



U.S. DEPARTMENT OF
ENERGY

Office of
Science

Basic Energy Sciences Update

Basic Energy Sciences Advisory Committee Meeting

April 5, 2022

Linda Horton, Bruce Garrett, and Andy Schwartz

Office of Basic Energy Sciences

Updates --

- ▶ **BES staff have returned to the office! First visitor is next week...**
- ▶ Organization Changes and Progress...
- ▶ FY 2022 funding and funding opportunity announcements (ALL)
- ▶ Strategic Planning (Bruce and Andy)
- ▶ FY 2023 funding

Office of Basic Energy Sciences

Associate Director
Linda Horton

BES Budget and Planning
Kara Beles, Financial Management
Donetta Herbert, Financial Management
Thomas Russell, Senior Technical Advisor
(Vacant, Senior Technical Advisor)

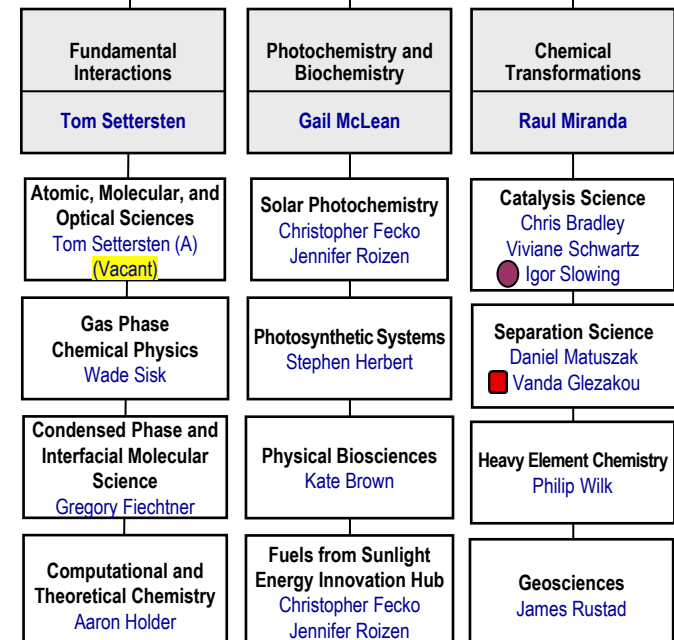
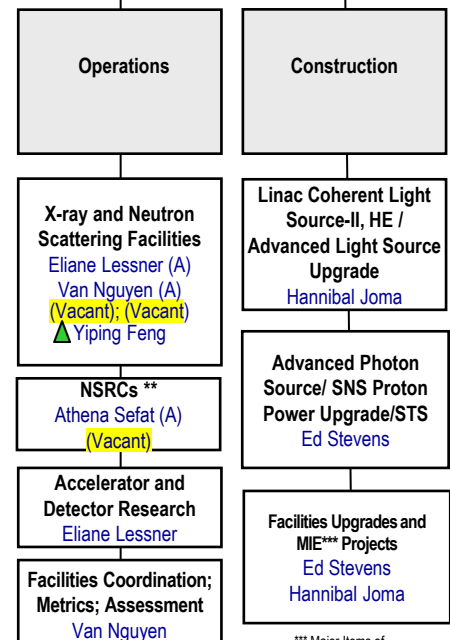
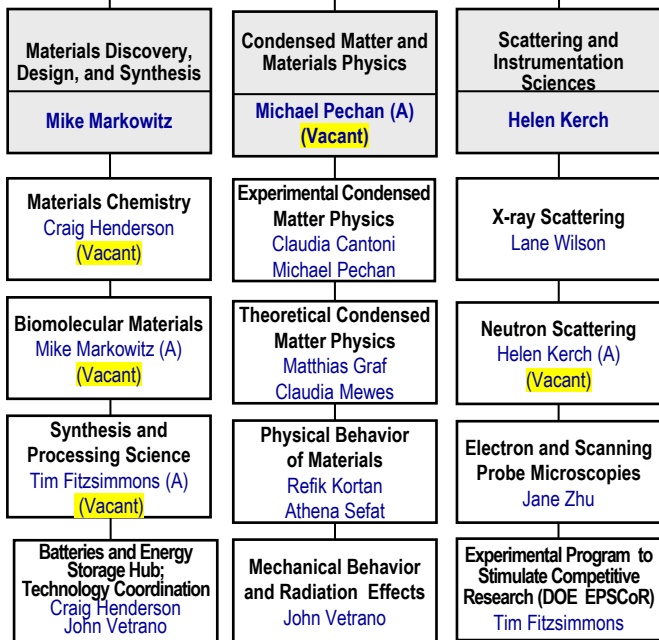
BES Operations
Teresa Crockett, Program Analyst
Robin Hayes, Program Manager
Kerry Hochberger, Program Analyst / BESAC*
Andy Schwartz, Senior Technical Advisor for EFRs (A)**
(Vacant, Program Support Specialist)

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

Materials Sciences and Engineering Division
Andy Schwartz, Director
Shawn Chen, AAAS Fellow

Scientific User Facilities Division
Linda Horton, Acting Director
Rocio Meneses, Program Support Specialist

Chemical Sciences, Geosciences, and Biosciences Division
Bruce Garrett, Director
Brandon Rohnke, AAAS Fellow



LEGEND

■ Detailee (50%) from PNNL ● Detailee (80%) from Ames

▲ Detailee (70%) from SLAC

(A) Acting

** Nanoscale Science Research Centers

*** Major Items of Equipment

New Materials Sciences and Engineering Division Director!



Dr. Andrew Schwartz

Division Director

Materials Sciences and Engineering Division

Expertise

- Experimental condensed matter physics (superconductors, oxides, organic/inorganic conductors, and semiconductors)
- Novel metrology for development and control of manufacturing processes for advanced integrated circuits

Experience

- Acting Division Director for Materials Sciences and Engineering
- Leads the microelectronics initiative for the Office of Science
- Interagency role for OSTP activities in nanotechnology (co-chair) and microelectronics
- Senior technical advisor in the BES Associate Director's office, leading the Energy Frontier Research Center team
- DOE-BES Program Manager for Experimental Condensed Matter Physics
- Technical Director, Solid State Measurements, Inc. and Neocera, Inc.
- Ph.D. in Physics from UCLA

