

Basic Energy Sciences Update

NASEM CMMRC

October 2, 2024

- ▲ Andy Schwartz
- ▲ Office of Basic Energy Sciences



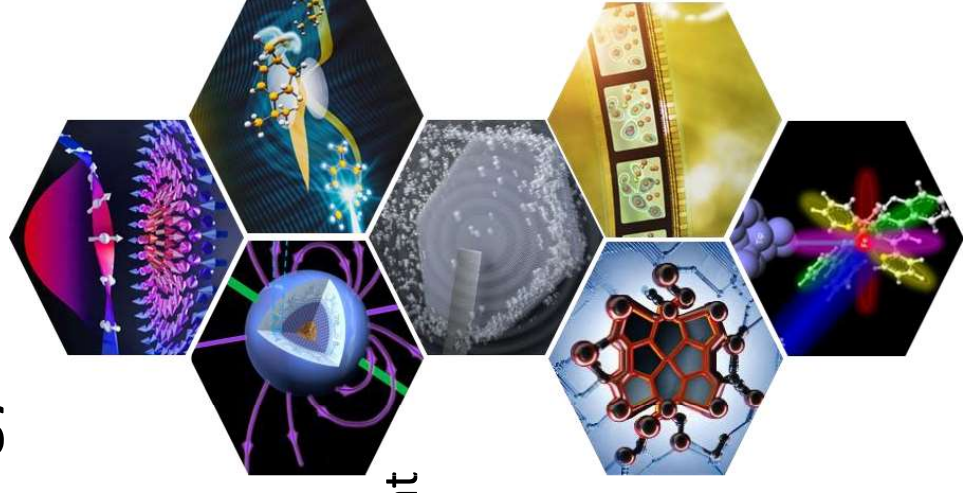
U.S. DEPARTMENT OF
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<https://science.osti.gov/>

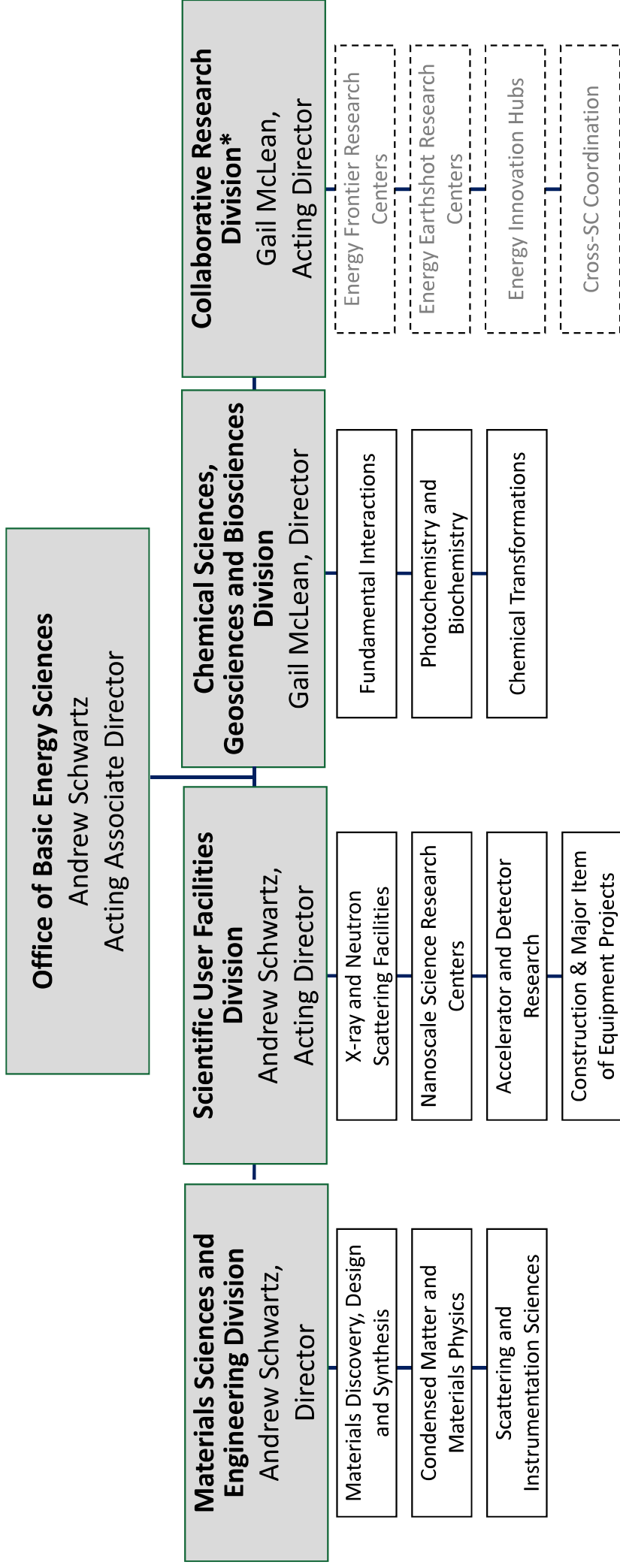
Basic Energy Sciences: Understanding Matter and Energy at Electronic, Atomic, and Molecular Levels

BES fulfills its mission through:

- Supporting **basic research**
 - “Grand Challenge” science
 - Discovery and design of materials and chemical processes that underpin a broad range of energy technologies
- Ensuring **broad participation** in the research portfolio
- Operating **world-class scientific user facilities** in X-ray, neutron, and nanoscale science
- Managing **construction and upgrade projects** to maintain **world-leading** scientific user facilities



