

Basic Energy Sciences Update

Basic Energy Sciences Advisory Committee Meeting
April 9, 2024

- ▶ Andy Schwartz and Gail McLean
- ▶ Office of Basic Energy Sciences



U.S. DEPARTMENT OF
ENERGY

Office of
Science

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

New Staff
Posted Positions
Vacancies

Office of Basic Energy Sciences

Associate Director (A)
Andy Schwartz

BES Budget and Planning

Kara Beles, Financial Management
 Donetta Herbert, Financial Management
 Adam Kinney, Senior Technical Advisor
 (Vacant, Senior Technical Advisor)

BES Operations

Teresa Crockett, Program Analyst
 Robin Hayes, Program Manager and Acting EFRC Co-Lead
 Kerry Hochberger, Program Analyst / BESAC*
 Angie Thevenot, Program Analyst
 (Vacant, Senior Technical Advisor)

* Basic Energy Sciences Advisory Committee

Chemical Sciences, Geosciences, and Biosciences Division

Gail McLean, Director

Gregory Fiechtner, EFRC Team Co-Lead (A)
 (Vacant)

Collaborative Research Division

Gail McLean, Director (A)

Materials Sciences and Engineering Division

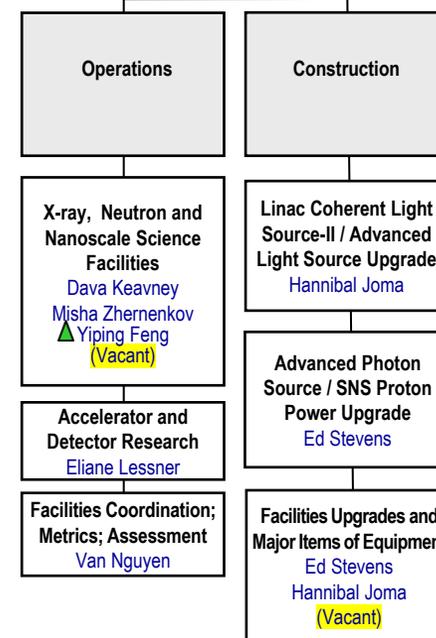
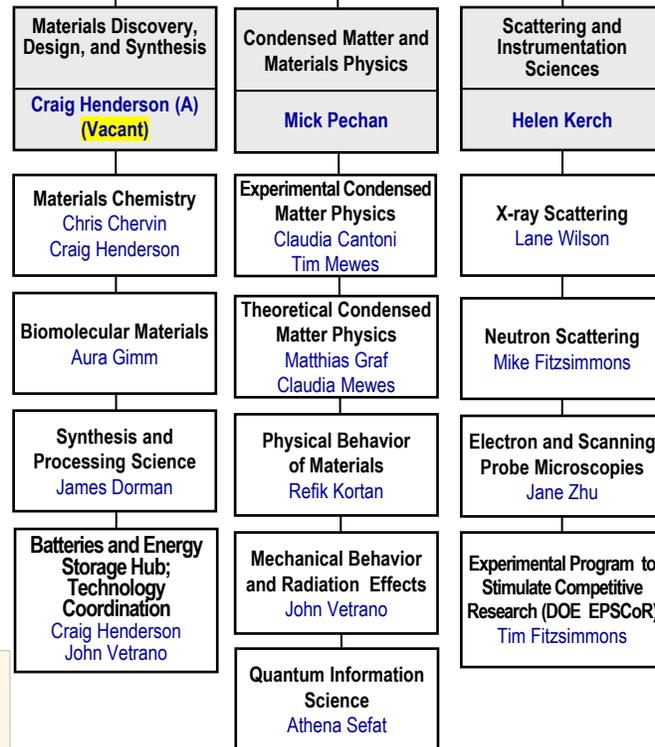
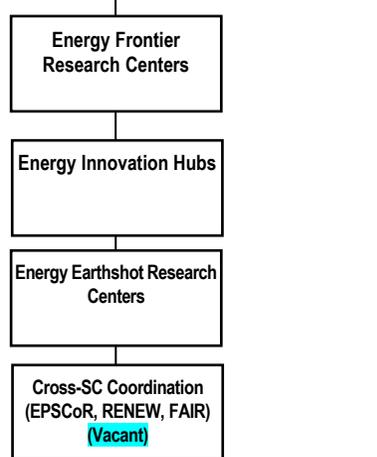
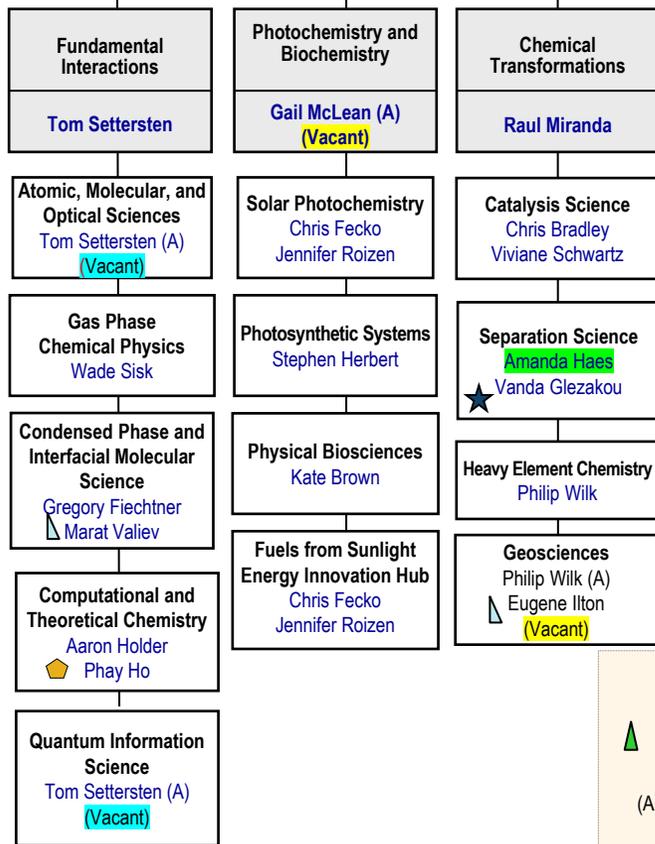
Andy Schwartz, Director