New Hire – Physical Biosciences Program



Dr. Kate Brown

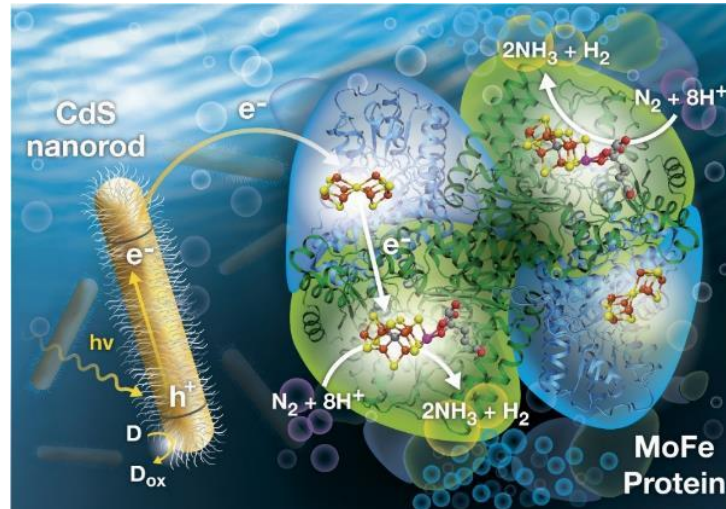
Program Manager, Physical Biosciences
Chemical Sciences, Geosciences and Biosciences Division

Expertise

- Redox biochemistry
- Chemistry and photocatalysis
- Biohybrid methods

Experience

- National Renewable Energy Laboratory (NREL), Scientist
- National Renewable Energy Laboratory (NREL), Postdoctoral Fellow
- Massachusetts Institute of Technology, Ph.D.



Light-driven reduction of nitrogen to ammonia by coupling nitrogenase enzyme to light-harvesting cadmium-sulfide nanorods

New Fundamental Interactions Team Lead



Dr. Tom Settersten

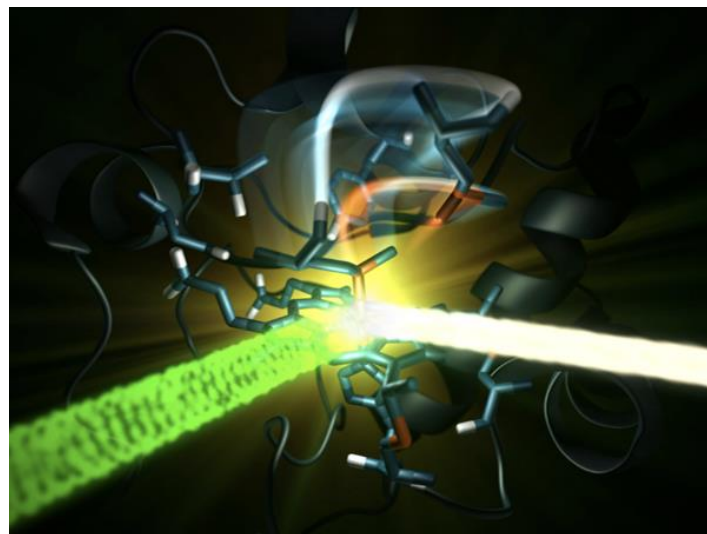
Team Lead, Fundamental Interactions
Chemical Sciences, Geosciences and Biosciences Division

Expertise

- Chemical Physics
- Photon-molecule interactions
- Nonlinear laser spectroscopy

Experience

- Program Manager, Atomic, Molecular, and Optical Sciences (AMOS)
- Sandia National Laboratories (SNL), Technical Manager, Combustion Chemistry and Diagnostics
- SNL, PI, Gas-Phase Chemical Physics
- Colorado School of Mines, Ph.D.



Advances in Ultrafast Science enabled by AMOS support: Combined ultrafast x-ray scattering and spectroscopy study identified the electronic state that triggers Fe-S bond dissociation in the protein cytochrome C. *Nature Comm 12, 1086 (2021)*

New Construction Project Program Manager, Scientific User Facilities Division



Hannibal Joma

Project Program Manager
Scientific User Facilities Division

Expertise

- Science and engineering management for large, strategic projects and programs
- DOE Federal Project Director of the Year, 2012

Experience

- Detail (50%) to BES, Scientific User Facilities construction program manager
- Federal project director, Bay Area SC site office, for BES (ALS-U), FES, and HEP projects
- Program manager, DOE-NNSA, Nuclear Stockpile Stewardship (Livermore)
- Bachelor's degree from Temple University in Geology with a Physics minor; post bachelor's work in Physics at CalState Northridge; certificate in risk management at George Washington University

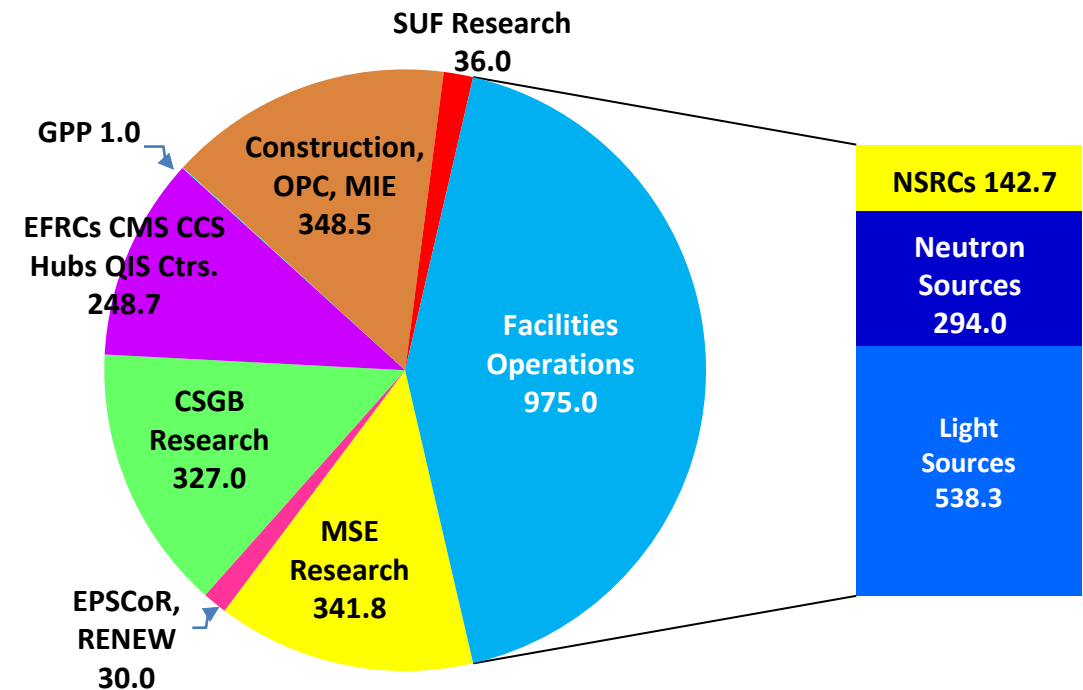
FY 2022 Enacted: \$2,308M (+\$63M or +2.8% above FY 2021)