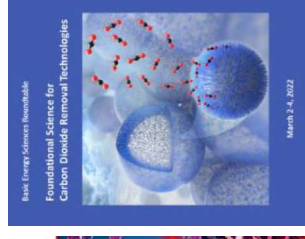
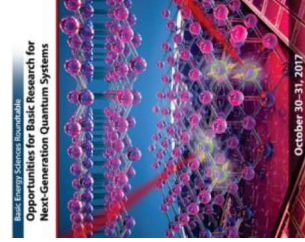
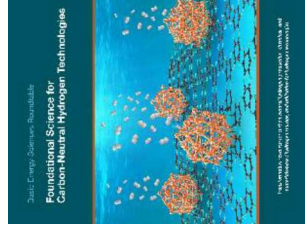
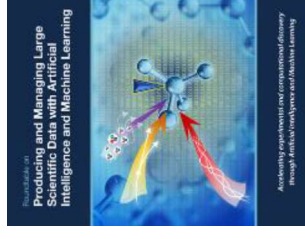
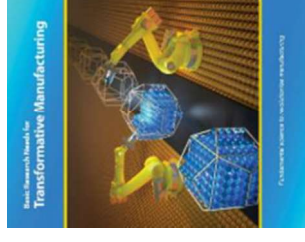
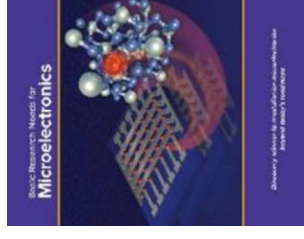
Basic Energy Sciences – Organization



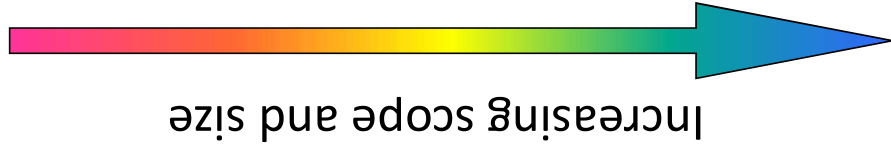
Research grouped by scientific topics, each impacting many energy technologies

Current Research Priorities

- Science in support of clean **energy and sustainable manufacturing**
 - Supported by strategic planning and cross-DOE initiatives, including Energy Earthshots
 - Strategic planning reports in the past 5 years include hydrogen, carbon dioxide removal, solar fuels, microelectronics, manufacturing, nuclear energy (in draft)
- Science addressing **national priorities**
 - Quantum Information Science, including National QIS Research Centers
 - Microelectronics
 - Data, artificial intelligence, and machine learning
 - Biopreparedness capabilities
 - Transition of science advances to technologies
 - Critical materials
- Forefront science in **core research foundations**
 - BESAC charge to provide advice on prioritization strategies – report out at the September 24th meeting)
- Support to **broaden participation** in research (Early Career, RENEW, and FAIR)



Fundamental Research Supported in All BES Research Modalities



Increasing scope and size

Core Research

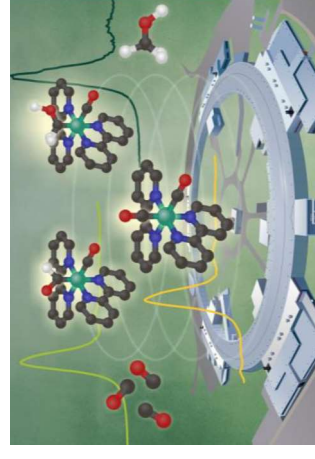
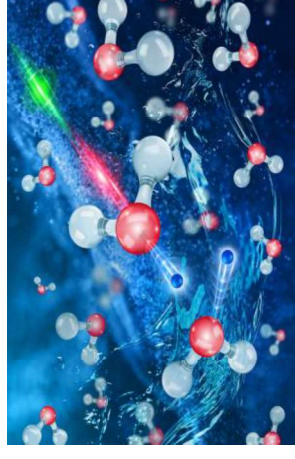
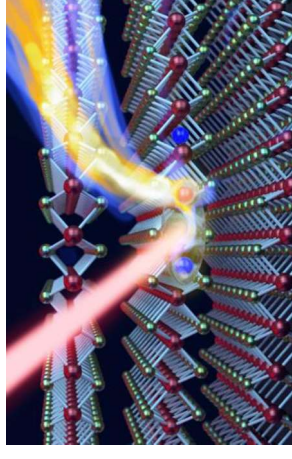
Fundamental materials & chemical sciences research. Supports single investigators (~\$150K+/year) & small groups (\$500K-\$2M/yr, 3-yr).

Energy Frontier & Energy Earthshot Research Centers, Computational Chemical and Materials Science Centers, and Microelectronics Research Centers

Fundamental, use-inspired research per Basic Research Needs Workshop reports. Supports larger teams (\$2-5M/yr, up to 4-yr).

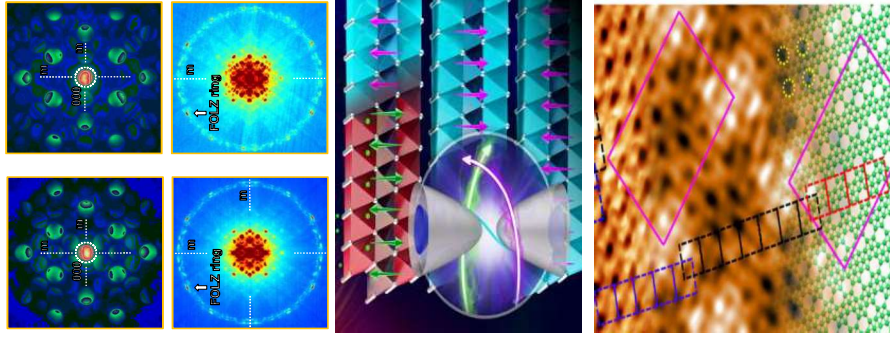
Energy Storage & Fuels from Sunlight Energy Innovation Hubs; Quantum Information Science Research Centers

Fundamental research on topics that have proven challenging for traditional funding modalities. Large-team research awards (\$8-25M/yr, 5-yr). Have defined research goals, milestones, and management.