John Vetrano, EFRC Team Co-Lead (A)
 Shawn Chen

Scientific User Facilities Division

Andy Schwartz, Director (A)

Rocio Meneses, Program Support Specialist



LEGEND

- ▲ IPA from SLAC
- (A) Acting
- ★ Detailee (50%) from ORNL
- ◆ Detailee (50%) from ANL
- ▽ Detailee (50%) from PNNL

Revised 4-07-2024

New Separation Science Program Manager Chemical Sciences, Geosciences and Biosciences



Dr. Amanda Haes

Expertise

- ◆ Experimental physical chemistry and quantitative analytical chemistry
- ◆ Small molecule separations
- ◆ Environmental and sustainable chemistry

Experience

- ◆ Joined BES in January 2024 as the program manager for Separation Science
- ◆ Professor in Chemistry at the University of Iowa (2006-2024) conducting studies of plasmonic nanostructures and metal oxide reactivity and transformations using vibrational and surface-enhanced spectroscopies
- ◆ Rotating program director at the National Science Foundation (2020-2023)
- ◆ Ph.D. and M.S. in Chemistry from Northwestern; B.A. in Chemistry and Physics from Wartburg College

In Memoriam: Mike (Michael) Markowitz

Prior to DOE (1992-2008):

Research Chemist

Center for Bio/Molecular Science and Engineering, Naval Research Laboratory (NRL), Washington, DC

Research on:

- Bio-inspired materials functionality
- Self-assembly mechanisms
- Sol-gel chemistry
- Interfacial recognition functions
- >50 peer-reviewed papers, review articles, book-chapters, and several patents.

Education:

Post-doc, NRL, 1990-1992

Post-doc, Lehigh University, 1987-1990

Ph.D., Chemistry, Univ. of Chicago, 1987

B.A., Chemistry, Univ. of Pennsylvania, 1981



Team Lead (2019-2023)

Materials Discovery, Design, and Synthesis

Program Manager (2008-2022)

Biomolecular Materials (BMM)

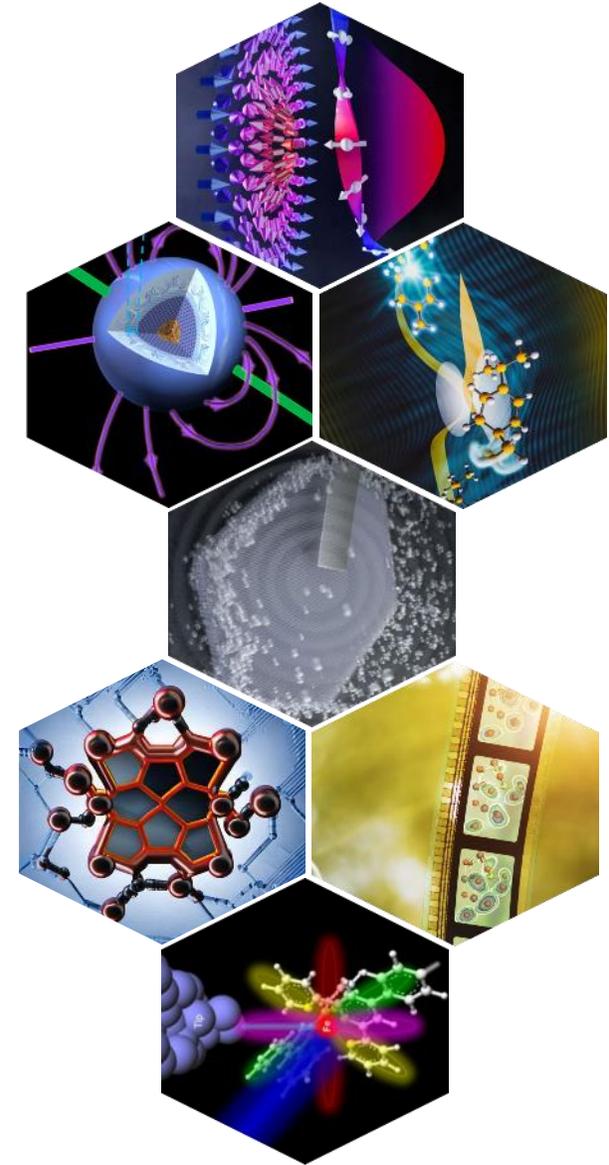
Remembrances and reflections:

- Calm and thoughtful leader
- Avid supporter of basic sciences and the local arts
- Enjoyed colleagues, family, friends, and the outdoors, often through the lens of a camera.