Research programs $\Delta = +\$117.2M$

- ▶ Research (\$696.8M, +\$99.5M) includes new and expanded investments in research for clean energy, manufacturing, microelectronics, critical materials and minerals, BRaVE, and RENEW (\$3M, Reaching a New Energy Sciences Workforce)
 - ▶ EPSCoR continues (\$25M)
- ▶ Computational Materials and Chemical Sciences, Energy Innovation Hubs, and National QIS Research Centers continue (\$118.7M, +\$2.7M)
- ▶ Energy Frontier Research Centers continue (\$130M, +\$15M**)

Scientific user facilities $\Delta = +\$15.8M$

- ▶ Operations of 12 facilities continue at ~97% of historic optimal (\$975.0M)
- ▶ Facilities research (\$36M) continues AI/ML; increases accelerator R&D; plus RENEW +\$2M



Construction/MIE* $\Delta = -\$70M$

- ▶ APS-U (\$106M); LCLS-II (\$32.4M); LCLS-II-HE (\$53M); ALS-U (\$75.1M); PPU (\$17M); STS (\$32M); CRMF (\$3M)
- ▶ MIEs: NSRC Recap (\$15M); NEXT-II (\$15M)

*includes OPC, **includes SBIR

FY 2022 FOAs: Preapplication Response Indicates oversubscription by 5 to 10X

- ▶ **Early Career:** 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.
 - ❖ Typical funding: University: \$150K/yr for 5 years (forward funded); DOE Lab: \$500K/yr for 5 years
 - ❖ Approximately 30 awards anticipated; proposals received January 20, in review
- ▶ **CCS:** Basic research by teams to develop validated, open-source codes that can effectively use exascale computing capabilities to model and simulate complex chemical systems.
 - ❖ Up to \$6.5M/year for 3-year awards; ~6-10 awards anticipated; proposals received March 25

FY 2022 FOAs: (continued)

- ▶ **CEM**: Basic research by small teams and single PIs to advance priorities for clean energy and low-carbon manufacturing.
 - ❖ Includes hydrogen, solar energy, carbon dioxide removal, energy storage, nuclear energy, and science for decarbonization and sustainable manufacturing; critical materials is a crosscutting, enabling topic
 - ❖ Up to \$50M/year for 3-year awards; ~50 awards anticipated; proposals due May 17

FY 2022 FOAs: Continued

- ▶ **EPSCoR**: Early-stage, fundamental scientific and engineering research to advance the geographic diversity of researchers conducting energy-related research through collaborative partnerships with DOE National Labs. Coordinated with SC, EERE, NE, FECM, and OE
 - ❖ \$24M for 3-year awards (fully funded); ~35 awards anticipated
 - ❖ Proposals due April 14
- ▶ **EFRCs**: Multi-disciplinary teams performing discovery science and use-inspired basic research that addresses priority research directions and opportunities identified by BES workshop and roundtable reports.
 - ❖ Emphasis on science for clean energy and advanced manufacturing, as well as other priority areas including quantum information science and quantum materials
 - ❖ Up to \$100M/year for 4-year awards; 30-35 awards anticipated; proposals due May 3

RENEW FOA: Reaching a New Energy Sciences Workforce

- ▶ Planned BES FOA to expand the community and provide training for materials and chemical sciences in science topics relevant to clean energy and advanced manufacturing
 - ❖ Eligible Institutions: Non-R1 MSIs as the primary recipients
 - ❖ Partnerships with, and internships at, DOE laboratories including BES user facilities (~20% of awarded funds to DOE Labs)
 - ❖ Program includes emphasis on outcomes/impacts and tracking of participants
 - ❖ \$5M for 3-year awards (renewable); up to 10 awards anticipated
 - ❖ Letters of Intent will be required; 1 application per lead institution

DOE Energy Earthshots Initiative – Bipartisan Infrastructure Law Investment in Technology Offices

Hydrogen Shot – announced June 7, 2021

Goal: \$1 per 1 kg in 1 decade (1-1-1)

- ▶ Cross-DOE activity led by EERE-HFTO, co-led by SC-BES and FECM, with NE and ARPA-E



1 Dollar



1 Kilogram



1 Decade

Long Duration Storage Shot – announced July 14, 2021

Goal: Reduce storage costs by 90% from Li-ion baseline to storage systems that deliver 10+ hours of duration, in 1 decade

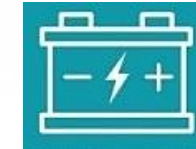
- ▶ Cross-DOE activity led by Offices of Electricity (OE) and EERE, with participation by multiple offices including SC, FECM, ARPA-E, NE

Long Duration Storage Shot



Reduce storage costs by 90%*...

*from a 2020 Li-Ion baseline



...in storage systems That deliver 10+ hours of duration



...in 1 decade

Carbon Negative Shot – announced November 5, 2021

Goal: Durable and scalable carbon dioxide removal under \$100/net metric ton within a decade

- ▶ Cross-DOE activity led by FECM, co-led by SC-BES, EERE-BETO, and ARPA-E



<100 Dollars



1 Ton

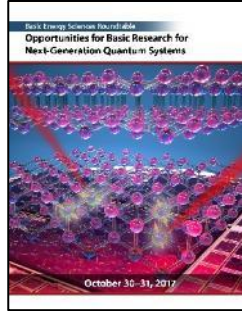
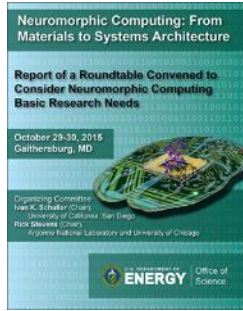
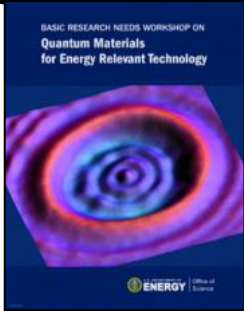


1 Decade

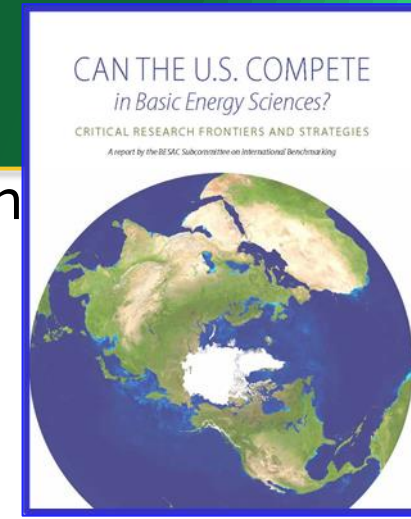
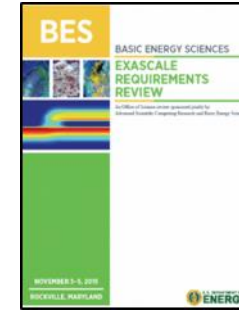
<https://www.energy.gov/policy/energy-earthshots-initiative>