Materials Sciences and Engineering Research

Broad Portfolio of Grand Challenge and Energy Use-Inspired Fundamental Research



Scattering and Instrumentation Sciences:

Investigation of photon, neutron, and electron interactions with matter to characterize structures, dynamics, and functionality

Condensed Matter and Materials Physics:

Exploration of phenomena in condensed matter, such as quantum behavior and response to environmental stimuli

Materials Discovery, Design, and Synthesis:

Understanding synthesis and dynamics to discover/design new materials via innovative physical, chemical, and bio-molecular routes

Crosscutting Research Themes: Energy-inspired materials research; Quantum and electronic materials; Theory, computation, data science; Synthesis; Science across length and time scales; Non-equilibrium dynamics; In-situ, operando, and multi-modal characterization

Administrative Staff

Teresa Crockett



Andy Schwartz
Director

Materials Science and Engineering Division

PM – Shawn Chen



Contact info for all PMs is
on the BES-MSE Website

Materials Discovery, Design, and Synthesis Team



Acting Team Lead – Craig Henderson



Materials Chemistry

PMs – Craig Henderson and Chris Chervin



Biomolecular Materials

PM – Aura Gimm



Synthesis and Processing Science

PM – James Dorman



Batteries and Energy Storage Hub & Integrated Energy Research

PMs – Craig Henderson and John Vetrano



Condensed Matter and Materials Physics

Team Lead – Mick Pechan



Experimental Condensed Matter Physics

PM – Claudia Cantoni and Tim Mewes



Theoretical Condensed Matter Physics

PMs – Claudia Mewes and Matthias Graf



Physical Behavior of Materials

PM – Refik Kortan



Mechanical Behavior and Radiation Effects

PM – John Vetrano



Quantum Information Science

PM – Athena Sefat



Scattering and Instrumentation Sciences

Team Lead – Helen Kerch



X-Ray Scattering

PM – Lane Wilson



Neutron Scattering

PM – Mike Fitzsimmons



Electron and Scanning Probe Microscopies

PM – Jane Zhu

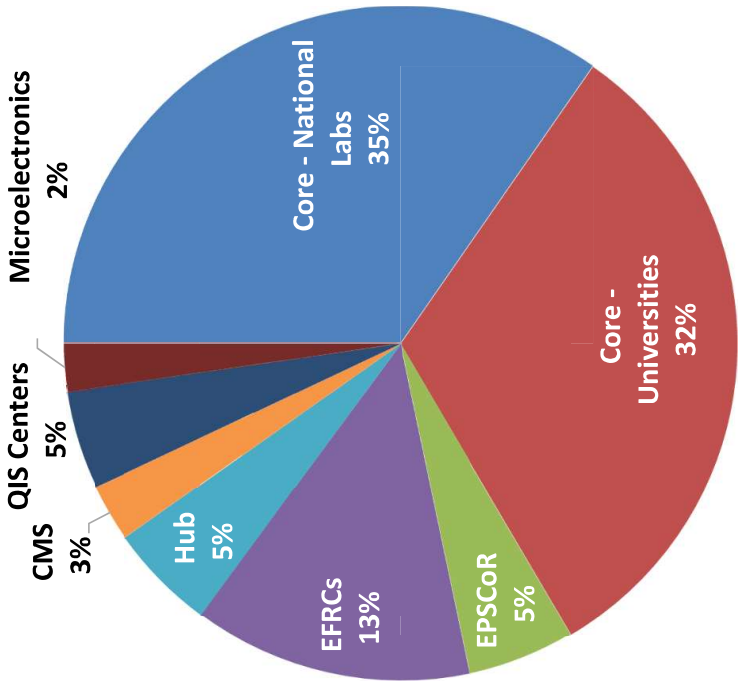
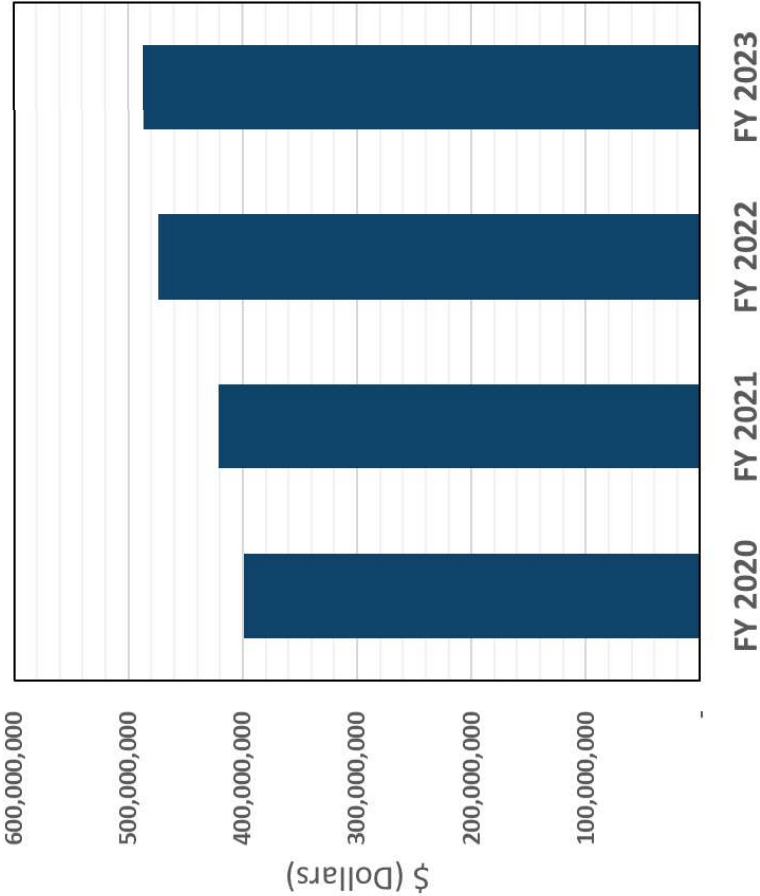


Experimental Program to Stimulate Competitive Research (DOE EPSCoR)

PM – Tim Fitzsimmons

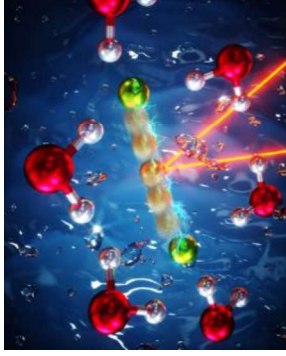
Updated January 2024

BES-MSE Budget



Chemical Sciences, Geosciences & Biosciences Research

Broad Portfolio of Grand Challenge and Energy Use-Inspired Fundamental Research



Fundamental Interactions:

Control chemical reactivity and dynamics in gas and condensed phases and at interfaces

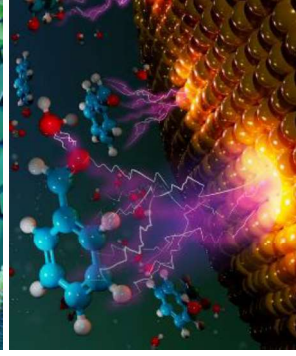
Photochemistry and Biochemistry:

Molecular mechanisms of light energy capture and its conversion into chemical and electrical energy