BES By the Numbers – FY 2023

- ◆ FY 2023 BES Budget: \$2.5B
 - \$1.10B Research
 - \$1.07B Facility Operations
 - \$362.7M Projects (Construction/OPC/MIEs)
- ◆ FY 2023 BES funding spanned:
 - 16 National laboratories
 - 224 Academic, Nonprofit, and Industrial Institutions
 - 46 states plus Puerto Rico, District of Columbia, and Guam
- ◆ Over 13,000 users
 - 73% Onsite/27% Remote
- ◆ 30% Average New grant success rate
- ◆ 51 Energy Frontier Research Centers
- ◆ 2 Energy Innovation Hubs
- ◆ 25 core research areas



FY 2024 Enacted: \$2,625M (+\$91.6M or 3.6% above FY 2023 Enacted)

Research programs $\Delta = -\$25M$

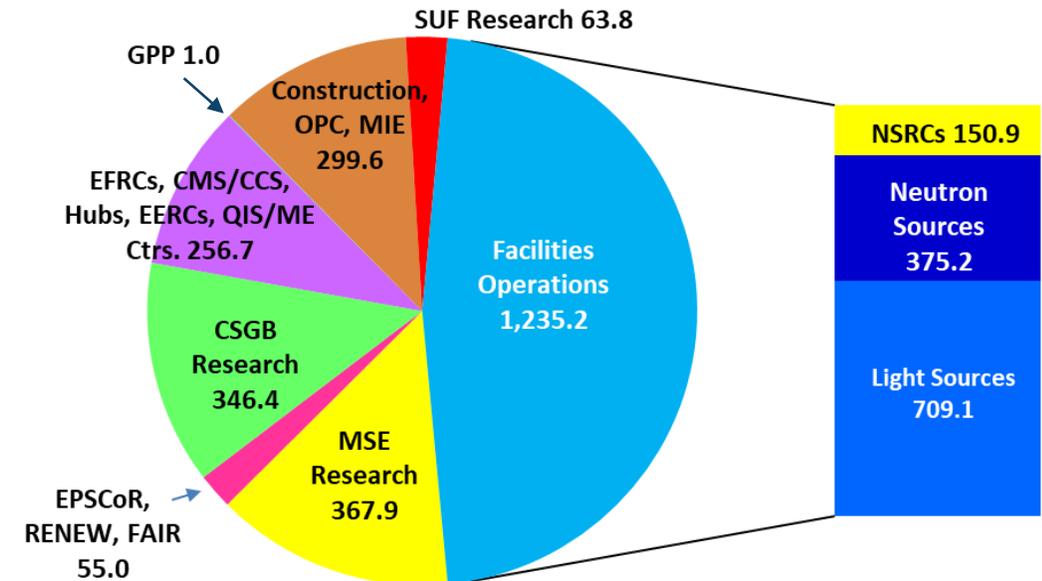
- ◆ Continued investments in research for clean energy, manufacturing, critical materials, FAIR, and RENEW
- ◆ Computational Materials & Chemical Sciences, Energy Innovation Hubs, and National QIS Research Centers continue (\$119.7M)
- ◆ Increase to advance next generation electronics, with planned investment in a network of multiple team awards to comprise Microelectronics Science Research Centers (+\$10M)
- ◆ Energy Frontier Research Centers continue (\$130M)
- ◆ Continued investments in SC Energy Earthshots initiative (-\$40M)

Scientific user facilities $\Delta = +\$179.7M$

- ◆ Operations of 12 facilities supported at ~93% of funding required for re-baselined, normal operations (\$1,235.2M)
- ◆ Facilities research (\$63.8M): Accelerator & Detectors; AI/ML; BRaVE; preliminary planning for future MIEs

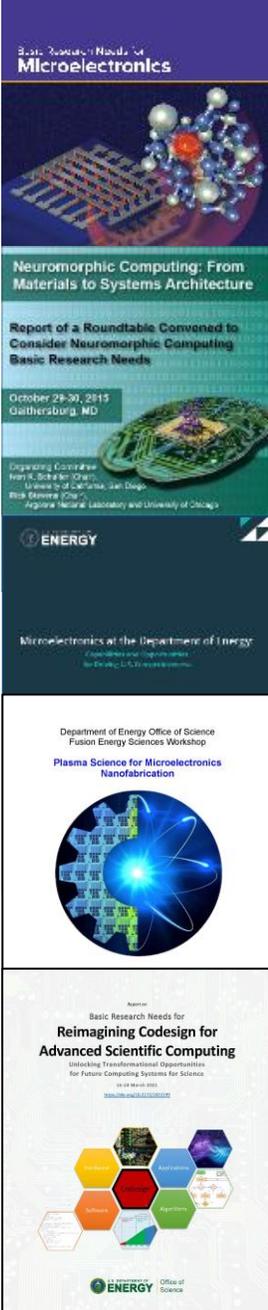
Construction/MIE $\Delta = -\$63.1M$ (includes OPC)

- ◆ LCLS-II-HE (\$120M); ALS-U (\$57.3M); PPU (\$15.8M); STS (\$52M); CRMF (\$10M)
- ◆ **New starts: HFIR Pressure Vessel Replacement (\$13M); NEXT-III (\$6.6M)**
- ◆ MIEs: NSRC Recap (\$5M); NEXT-II (\$20M)