Defining Research Priorities: Basic Research Needs Strategic Planning Workshops and Roundtables

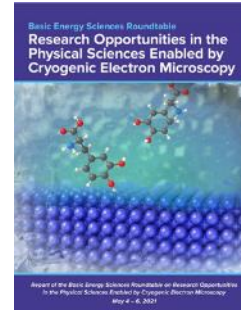
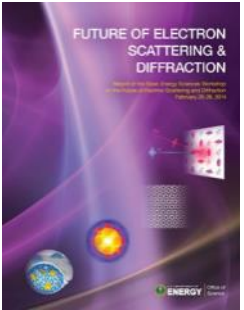
Quantum Science



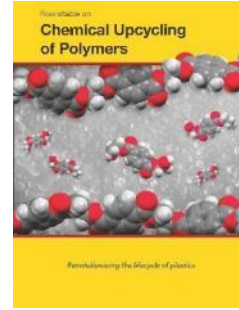
Theory, Modeling & Computation



Characterization

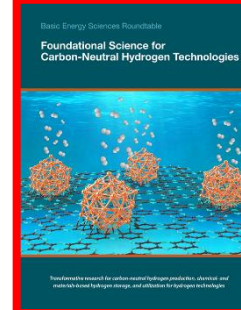
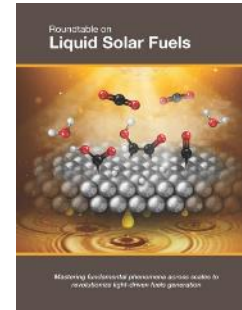
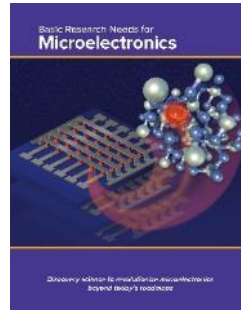
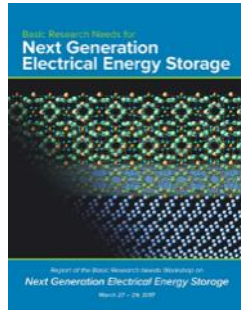
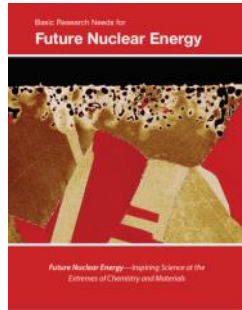
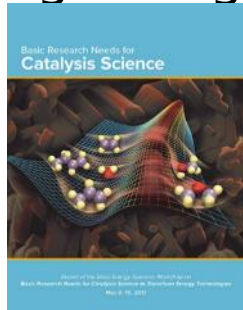
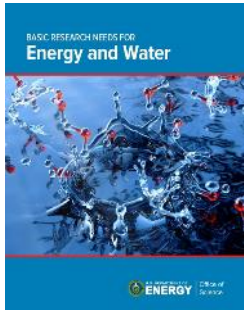


Synthesis



BES Advisory Committee: International Benchmarking Report

Cross-Cutting Energy



Priority Research Opportunities to Advance Foundational Science for Carbon Dioxide Removal Technologies

- ❖ Master Interfacial Processes of CO₂ Transport and Reactivity Across Multiple Length and Time Scales
- ❖ Design and Synthesize Materials that Simultaneously Achieve Multiple Functions for CO₂ Capture and Conversion
- ❖ Discover Unconventional Pathways and Materials for Energy-Efficient CO₂ Capture, Release, and Conversion
- ❖ Control Multiphase Interactions Required for CO₂ Conversion into Molecules, Minerals, and Materials
- ❖ Achieve Predictive Understanding of Complex Subsurface Processes to Enable Secure Carbon Storage



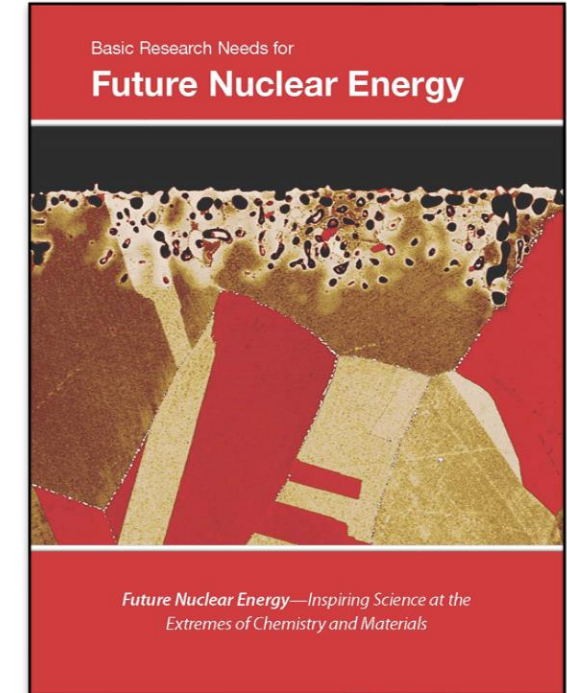
Roundtable held virtually
March 2-4

Chairs:

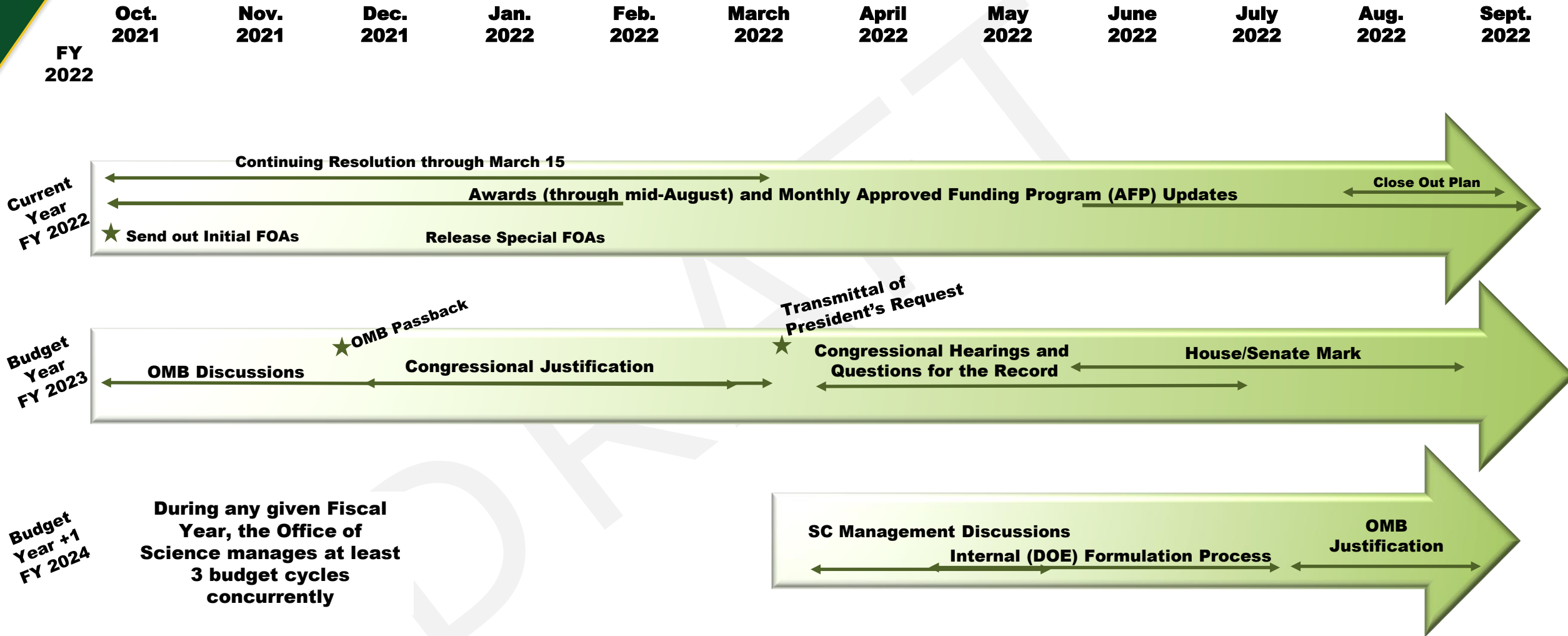
- Krista Walton (Georgia Tech)
- James De Yoreo (PNNL)