Chemical Transformations:

Chemical catalysis, synthesis, separation, stabilization, and transport processes, from atomic to geologic scales

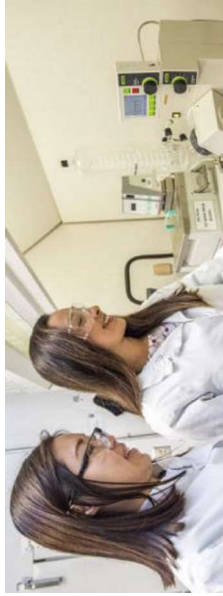


Crosscutting Research Themes: Mechanisms for Clean Energy; Ultrafast

Chemistry; Complex Interfaces; Charge Transport and Reactivity;

Reaction Pathways in Diverse Environments; Aqueous Environments

BES has Strong Participation in SC Programs to Broaden Participation



RENEW

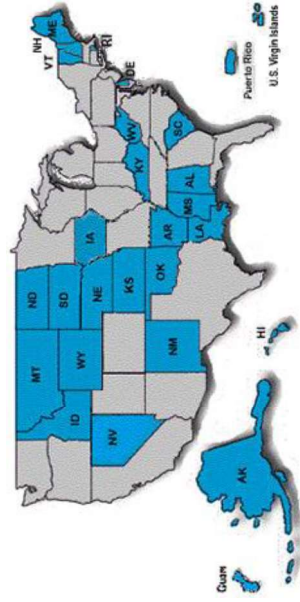
Reaching a New Energy Sciences Workforce

- Internships for non-R1 emerging research institutions and non-R1 minority serving institutions



FAIR

Funding for Accelerated, Inclusive Research

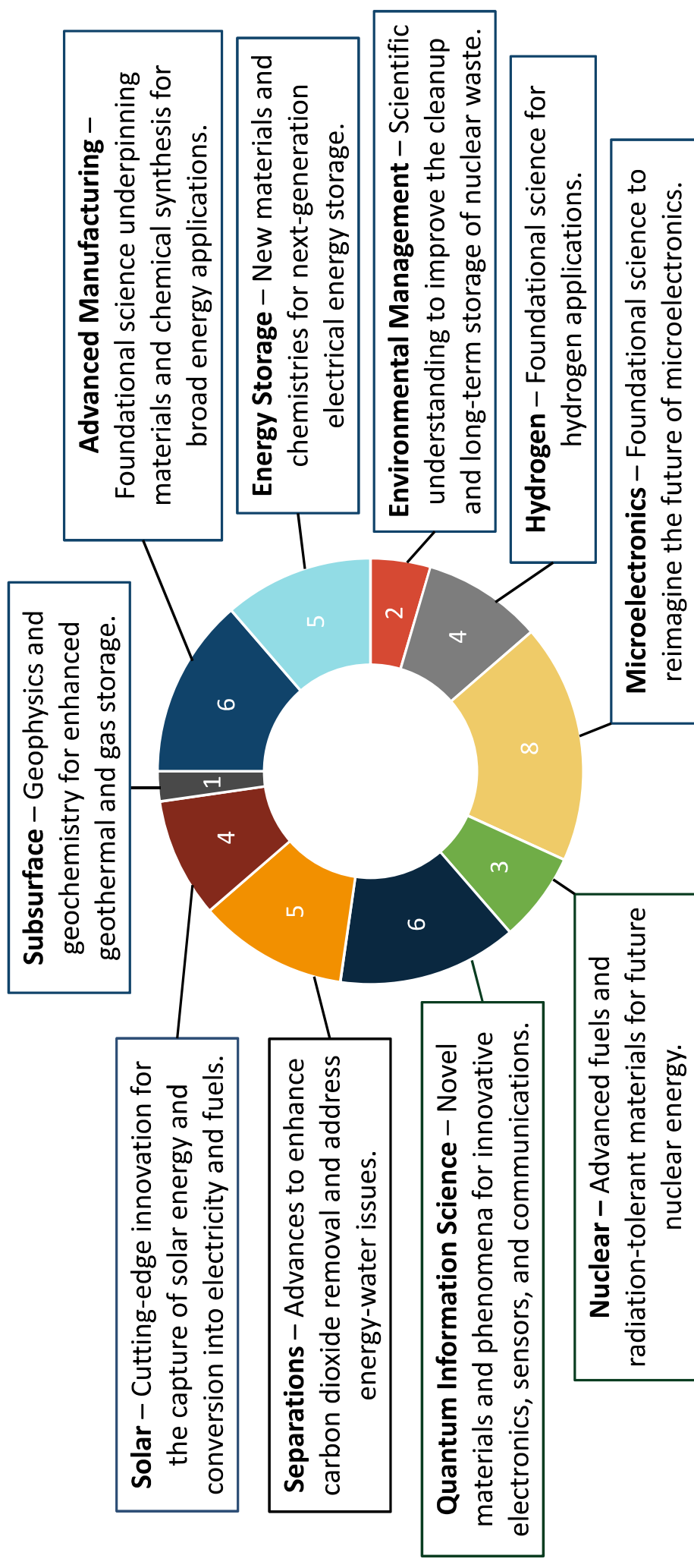


EPSCoR

Established Program to Stimulate Competitive Research

- BES manages the cross-SC Established Program to Stimulate Competitive Research that Promotes Geographically Inclusive and Equitable Research

44 Energy Frontier Research Centers Support National Priorities



SC Energy Earthshots Initiative

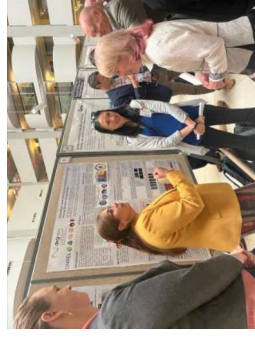
- ♦ Fundamental research to accelerate breakthroughs required to address challenges for the stretch goals of the DOE Energy Earthshots
 - Eight Energy Earthshots have been announced. The first six Earthshots are supported with SC awards announced in FY 2023. Two additional Earthshots were announced in FY 2023 (Affordable Home Energy and Clean Fuels & Products Shots).
- ♦ Energy Earthshot Research Centers (EERCs) established in FY 2023
 - Advances foundational knowledge and state-of-the-art capabilities in experimental, theoretical, and computational sciences needed to realize new approaches and solutions.
 - Large, multi-investigator, multi-disciplinary national laboratory-led teams.
 - Close coordination with the Energy Technology Offices and existing research consortia/demonstration projects to enhance cross-office research cooperation.
- ♦ EERCs are complemented by small group awards focused on use-inspired fundamental research to address knowledge gaps that limit achievement of the Energy Earthshot goals