Advanced Microelectronics in DOE SC

- ◆ Continues coordinated SC support for multi-disciplinary research to accelerate innovation and advance microelectronic technologies in a co-design ecosystem.
 - Support for fundamental microelectronics research through co-design awards (ASCR, BES, FES, HEP) and EFRCs (BES).
 - Includes fundamental research on materials, chemistries, processing, isotopes, devices, systems, architectures, algorithms, and software
 - Builds on capabilities at SC user facilities for computation, fabrication, and characterization
- ◆ Research provides foundational knowledge for development of next-generation technologies in computing, communications, sensing, and power
- ◆ Anticipated new SC Microelectronics Science Research Centers would likely be networks of multi-disciplinary team awards focused on common research goals
- ◆ This basic research complements later-stage investments being made by other agencies through the CHIPS Act (e.g., Commerce, Defense)



FY 2024 BES Funding Opportunities – Released

- ◆ **Annual Open Solicitation:** Supports grants for research in the topical areas supported by the Office of Science. **Accepts applications continuously.**
- ◆ **EPSCoR-State/National Laboratory Partnerships.** Supports collaborations between EPSCoR-eligible institutions and DOE national laboratories on fundamental, early-stage energy science research. **Proposals under review.**
- ◆ **Annual Early Career FOA:** Supports outstanding scientists early in their careers in research areas supported by the Office of Science; all BES core research areas and facilities capabilities research. **Proposals encouraged.**
- ◆ **Energy Frontier Research Centers:** Supports multi-disciplinary, multi-institutional centers to enable transformative advances in energy-relevant basic science, emphasizing QIS, microelectronics, transformative manufacturing, and environmental management. **Proposals encouraged.**
- ◆ **Computational Materials Sciences – Exploratory Research at the Exascale:** Computational codes and associated databases for the design of materials with advanced functionalities. **Proposals under review.**
- ◆ **RENEW, FAIR:** Supports efforts to broaden participation within the SC research community through training opportunities leveraging the DOE complex and direct research support at non-R1 MSIs and ERIs (incl. DOE lab and R1 MSI partners). **Pre-applications due April 24 (FAIR) and April 30 (RENEW).**

SC Energy Earthshots (FY 2024 BES Enacted: \$10M)

- ◆ The SC Energy Earthshots Initiative addresses key scientific challenges that underpin stretch goals for the first 6 DOE Energy Earthshots.
 - Closely coordinated with the Energy Technology Offices.
- ◆ SC announced 29 awards in FY 2023: 18 scientific foundations grants (~\$2-5M/award over 3 yrs) and 11 EERCs (recommended ~\$4.8M/yr/EERC).
- ◆ BES supported 8 Energy Earthshot Research Centers (EERCs).
 - Multi-disciplinary, multi-institutional teams led by DOE labs focused on fundamental research addressing key research challenges for Earthshots.
- ◆ BES supported 9 foundational science, small group awards.
 - Led by academic or private sector institutions, focused on use-inspired fundamental research to address knowledge gaps that limit achievement of Earthshot goals.

Enhanced Geothermal Shot



90% Reduction



2035

Floating Offshore Wind Shot



>70% Reduction



2035

Industrial Heat Shot



85% Reduction



2035

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

Hydrogen Shot



1 Dollar



1 Kilogram

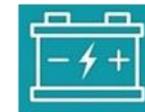


1 Decade

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

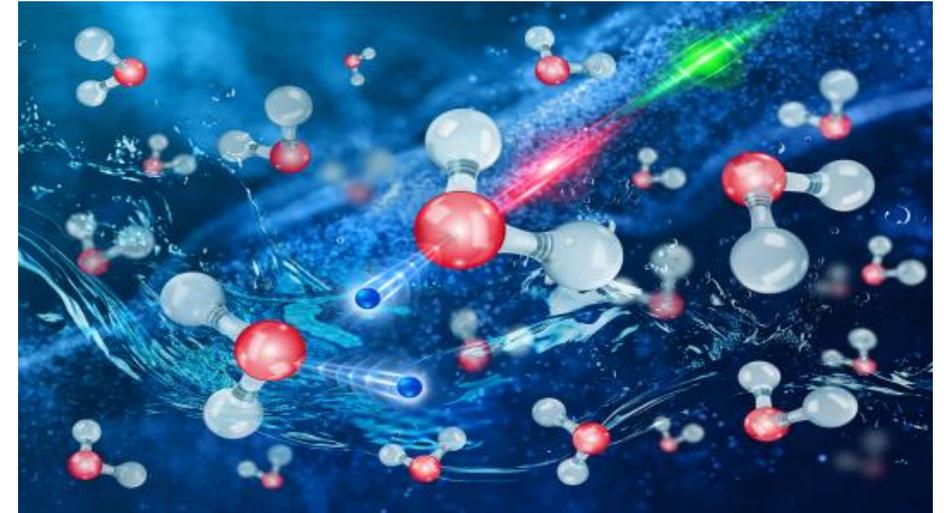
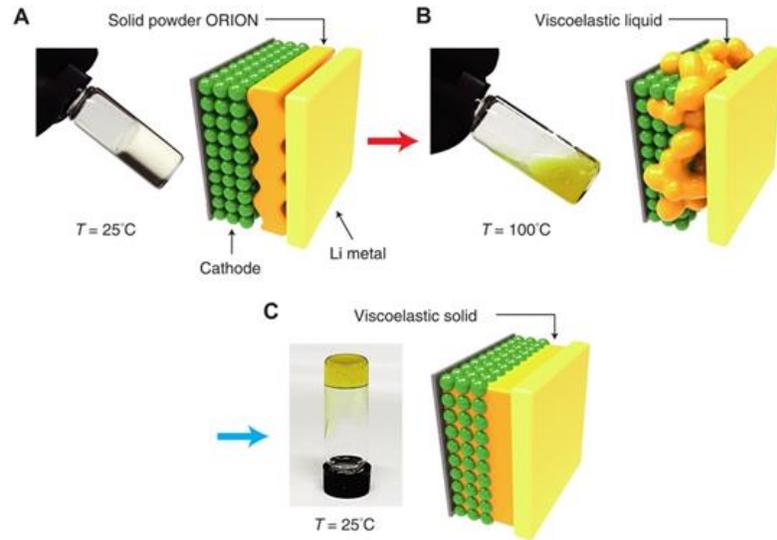