In planning – Roundtable to Identify Priority Research Opportunities for Fundamental Science to Accelerate Nuclear Energy Innovation

- ❖ Complement the research priorities in the 2017 BES Workshop report on Basic Research Needs for Future Nuclear Energy
- ❖ Will consider the impact of new technological innovations such as the growing use of artificial intelligence and machine learning tools
- ❖ Will address challenges that have emerged for nuclear energy including materials, coolant, and fuel challenges for advanced reactor concepts
- ❖ Co-organized by BES, Advanced Scientific Computing Research, Fusion Energy Sciences, and Nuclear Energy
- ❖ Virtual format – likely in July 2022
- ❖ Co-chairs: Rebecca Abergel (LBNL/UCB); Blas Uberuaga (LANL); Marianne Walck (INL)



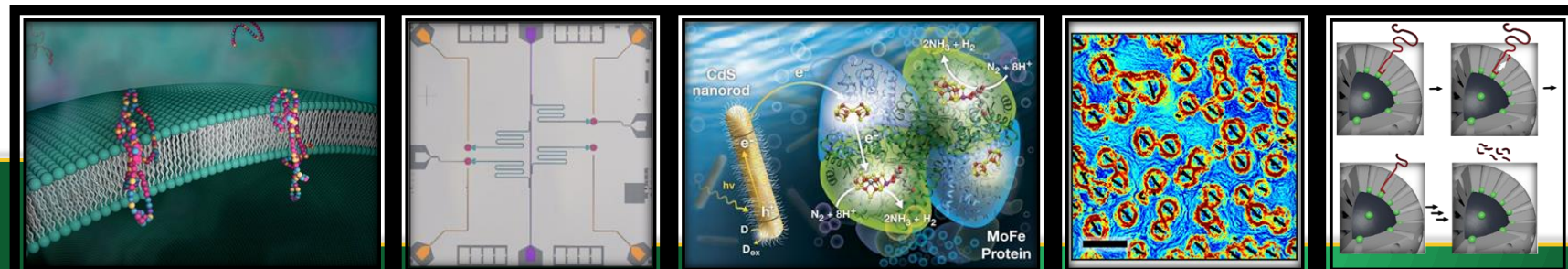
FY 2022 – FY 2024 Budget Timeline



Basic Energy Sciences

Understanding, predicting, and controlling matter and energy at the electronic, atomic, and molecular levels

- ▶ **The BES FY 2023 President's Request is ~\$2,420M, \$112M (4.9%) above FY 2022 Enacted, balancing funding among the major program components—research, user facilities operations, and construction and upgrade of facilities.**
- ▶ Research priorities include:
 - ❖ **SC Earthshot Initiative (+\$104M):** focuses BES research on the stretch goals of the DOE Energy Earthshots, including a new research modality (Energy Earthshot Research Centers) that will provide a solid bridge between SC and Energy Technology Offices
 - ❖ **National Competitiveness and Responsiveness:** fundamental science to **Accelerate** (+\$15M) transition of science innovations to emerging technologies, and expansion of user facilities capabilities to respond to biological threats (**BRaVE**,+\$12M). Continues support for **QIS** and **microelectronics**. **AI/ML** (+\$9M) to accelerate discovery science, for effective user facility operations, and interpretation of massive data sets
 - ❖ **Research Opportunities for Underrepresented Communities,** focus on Climate and Clean Energy research: **EPSCoR** (+\$10M), **RENEW** (+\$5M for MSI internships), **FAIR** (Funding to Accelerate Inclusive Research; +\$20M to build MSI research capacity/capabilities)
 - ❖ The **Batteries and Energy Storage** and **Fuels from Sunlight Energy Innovation Hub programs** continue with flat funding, including an open recompetition of the Batteries and Energy Storage Hub program. **Energy Frontier Research Centers** and **National QIS Research Centers** continue with flat funding.
- ▶ **BES user facilities** would operate at ~90% of optimal. For international competitiveness, BES continues support for **major facility upgrades** (+\$12M) per BESAC report recommendations, MIEs for NSLS II beamlines, and recapitalization of the NSRCs.



FY 2023 SC Energy Earthshot Initiative (+\$104M)

- ▶ Addresses key research challenges at the interface between basic research and applied research and development activities to bridge the R&D gap and realize the stretch goals of the DOE Energy Earthshots
- ▶ BES, with other SC Offices, will initiate a new research modality of Energy Earthshot Research Centers (EERCs)
 - ❖ Modeled on the Energy Frontier Research Centers, BES will support large teams that are multi-investigator, multi-disciplinary, and multi-institution (academic, national laboratory, industrial) to advance foundational knowledge and enabling capabilities in experimental and computational chemical and materials sciences to address Earthshot goals
 - ❖ BES will coordinate closely with the Energy Technology Offices and existing research consortia/demonstration projects, to establish teams that span the R&D continuum and accelerate both science and technologies – providing a strong bridge between BES and technology research
- ▶ BES will complement EERCs with small group awards
 - ❖ Focus on use-inspired fundamental research to address knowledge gaps that limit achievement of the Energy Earthshot goals

Hydrogen Shot



1 Dollar



1 Kilogram



1 Decade

Long Duration Storage Shot



Reduce storage costs by 90%*...