Affordable Home Energy Shot   		50%+ Technology Cost Reduction 20% Lower Cost Within the Decade
Floating Offshore Wind Shot  		>70% Reduction 2035
Industrial Heat Shot  		85% Reduction 2035
Enhanced Geothermal Shot  		90% Reduction 2035
Clean Fuels and Products  		85% Reduction 2035

Hydrogen Shot   		1 Dollar 1 Kilogram 1 Decade
Long Duration Storage Shot 		Reduce storage costs by 90%*in storage systems That deliver 10+ hours of duration ...in 1 decade *from a 2020 Li-Ion baseline
Carbon Negative Shot   		<100 Dollars 1 Ton 1 Decade

Science Summit for Energy Earthshot Innovation

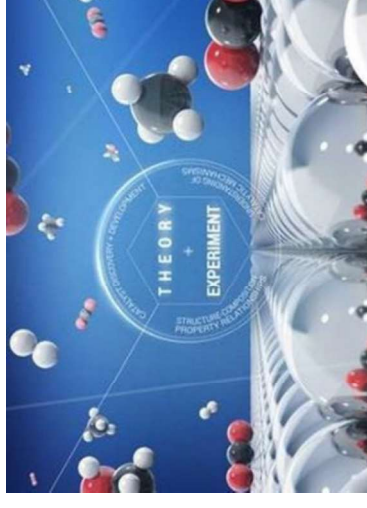
- **Goal:** Opportunity for multi-disciplinary teams funded in ASCR, BES, and BER to collaborate, engage, and discuss foundational research needed to support the DOE Energy Earthshot portfolio
- Held **September 4-5th, 2024** in Rockville, MD
- Over 200 attendees
 - Energy Earthshot Research Centers (EERCs)
 - Science Foundations for the Energy Earthshots (SFEEs)
 - Bioenergy Research Centers (BRCs)
 - Energy Frontier Research Centers (EFRCs)
 - Mathematical Multifaceted Integrated Capability Centers (MMICCs)
 - ASCR Software Stewardship projects
 - Fuels from Sunlight Energy Innovation Hubs
 - User Facilities and other SC Resources
 - S4, SC PMs & upper management, DOE Technology Offices
- Agenda included plenary talks, poster sessions, and discussion-based breakout sessions on DOE Energy Earthshot Research and Cross-cutting Foundational Science topics



BES Supports 2 Energy Innovation Hub Topics

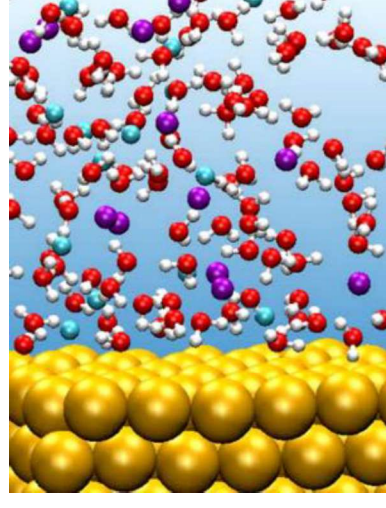
- **Fuels from Sunlight:**

- Build the scientific foundation for a scalable technology that converts carbon dioxide into renewable transportation fuels with only solar energy added
- Joint Center for Artificial Photosynthesis (JCAP) 2010-20
- 2 new awards in FY 2020 (5 years): Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE, UNC) and Liquid Sunlight Alliance (LiSA, Caltech)



- **Batteries and Energy Storage:**

- Build the scientific foundation for disruptive, high-performance batteries that go beyond today's commercial products and meets challenging performance requirements for grid or transportation applications
- Joint Center for Energy Storage Research (JCESR, led by Argonne National Laboratory (ANL), 2014-2023).
- 2 new awards in FY 2024 (5 years): Energy Storage Research Alliance (ESRA, ANL) and Aqueous Battery Consortium (ABC, Stanford University)



National Quantum Information Science (QIS) Research Centers

Established in FY 2020, DOE's National QIS Research Centers are a large-scale effort across the technical breadth of SC. The Centers, coupled with SC's core research portfolio, form an ecosystem to foster and facilitate advancement of QIS.



Q-NEXT • Next Generation
Quantum Science and
Engineering
(David Awschalom, ANL)



C²QA • Co-design Center for
Quantum Advantage
(Andrew Houck, BNL)



SQMS • Superconducting
Quantum Materials and Systems
Center
(Anna Grassellino, FNAL)



QSA • Quantum Systems
Accelerator (LBNL)
(Rick Muller, SNL)



QSC • The Quantum Science
Center
(Travis Humble, ORNL)

FY 2024 BES Funding Opportunities

- ◆ **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. **Awards announced Aug. 22, 2024 - \$36M for 39 awards in 19 states**
- ★ ◆ **Computational Materials Sciences – Exploratory Research at the Exascale:** Computational codes and associated databases for materials design with advanced functionalities. **Awards announced August 28, 2024 - \$14M for 4 DOE lab awards.**
- ★ ◆ **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. **Awards announced Sept. 4, 2024 - \$118M for 10 new and renewing Centers led by 6 universities and 4 DOE Laboratories with 65 additional partner institutions.**
- ★ ◆ **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. **Awards announced Sept. 10, 2024 - \$58M for 46 BES awards at 32 unique universities and 8 unique DOE Lab.**
- ◆ **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). **Proposals under review. Announcements anticipated early FY 2025.**