1 Decade

BES SBIR/STTR Update

- ◆ **Annual SBIR/STTR FOA:** Topics support research that is ready for commercialization, including topics related to accelerators, detectors, and nanoscale instrumentation
- ◆ **FY 2024 Awards Issued:** SC facilities were made exempt from SBIR/STTR taxes in FY 2023, reducing available BES funding for awards by ~50% from previous years. FY 2024 awards total \$38.3M
 - Phase I: 26 SBIR/7 STTR
 - Phase II: 25 SBIR/3 STTR (1 co-funded award with Advanced Scientific Computing Research)
- ◆ **FY 2025 FOA:** Will be released July 15, 2024
 - BES-funded topics TBD
 - Coordination with NE, EERE, and FECM will continue
- ◆ **SBIR Success Story:** STEM manufacturer Nion acquired by Bruker Corporation, January 2024
 - 5 Phase I and 3 Phase II awards from BES totaling \$3.5M over 20 years supported development of leading-edge hardware and software for STEM instrumentation.

Selected Recent Scientific Highlights



Closed-loop cathode recycling in solid-state batteries enabled by supramolecular electrolytes

Users and staff at LBNL's Molecular Foundry developed a new class of viscoelastic solid electrolytes that can be used in solid state batteries (SSBs) to enable direct cathode recycling. The new electrolyte showed excellent performance in new and refurbished SSBs.

Ref.: [Science Advances, 9\(32\), 2023](#)

The first “freeze-frame” of liquid water using an X-ray Free Electron Laser

An international team from the US and Germany measured, for the first time, the real-time energetic motion of an electron prior to the motion of the atomic nucleus in liquid water using new methodology that leverages the attosecond X-ray pulses available at LCLS.

Source: PNNL, ANL, SLAC, U. Washington, DESY (Germany)

Ref.: [Science, 383 \(6687\), pp. 1118-1122 \(2024\)](#)

Facilities Project Updates and Major Milestones

- ◆ **Advanced Photon Source Upgrade (ANL):** Installation of the multi-bend achromat storage ring is complete! Testing and checkout is ongoing. Commissioning is planned to begin this week with completion estimated for June and users returning in July 2024.
- ◆ **Proton Power Upgrade (ORNL):** Installation nears completion. Project is on-track to deliver neutrons for the user program in July 2024, with early project finish in January 2025.
- ◆ **Linac Coherent Light Source – II – High Energy (SLAC):** A combined Critical Decision 2/3 (Approve Performance Baseline & Start of Construction) is anticipated in FY 2024.
- ◆ **NSRC Recapitalization (multiple Labs):** 16 of 18 instrument awards have been made, with 3 instruments delivered.



Installation of the kicker absorber in APS Sector 39, the **final** component of the MBA storage ring, completing installation.

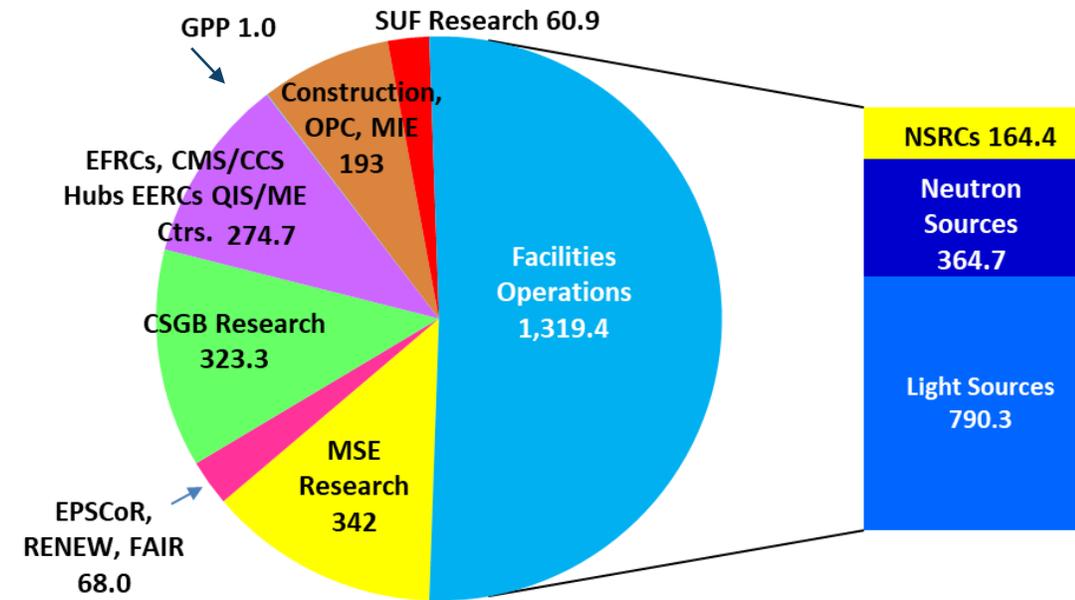
FY 2025 Request: \$2,582.3M (-\$43.3M or 1.65% below FY 2024 Enacted)

