A.C. Walls, M.A. Tortorici, S. Biachi, S. Jaconi, K. Culap, F. Zatta, A. De Marco, A. Peter, B. Guarino, R. Spreafico, E. Cameroni, J.B. Case, R.E. Chen, C. Havenar-Daughton, G. Snell, A. Telenti, H.W. Virgin, A. Lanzavecchia, M.S. Diamond, K. Fink, D. Veesler, and D. Corti, *Nature*, doi:10.1038/s41586-020-2349-y (2020). Work was performed at Lawrence Berkeley National Laboratory, ALS/BCSB Beamline 5.0.2. Operation of the ALS is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences program.

BES Construction/MIE Funding Profiles: 2000 – 2019

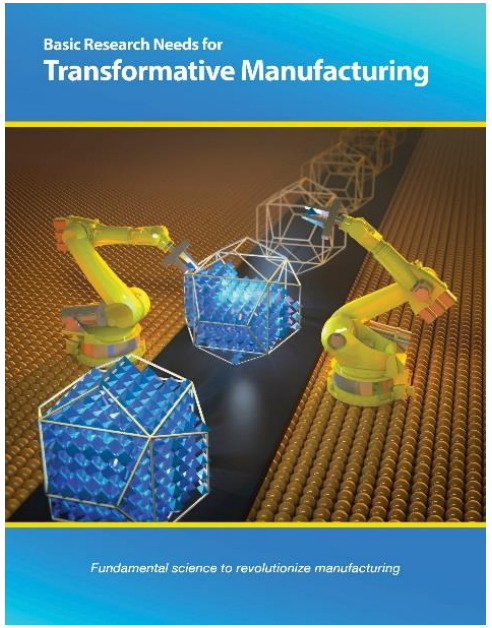


Research Directions to Advance Transformative Manufacturing

The BES Goal: a basic science strategy that underpins applied technology research and lays the scientific foundation to go beyond incremental improvements to create new, transformative technologies for manufacturing that are energy efficient and sustainable

Priority Research Directions for BES research:

- Achieve precise, scalable synthesis and processing of atomic-scale building blocks for components and systems
- Integrate multiscale models and tools to enable adaptive control of manufacturing processes
- Unravel the fundamentals of manufacturing processes through innovations in operando characterization
- Direct atom and energy flow to realize sustainable manufacturing
- Co-design materials, processes, and products to revolutionize manufacturing



Workshop in March 2020 chaired by Cynthia Jenks (ANL), Jennifer Lewis (Harvard), and Ho Nyung Lee (ORNL)

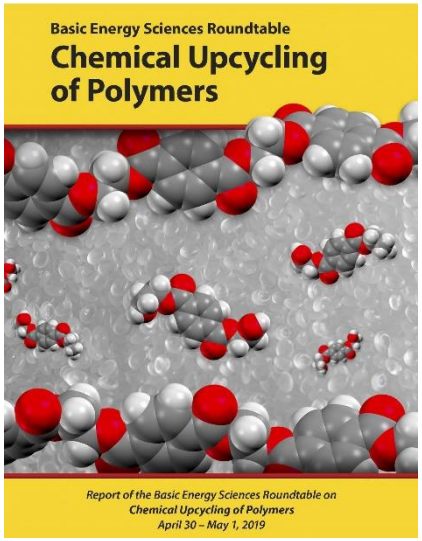
Opportunities to Advance Chemical Upcycling of Polymers

Report based on BES Roundtable in April 2019

The BES Goal: provide foundational knowledge for designing new chemical processes and polymeric materials to shift the paradigm of discarded plastics from wastes to a resource for making high-value fuels, chemicals, and new polymeric materials

Priority Research Opportunities for a BES research agenda:

- Master the mechanisms of polymer deconstruction, reconstruction and functionalization
  - *How do we develop selective and integrated chemical processes to upgrade a discarded plastic into a desirable product?*
- Understand and discover integrated processes to upcycle mixed plastics
  - *How can we directly transform mixed discarded plastics to desirable products?*
- Design next generation of polymers for chemical circularity
  - *How can we design new polymers that have the properties of today's polymers and enable simple reuse of the molecular building blocks?*
- Develop novel tools to discover and control chemical mechanisms for macromolecular transformations
  - *What experimental and computational tools are needed to elucidate the macromolecular transformations of plastics in complex, non-equilibrium media?*



BES convened a Roundtable in April 2019 chaired by Phil Britt (ORNL), Geoff Coates (Cornell), and Karen Winey (U Penn)

Used as source document for 2020 EFRC FOA – 2 awards made