★ Details on subsequent slides

Computational Materials Science – Exploratory Research at the Exascale

- ◆ Scope: Produce widely applicable, validated public-access community codes and associated databases for functional materials that leverage the exascale software stack and ECP work.
- ◆ Requirements: Fully integrated, multi-investigator teams led by DOE labs and exascale-ready software
- ◆ Topics: (1) Computational discovery and design of functional materials with unique physical properties; (2) computational modeling of emergent and ordered magnetic, superconducting, and/or ferroelectric phases, including their dynamics.
- ◆ [Awards](#) - \$14M for 4 new and renewal awards led by 4 DOE labs with 12 partner institutions
 - **Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM)** | Lead: Steven Louie - Lawrence Berkeley National Laboratory (Renewal)
 - **Center for Predictive Simulation of Functional Materials (CPSFM)** | Lead: Paul Kent - Oak Ridge National Laboratory (Renewal)
 - **Accelerating the discovery and design of advanced functional materials using AI/ML and exascale computing** | Lead: Cai-Zhuang Wang - Ames National Laboratory (New)
 - **Navigating the Design Space of Heterostructures: Advancing Functionality of Modeling for 2D Materials and Transition Metal Oxides** | Lead: Eric Bylaska - Pacific Northwest National Laboratory (New)

Energy Frontier Research Centers

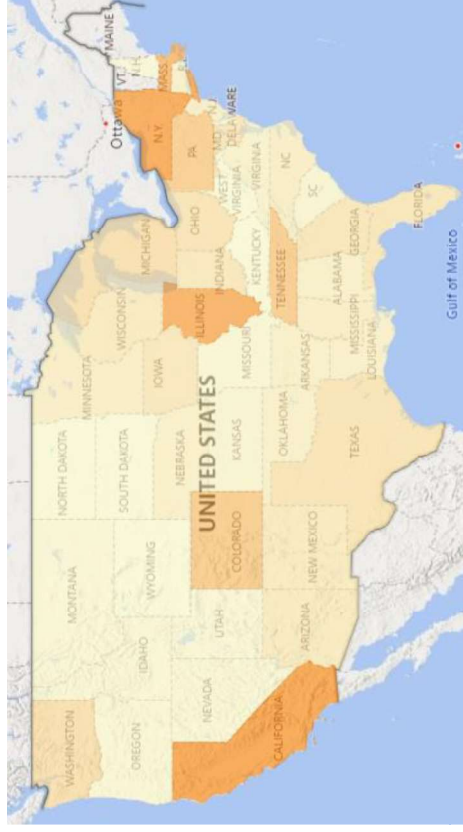
◆ Topics:

- Renewals: (1) Transformative manufacturing; (2) Quantum information science; (3) Environmental management
- New: (1) Co-design of materials and processes to revolutionize microelectronics and/or QIS fabrication; (2) Environmental management
- ◆ Awards: 10 new and renewal awards led by 6 universities and 4 DOE Labs (75 partner institutions)
 - **A Center for Power Electronics Materials and Manufacturing Exploration (APEX)** | Lead: Nancy Haegel – NREL (new)
 - **Quantum Photonic Integrated Design Center (QuPIDC)** | Lead: Libai Huang – Purdue University (new)
 - **Center for Plastics Innovation (CPI)** | Lead: LaShanda Korley – University of Delaware (renewal)
 - **Ion Dynamics in Radioactive Environments and Materials (IDREAM)** | Lead: Carolyn Pearce – PNNL (renewal)
 - **Institute for Cooperative Upcycling of Plastics (iCOUP)** | Lead: Aaron Sadow – Ames National Laboratory (renewal)
 - **Center for Energy Efficient Magnonics (CEEMag)** | Lead: Yuri Suzuki – SLAC (new)
 - **Center for 3D Ferroelectric Microelectronics Manufacturing (3DFEM2)** | Lead: Susan Trolier-McKinstry – Pennsylvania State University (renewal)
 - **Center for Molecular Quantum Transduction (CMQT)** | Lead: Michael Wasielewski – Northwestern University (renewal)
 - **EFRC for Quantum Sensing and Quantum Materials (QSQM)** | Lead: Peter Abbamonte – University of Illinois Urbana Champaign (renewal*)
 - **Ultra Materials for Resilient, Smart Electricity Grid (ULTRA)** | Lead: Arizona State University (renewal*)

* Two-year transition

Early Career Research Program (ECRP)

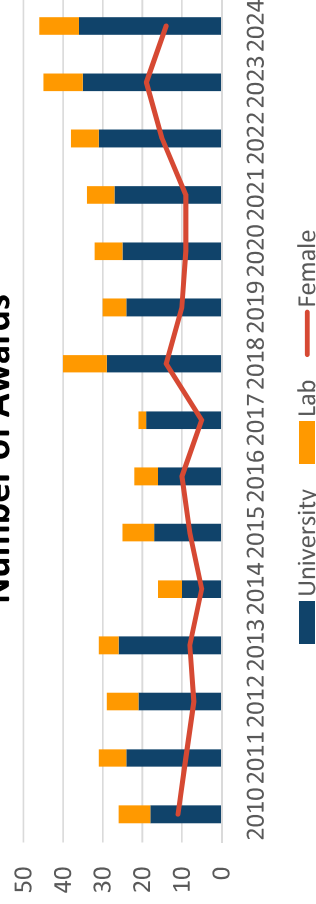
Location of all 466 BES ECRP Awards from 2010 - 2024



Location of 46 BES ECRP Awards in 2024



Number of Awards

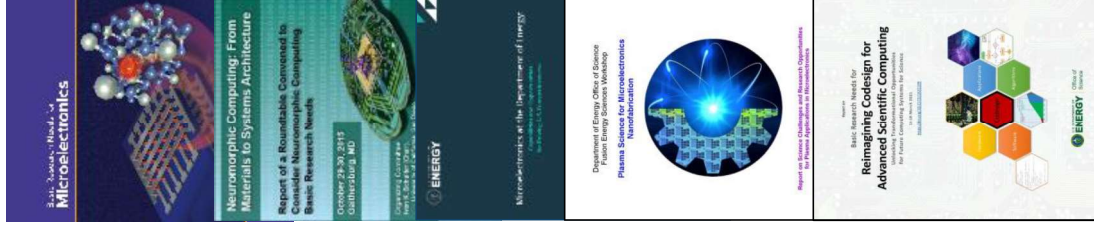


BES ECRP Awards in 2024

- 22 states and 40 unique institutions
- 5 new institutions (since program inception)
- 4 awards to EPSCoR institutions
- 8 HSI awards