Research programs $\Delta = -\$18.1M$

- Continued investments in research for clean energy, critical materials, FAIR and RENEW (+\$13M).
- Support for AI/ML increases (+\$8M), emphasizing research to accelerate discovery, translate large datasets into scientific understanding.
- Continued investments in microelectronics research, including networked team awards that comprise Microelectronics Science Research Centers.
- EFRCs, NQISRCs (recompeted/renewed), CMS/CCS, Fuels from Sunlight (renewal) and Batteries and Energy Storage Energy Innovation Hub awards, and DOE EPSCoR are flat funded.
- Expanded investments in SC Energy Earthshots initiative (+\$45M)

Scientific user facilities $\Delta = +\$81.4M$

- Operations of 12 facilities supported at 90% of funding required for re-baselined, normal operations (\$1,319.4M)
- Facilities research (\$60.9M): Accelerator & Detectors; AI/ML (+9M); BRaVE; preliminary planning for future MIEs



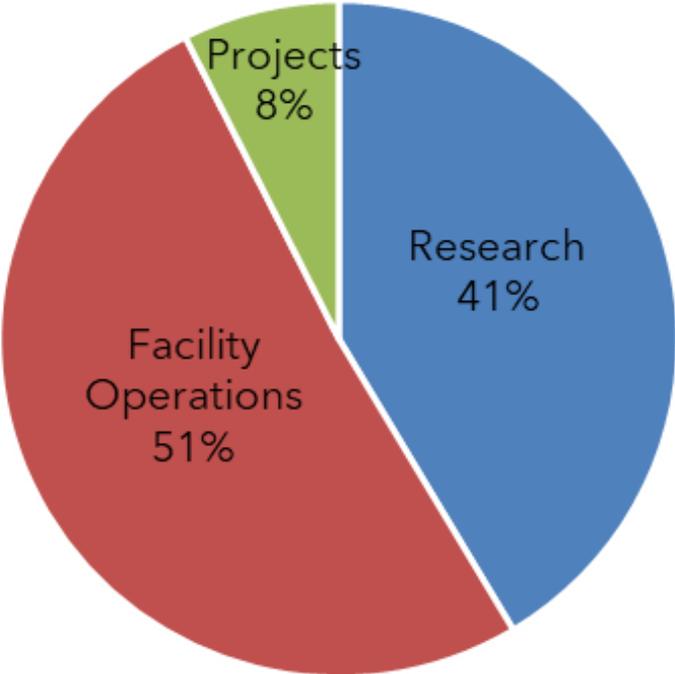
Construction/MIE $\Delta = -\$106.6M$ (includes OPC)

- LCLS-II-HE (\$100M); STS (\$52M); CRMF (\$20M); HFIR Pressure Vessel Replacement (\$11M); NEXT-III (\$10M)
- No Major Items of Equipment requested

BES Funding: Research, Facility Operations, Projects

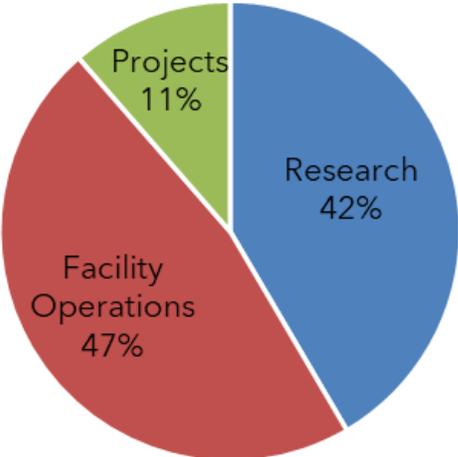
FY 2025 President's Request is \$2,582M, \$43.3M (1.65%) below FY 2024 Enacted -- balances major program components.