*from a 2020 Li-Ion baseline



...in storage systems That deliver 10+ hours of duration



...in 1 decade

Carbon Negative Shot



<100 Dollars



1 Ton

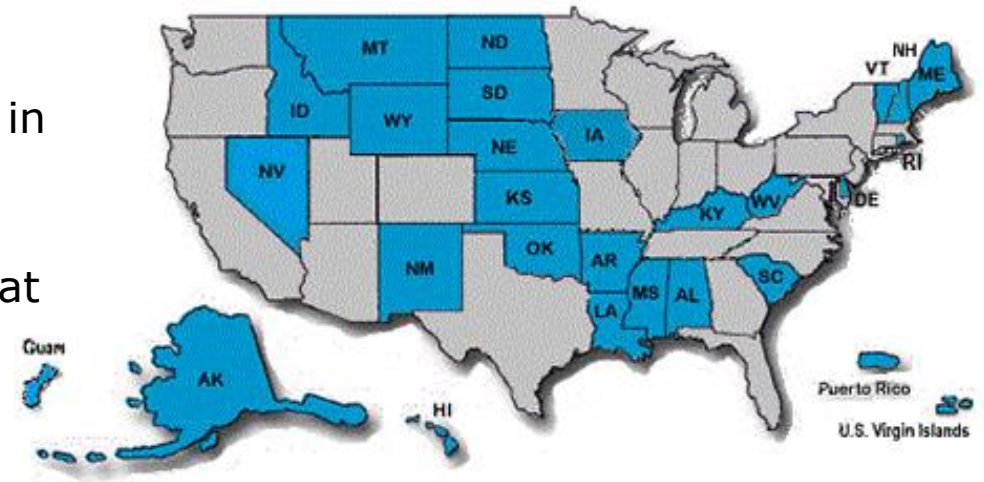


1 Decade

Research Opportunities for Underrepresented Communities

BES will build stronger programs with underrepresented institutions and regions, including strengthening awareness to address environmental justice issues

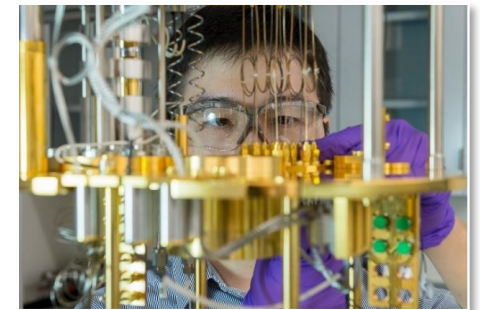
- ▶ **FAIR (+\$20M) - Funding to Accelerate Inclusive Research.** Enhancing research on clean energy, and related topics at minority serving institutions (MSIs). The activities will improve the infrastructure, capacity, capability, and expertise of MSIs to perform and propose competitive research and will build beneficial relationships between MSIs and DOE National laboratories and facilities, complementing the RENEW workforce initiative.
- ▶ **RENEW (+\$5M)** – Doubling the FY 2022 investment, BES increases support for the SC-wide RENEW initiative that leverages SC's world-unique National laboratories and user facilities to provide internships for students at academic institutions currently under-represented in the BES research portfolio, focused on clean energy topics.
- ▶ **EPSCoR (+\$10M)** - The increased funding in the DOE EPSCoR program will support clean energy and climate-related research in U.S. states and territories that do not have large federally-supported academic research programs. The FY 2023 funding opportunity will focus on larger-team implementation awards that facilitate development of research infrastructure in the EPSCoR jurisdictions.



FY 2023 Funding to Accelerate Inclusive Research (FAIR)

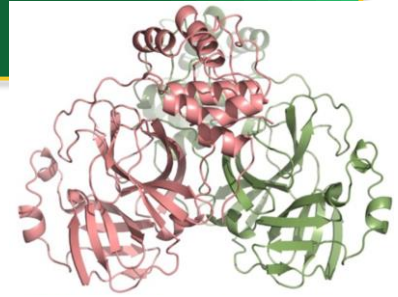
FAIR will enhance research on clean energy, climate, and related topics at minority serving institutions (MSIs), including underserved and environmental justice regions

- ▶ Builds research capacity, infrastructure, and expertise at MSIs
- ▶ Develops mutually beneficial relationships between MSIs and DOE national laboratories and user facilities
- ▶ Complements the RENEW initiative (internships at national laboratories for workforce development)
- ▶ Provides support of single PI or research teams, and includes an equipment or infrastructure element
- ▶ Majority of funds will go directly to HBCUs/MSIs, a portion will fund the partnering institution (Lab, university)

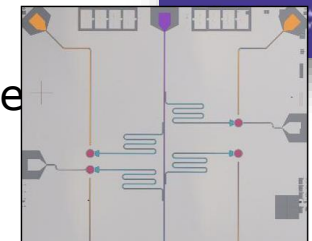
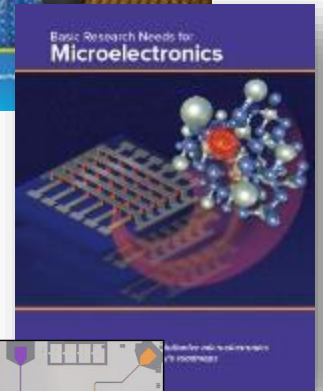


FY 2023 National Competitiveness

- ▶ **Accelerate Innovations in Emerging Technologies (Accelerate, +\$15M):** BES will support research to accelerate the transition of science advances to clean energy technologies, including future-generation microelectronics, low-carbon manufacturing, and emerging technologies to move from laboratory to industrial prototypes.
- ▶ **Biopreparedness Research Virtual Environment (BRaVE, +\$9M):** BES will support critical analytical capabilities foundational to responses for future emergencies, focusing on advanced end stations at DOE light and neutron user facilities plus cryoelectron microscopy and related imaging techniques.
- ▶ **Manufacturing and Microelectronics:** BES will continue to support multi-disciplinary basic research to advance new materials, chemistry, synthesis, and fabrication research that accelerates the advancement of low-carbon manufacturing and microelectronic technologies in a co-design innovation ecosystem.
- ▶ **Quantum Information Science (QIS):** BES will continue research to understand and control quantum coherence and entanglement in atomic, molecular, and materials systems; develop systems with properties needed for quantum computing and sensing; advance approaches and algorithms to harness quantum computers for BES research; and establish the QIS infrastructure needed to support the nation's research efforts.
- ▶ **Artificial Intelligence and Machine Learning (+\$9M):** BES will support data science to accelerate BES discovery science, and to aid in effective user facility operations and interpretation of massive data sets