Advanced Microelectronics Lab Call

- ◆ Microelectronics Science Research Centers will comprise a network of multiple multi-disciplinary team awards
 - Perform mission-driven research to address foundational challenges in the design, development, characterization, prototyping, demonstration, and fabrication of microelectronics
 - Each Center will be made up of individual team awards that focus on research required for a common Center goal
 - Teams will include researchers from universities, national laboratories, and industry
 - **Lab Call released May 8, 2024; awards to be announced early FY 2025.**
- ◆ Continued coordinated SC support for multi-disciplinary research to accelerate the innovation and advancement of microelectronic technologies in a co-design ecosystem
 - 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
 - Provides foundational knowledge for development of next-generation technologies in computing, communications, sensing, and power
- ◆ Basic research in microelectronics complements later-stage investments being made by other agencies through the CHIPS Act



FY 2025 FOA: EPSCoR Implementation Awards

- Solicitation Scope ([DE-FOA-0003444](https://www.fda.gov/oc/foia/epscor-0003444)) – Issued September 12, 2024):
 - Enhance S&T capabilities of designated jurisdictions to conduct nationally competitive research relevant to DOE’s science and energy missions; promote geographic and institutional diversity, including training of scientists and engineers in geographically underserved jurisdictions.
- Program Planning/Context:
 - On behalf of DOE, BES publishes the EPSCoR Implementation Award FOA biennially
- Program Coordination:
 - Coordination across DOE, with ~10% matching funds from participating Offices
 - Since FY 2023, EPSCoR funds are distributed among SC Offices: \$25M BES, \$2M in ASCR, BER, FES, HEP & NP (\$35M Total).
- Planned application requirements:
 - Eligible Institutions: Using NSF criteria (<https://new.nsf.gov/funding/initiatives/epscor-epscor-criteria-eligibility>) - colleges/universities in 28 jurisdictions
 - Estimated award size/duration: Up to \$1,500/2,500K per year for new/renewal awards with a duration of two years and up to two 2-year renewal options for new awards.
 - Funding: Up to \$35M in FY 2025 (pending appropriation)
 - Pre-applications will be required. Limitation of 1 pre-application and applications per institution per topical area (by SC program and Technology Offices, with EERE divided into three sectors). 1 application per lead PI.