FY 2025 President's Request

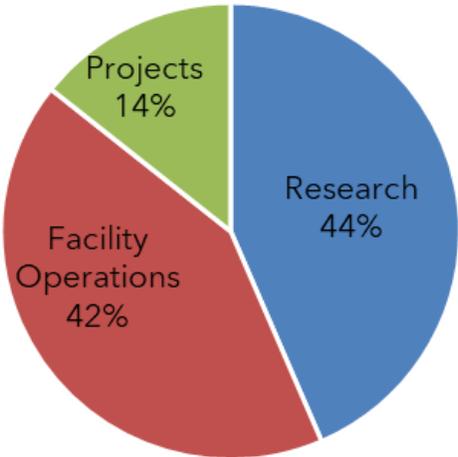


	FY 2023 Enacted	FY 2024 Enacted	FY 2025 Request
Research	1,101,653	1,089,823	1,068,824
Facility Operations	1,068,647	1,235,177	1,319,461
Projects	362,700	299,625	193,000
GPP	1,000	1,000	1,000
Total	2,534,000	2,625,625	2,582,285

FY 2024 Enacted



FY 2023 Enacted



Artificial Intelligence and Machine Learning

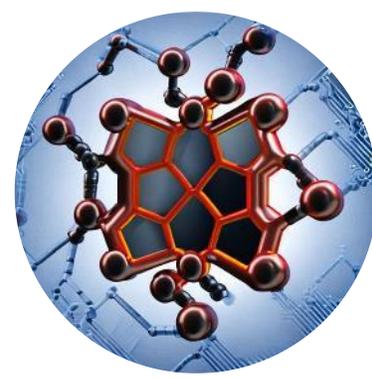
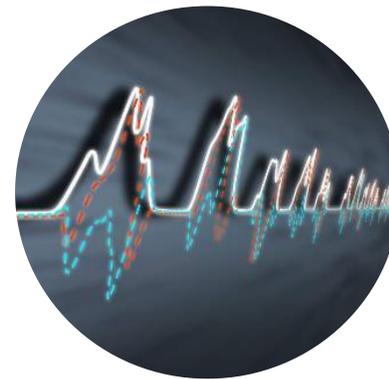
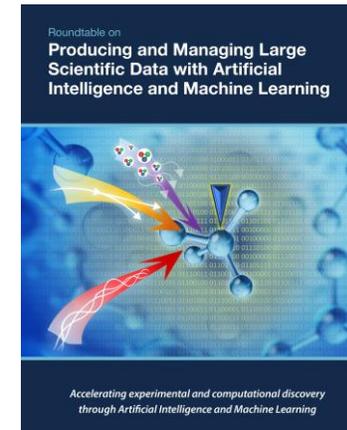
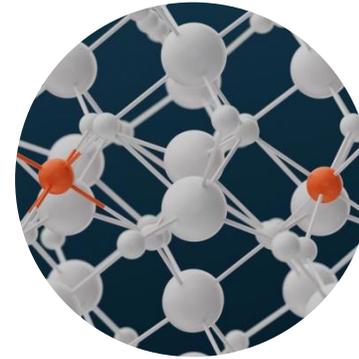
(+\$17.4M, 60% above FY 2024 Enacted)

◆ AI for Science

- Accelerate scientific discovery and realize broader insights from shared datasets
- Develop surrogate models for expensive or time-constrained experiments
- Learn from multi-modal, sparse, and/or noisy data

◆ AI for User Facilities

- Guided by BES Roundtable on Producing and Managing Large Scientific Data with AI/ML
- Enhance efficiency of facility operations and design of experiments
- Transform real-time analysis of data
- Predict and mitigate instrument/facility down time (e.g., use of digital twins)
- Enable self-driving, autonomous instrumentation and experiments

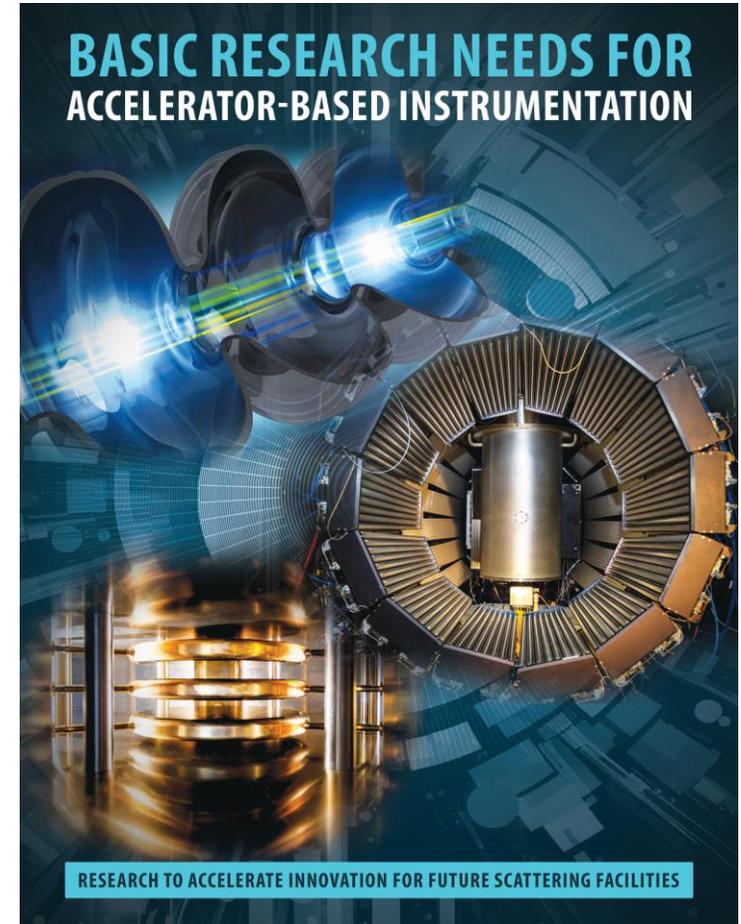


Update: BRN for Accelerator-Based Instrumentation

The brochure for the Workshop *Basic Research Needs for Accelerator-Based Instrumentation* available very soon on the BES website.