LCLS - SARS-CoV-2 structure



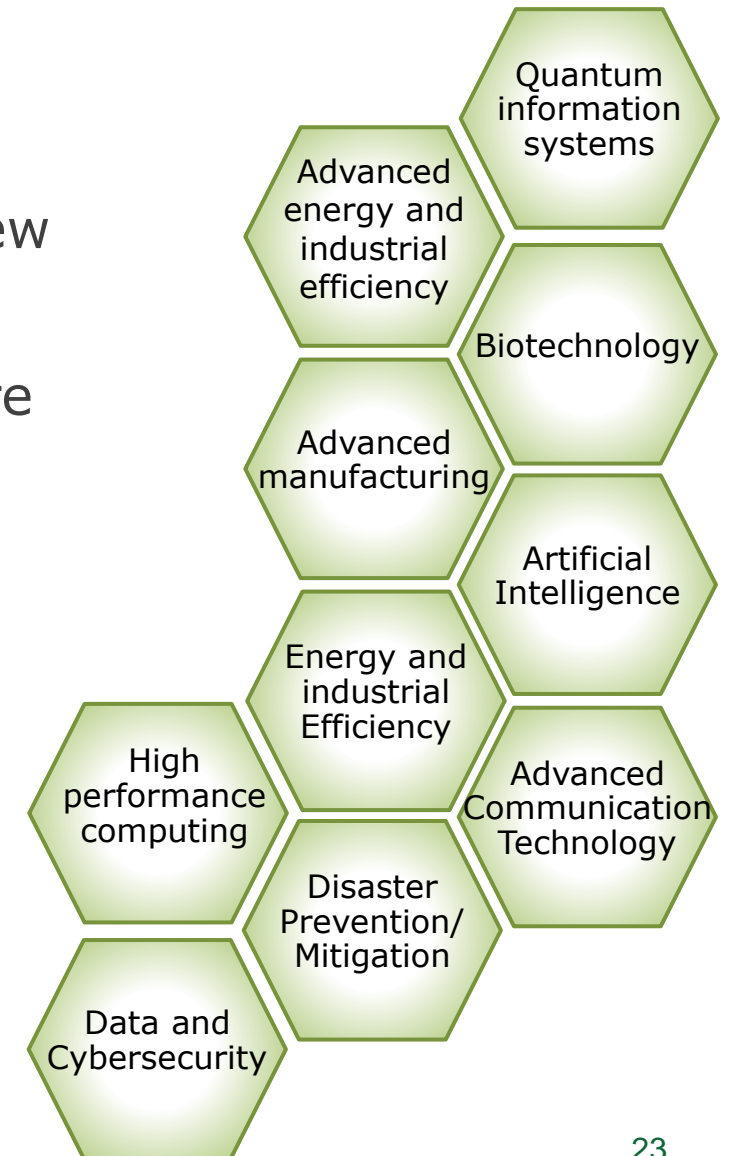
Superconducting multiqubit chip

FY 2023 Accelerate Innovations in Emerging Technologies

Initiative goals:

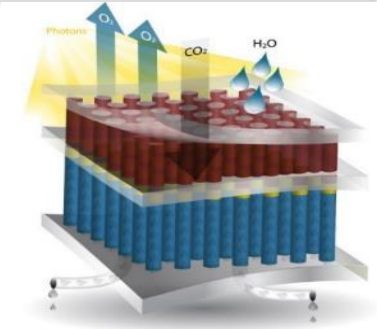
- ▶ To drive scientific discovery for sustainable production of new technologies across the innovation continuum
- ▶ To train a STEM workforce to support industries of the future
- ▶ To meet the nation's needs for abundant clean energy, a sustainable environment, and national security

Highly integrated research teams to accelerate the discovery, creation, production, and commercialization of new technologies to form the basis of future industries with public and economic impact

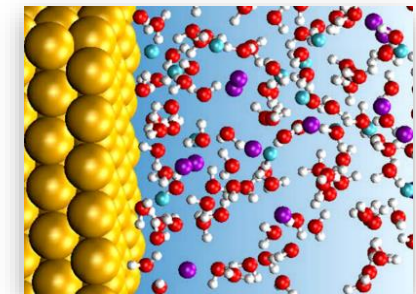


FY 2023 Team Science - Energy Frontier Research Centers, Energy Innovation Hubs, National QIS Research Centers, Computational Sciences

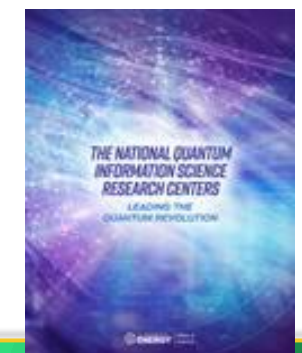
- ▶ In FY 2023 BES will continue to support major team science research centers that leverage advances in the core research programs and are critical to clean energy and QIS innovation
 - ❖ **Energy Frontier Research Centers** – Continued support for 4-year awards made in 2020 and 2022
 - ❖ **Fuels from Sunlight Energy Innovation Hub Program** – Continued support for two Hub projects initiated in 2020
 - ❖ **Batteries and Energy Storage Energy Innovation Hub Program** – After 10 years, open re-competition of the Hub program
 - ❖ **National QIS Research Centers** – Continued support for SC QIS Centers started in 2020
 - ❖ **Computational Sciences** – Re-competition of FY 2019 Computational Materials Sciences awards; Continued support for Computational Chemical Sciences