U.S. DOE Basic Energy Sciences User Facilities



BES User Facilities: Operating and Maintaining 12 World-leading Capabilities



Upgrade Underway

Advanced Light Source, LBNL



Stanford Synchrotron Radiation Lightsource, SLAC



Recapitalization Underway

Center for Nanophase Materials Sciences, ORNL



Recapitalization Underway

Center for Integrated Nanotechnologies, LANL



Recapitalization Underway

The Molecular Foundry, LBNL



2 Beamline Projects

National Synchrotron Light Source-II, BNL



Upgrade in Planning

High Flux Isotope Reactor, ORNL



Recapitalization Underway

Center for Nanoscale Materials, ANL



1 Upgrade Underway
+ Cryomodule Facility

Linac Coherent Light Source, SLAC



Recapitalization Underway

Center for Functional Nanomaterials, BNL



2 Upgrades Underway

Spallation Neutron Source, ORNL



Upgrade Underway

Advanced Photon Source, ANL

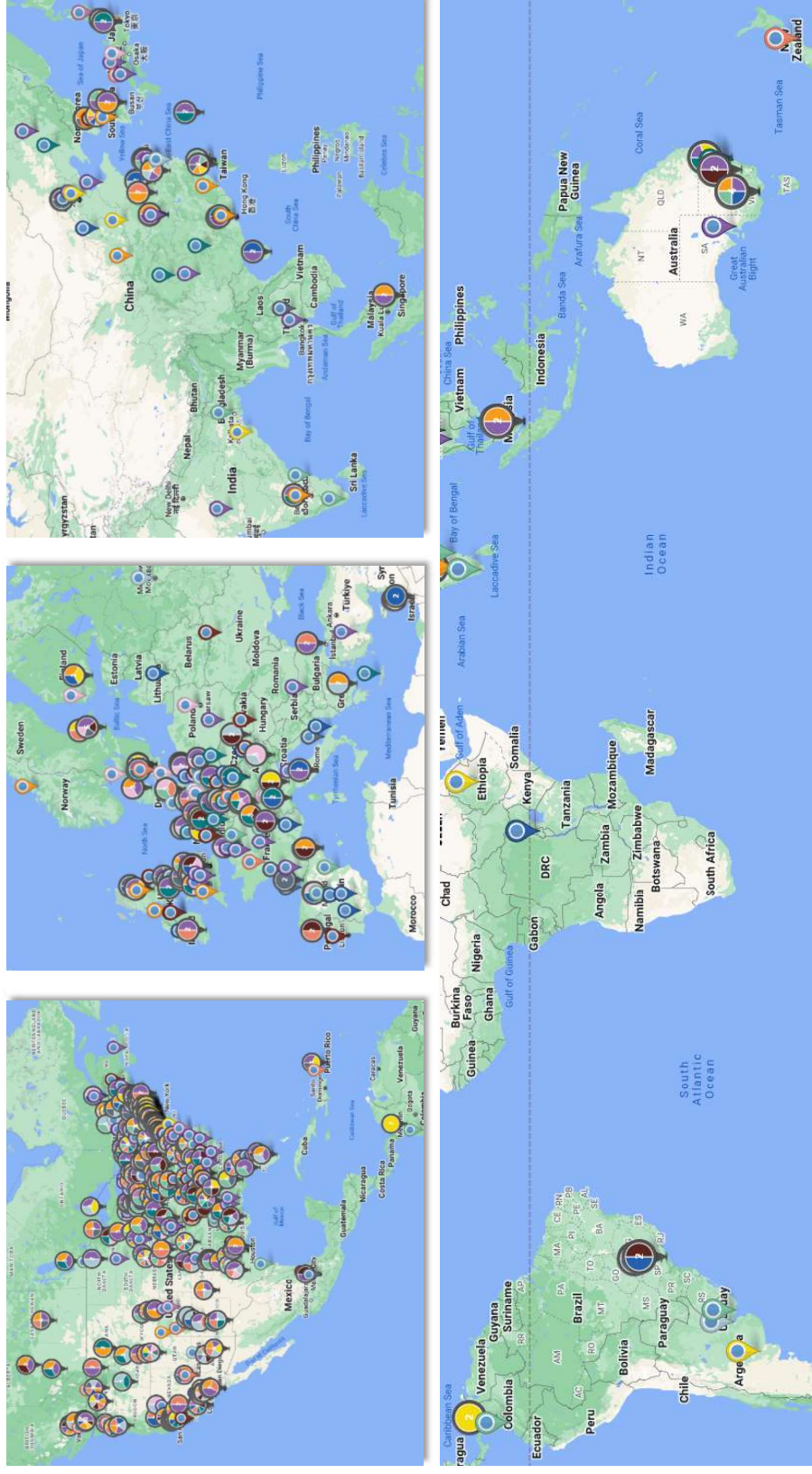


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Science

BES User Facilities: > 15,000 Users from Across the U.S. and the World

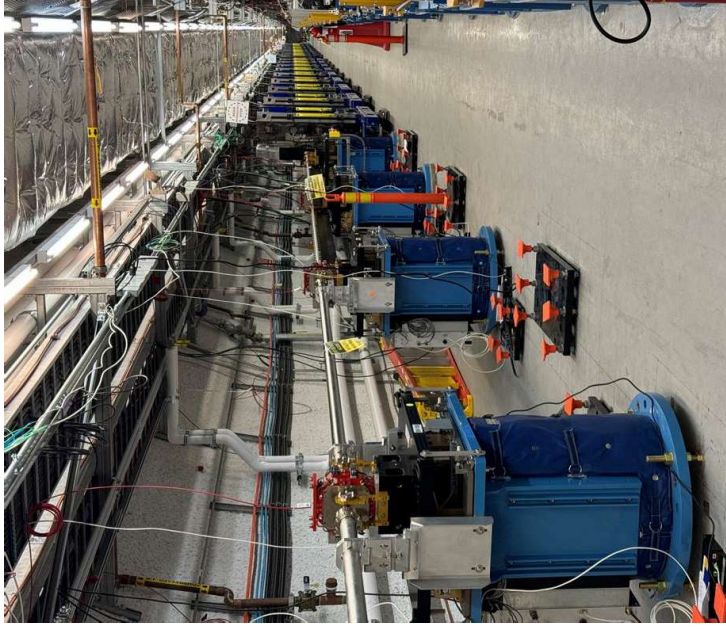
Users represent:

- Universities
- Industries
- National/Federal Laboratories
- Other Research Institutions



Facilities Project Updates and Major Milestones

- ◆ **Advanced Photon Source Upgrade (ANL):** Installation of the multi-bend achromat storage ring completed March 2024, with first light in June 2024 and a return of users in July 2024. Beamline installation and commissioning is ongoing.
- ◆ **Proton Power Upgrade (ORNL):** Operating at 1.7MW, 1.3 GeV since neutron production resumed in July 2024. Project delivered neutrons for the user program in July 2024. Planning underway for the Critical Decision (CD)-4 (Approve Project Completion) review in January 2025 with early finish expected in April 2025.
- ◆ **Linac Coherent Light Source – II – High Energy (SLAC):** A combined CD-2/3 (Approve Performance Baseline/Approve Start of Construction) was approved on September 18, 2024.
- ◆ **NSRC Recapitalization (multiple Labs):** 16 of 18 instrument awards have been made, with 5 instruments delivered (2 installed).
- ◆ **NSLS-II Experimental Tools-III (BNL):** CD-1 (Approve Alternative Selection and Cost Range) approved on September 13, 2024.



Space upstream of the existing Soft X-Ray (SXR) Undulator is prepared in August 2024 for the addition of nine LCLS-II-HE units.

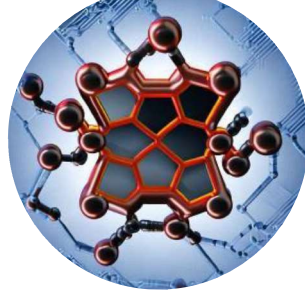
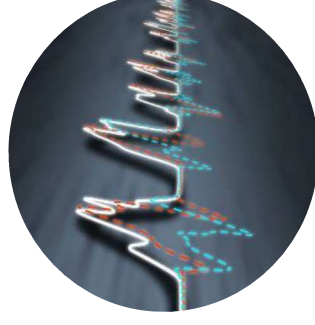
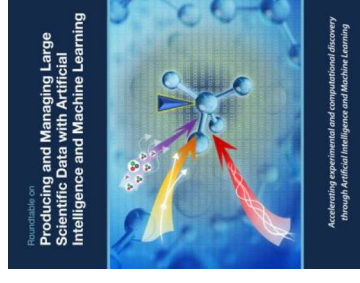
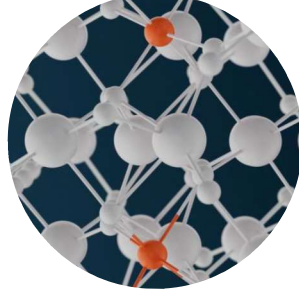
APS-U First Light

The upgraded APS achieved first light on June 17, 2024, with the resonant inelastic X-ray scattering program at 27-ID receiving the first X-rays.



Artificial Intelligence and Machine Learning

- ◆ 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



DOE-SC Roundtables: Transformational Science Enabled by Artificial Intelligence: October 28–31 & November 7–8, 2024



Analogous to community input on “first science” for new/upgraded user facilities, roundtable participants will identify Priority Research Opportunities (PROs) for using evolving AI capabilities to address the most significant challenges associated with the different scientific themes.

Complements focus of ASCR AI workshops

SC Office Hours

- ◆ As part of the efforts to improve outreach and accessibility, SC is holding monthly virtual office hours to share information and provide opportunities to ask questions.
- ◆ Starting in September, the Office of Science (SC) is transitioning to one SC-wide monthly virtual Office Hour to share information about our programs and provide opportunities to ask questions.
- ◆ All are welcome to attend; no existing relationship with DOE or the DOE national laboratories is required. Research administrators are also encouraged to attend.
- ◆ Schedule and details are on the office hour page at <https://science.osti.gov/officehours>
 - Prior BES Office Hours (slides & video) available at <https://science.osti.gov/bes/officehours>
- ◆ Upcoming Office Hours and Topics:
 - Tuesday, October 1, 2024, at 2pm ET – FY 2025 Annual Open Solicitation
 - Tuesday, November 12, 2024, at 2pm ET – TBD
 - Tuesday, December 3, 2024, at 2pm ET – TBD



THANK YOU!

Questions/Discussion