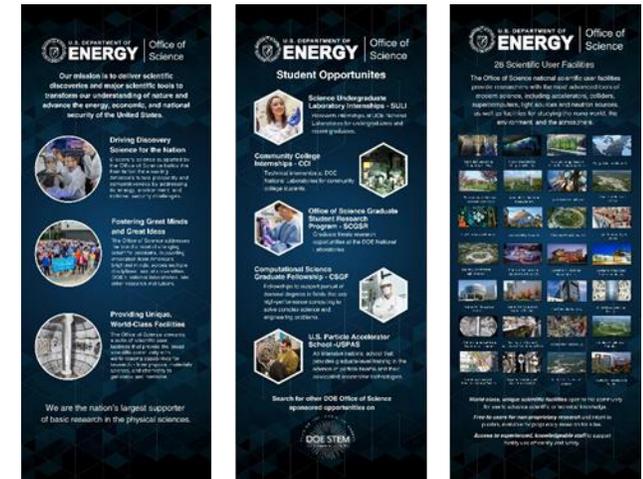
Five priority research directions to revolutionize accelerator-based instrumentation have been developed:

- Realize next-generation capabilities that achieve theoretical performance limits
- Tailor and control beams with unprecedented precision and speed to probe complexity in matter.
- Accelerate advanced modeling, real-time feedback, fully-integrated co-design, and physical-digital fusion.
- Lead innovation in new materials, system design, and advanced fabrication as a foundation for integration of technologies in accelerator-based facilities
- Understand Scientific Mechanisms that limit system performance and utilization



SC Coordinated Outreach Strategy

- ◆ Led by the Offices of Scientific Workforce Diversity, Equity, and Inclusion and Deputy Director for Science Program, SC has established a shared outreach strategy and increased both general and targeted outreach to broader audiences.
- ◆ SC program offices are leading outreach at one or more public events at major professional society meetings each year.
 - SC hosted panel discussions and promoted SC-sponsored research and internship program opportunities at over a dozen meetings in CY 2023 (e.g., National Society of Black Physicists, Society of Hispanic Professional Engineers, AAAS Annual Meeting).
 - Strong coordination with DOE laboratories.
 - Complements existing programmatic engagement with the community (e.g., conference attendance, public webinars)
- ◆ BES will be leading outreach for the Fall 2024 MRS Meeting in Boston, MA.



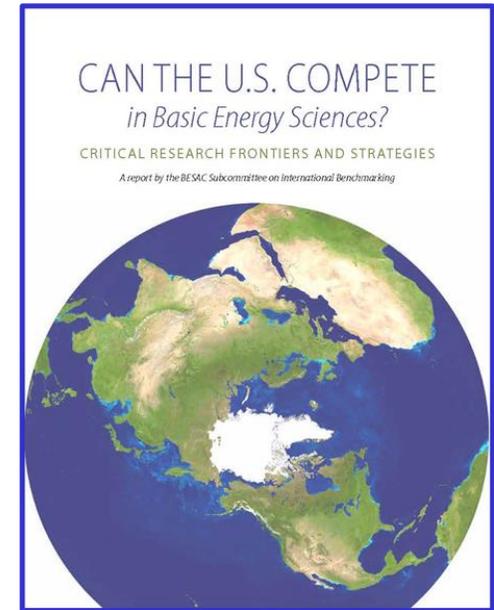
BES “Office Hours” (NEW)

- ◆ BES is holding virtual office hours on the third Thursday of the month, 2-3 pm ET
- ◆ Researchers, educators, and leaders within research administration from all institutional types are encouraged to join
- ◆ A primary goal of the virtual office hours is to broaden awareness of our programs; no prior history of funding from DOE is required to join
- ◆ Program managers are available to answer questions
- ◆ Topics include:
 - [Complete] Thursday, March 21, 2024 at 2pm ET – *Introduction to BES Materials Sciences and Engineering Division – Organization, priorities, and funding opportunities*
 - **Thursday, April 18, 2024 at 2pm ET – *Introduction to BES Scientific User Facilities Division – Capabilities and Access***
 - Thursday, May 16, 2024 at 2pm ET – *Introduction to BES Chemical Sciences, Geosciences, and Biosciences Division - Organization, priorities, and funding opportunities*
- ◆ Check the BES website (<https://science.osti.gov/bes/officehours>) for Zoom registration for upcoming office hours as well as slides/recordings from past sessions

Further Engagement on BESAC Charges

Two charges related to the 2021 BESAC International Benchmarking Report were briefed this morning (Additional discussion this afternoon):

- “...to propose **strategies for research investments** in BES-supported domains in the medium to long term” – status update at April BESAC; reporting out at the Fall 2024 BESAC meeting
- “to assess the **impact of the Nanoscale Science Research Centers (NSRCs)** to date and **provide strategies for selection of high-impact, future directions**” – reporting out at April BESAC



The third charge (SC-wide) is to “identify what **new or upgraded facilities** will best serve [SC’s] needs in the next ten years (2024-2034)” – reporting out tomorrow.

For the 8 projects identified, the subcommittee was charged with assessing:

- Potential to contribute to world-leading science in the next decade
- Readiness for construction

Questions?