*Photoelectrochemical
Solar-Fuel Generator*

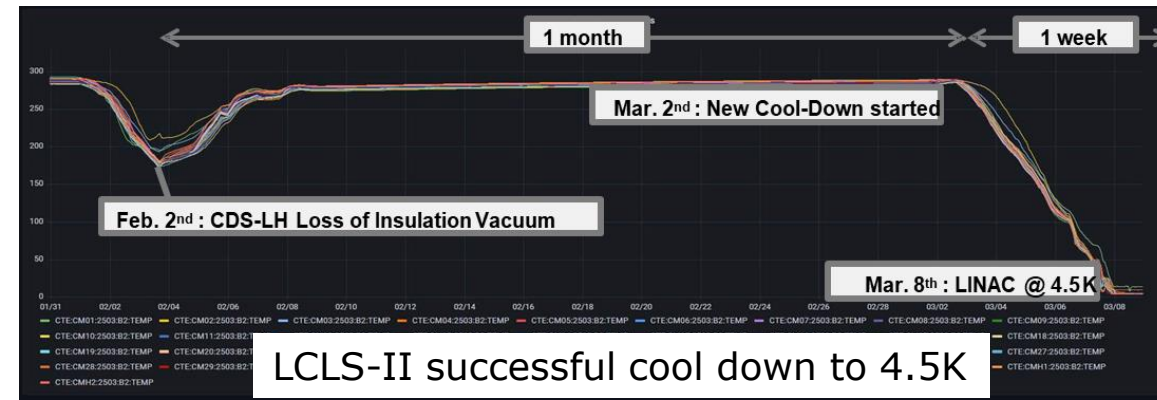


*Electrified Interfacial
Structure*

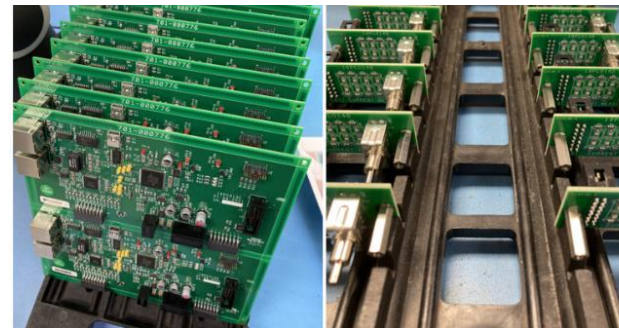


FY 2023/FY 2022 Highlights – Construction Projects

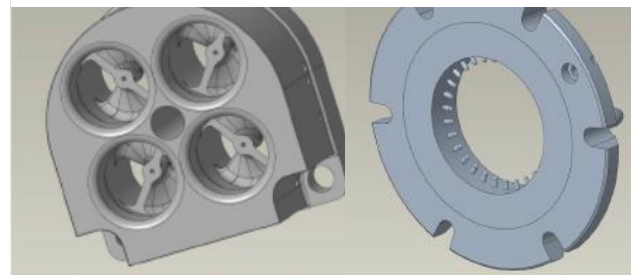
- ❖ **LCLS-II: Re-baseline** (10/13/2020) New TPC \$1,136M. Installation of remaining accelerator and x-ray systems and equipment commissioning activities. Both soft and hard x-ray undulators operational. CD-4 projected for 2Q FY 2024. (no funding required in FY 2023)
- ❖ **APS-U: CD-3** (7/25/2019) Continued procurement, testing of storage ring and experimental equipment, and long beamline building construction; dark time for installation projected to begin ~3Q FY 2023. CD-4 projected for 2Q FY 2026.
- ❖ **PPU: CD-2/3** (10/6/2020) Doubling the SNS accelerator beam power to 2.8 MW. Continued 2 MW target development; superconducting linac, magnet, and klystron procurements and installation; installation of cryomodules. CD-4 projected for 4Q FY 2028.
- ❖ **ALS-U: CD-2** (4/2/2021) Long-lead procurements, including accumulator ring installation during short downtimes. CD-3 projected for 1Q FY 2023; CD-4 for 4Q FY 2029.



APS-U bipolar power supply system printed circuit boards



PPU target successfully tested



"Swirl" type bubbler "IOB" type bubbler

ALS-U accumulator ring supports



FY 2023/FY 2022 Highlights – Construction and MIE Projects

- ❖ **LCLS-II-HE: CD-1** (9/21/2018), **3A** (5/12/2020) Scope includes a low-emittance superconducting electron gun & independent cryoplant (current TPC estimate is \$660M); R&D, design, prototyping, and long lead time procurements underway. COVID impacts and need for increased cost contingency delay CD-2/3 & could impact TPC. **CD-2/3 now planned for 4Q FY 2023**; CD-4 for 2Q FY 2031.
- ❖ **STS: CD-1** (11/23/2020) Continued design, R&D, and engineering activities. Project replanning underway due to long project duration; TPC range is \$1,800M to \$3,000M with a preliminary point estimate of \$2,242M. CD-2/3 projected for 2Q FY 2025; CD-4 for 2Q FY 2037.
- ❖ **CRMF: CD-0** (12/6/19) Continued conceptual design and analysis of alternatives. TPC range is \$70M to \$98M with a preliminary point estimate of \$94M. **CD-1/3A projected for 2Q FY 2023**.

Major Items of Equipment:

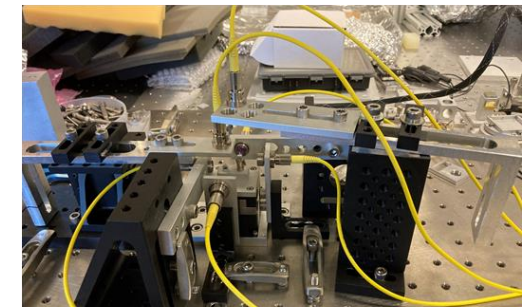
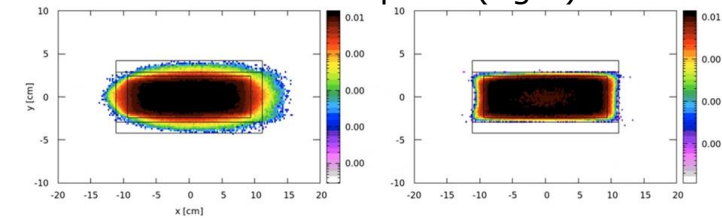
- ❖ **NEXT-II: CD-2/3 (10/13/2021)** Builds out 3 priority beamlines at NSLS-II. Procurement of beamline hutches and CDI photon delivery system; TPC is \$94.5M. CD-4 projected for 3Q FY 2028.
- ❖ **NSRC Recap: CD-2/3 (3/31/2022)** Provides 17 instruments to upgrade capabilities at the NSRCs. TPC is \$80M. CD-4 projected for 2Q FY 2028.

FY 2023: Other Project Cost Support to start planning for the **HFIR Pressure Vessel Replacement** (replace the pressure vessel for the High Flux Isotope Reactor) and **NEXT-III** (build out additional beamlines for NSLS-II).



LCLS-II-HE: Verification cryomodule (rec 02-2022)

STS: Calculation of beam profile using only quadrupoles for focus (left) and with addition of octupoles (right).



NEXT III: ARI-SXN beamline prototype sample holder test

Congratulations and Thank you to Bruce Garrett – Retirement!



Dr. Bruce Garrett

Division Director

Chemical Sciences, Geosciences and Biosciences Division

Expertise

- Computational and theoretical chemistry
- Fellow of the American Physical Society, the American Association for the Advancement of Science, and the Royal Society of Chemistry
- Strategic planning

Experience

- Joined BES in 2016
- Previous career -- 27 years at Pacific Northwest National Lab, Chief Scientist for Chemical Sciences
- While at BES, Bruce led or co-led –
 - ❖ >20 FOAs
 - ❖ Strategic planning for Energy and Water, Polymer Upcycling, Catalysis Science, Liquid Solar Fuels, Carbon Neutral Hydrogen, Quantum Computing for Chemical and Materials Sciences
 - ❖ Science and Energy Technology Teams and cross-DOE working groups
 - ❖ Hiring of 6 CSGB staff members

Questions?



U.S. DEPARTMENT OF
ENERGY

Office of
Science