

Basic Energy Sciences Update

Basic Energy Sciences Advisory Committee Meeting
December 12, 2023

- ▲ Linda Horton, Gail McLean, and Andy Schwartz
 - ▲ 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
Linda Horton

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

Andy Schwartz, Acting Director

Materials Sciences and Engineering Division

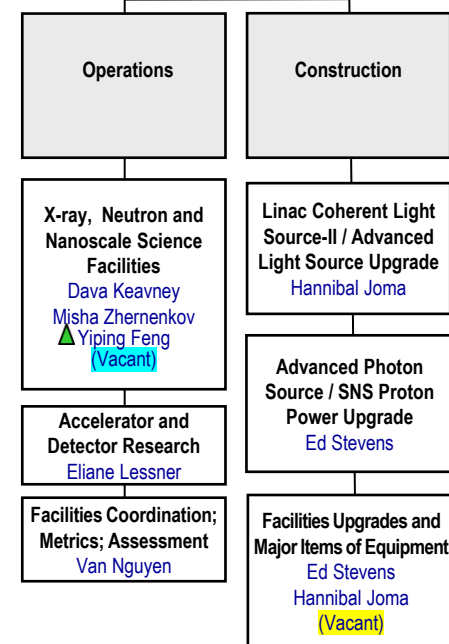
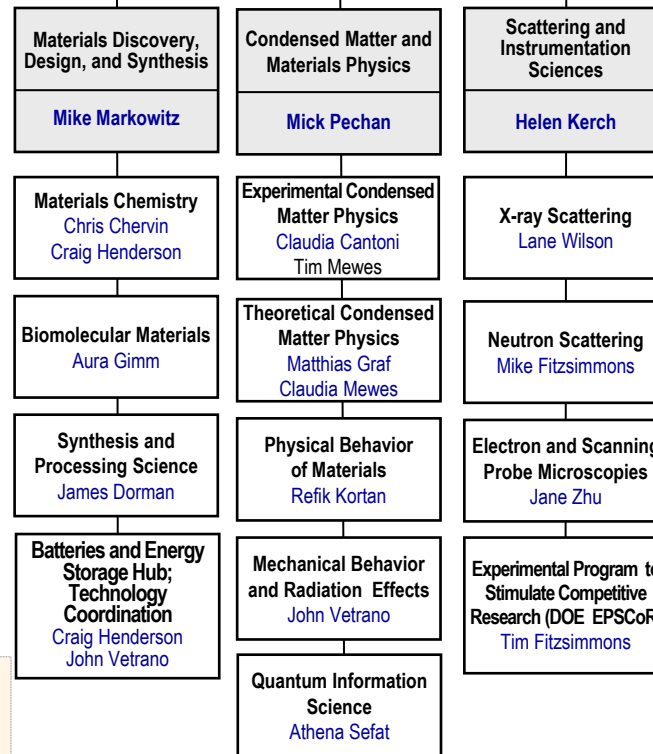
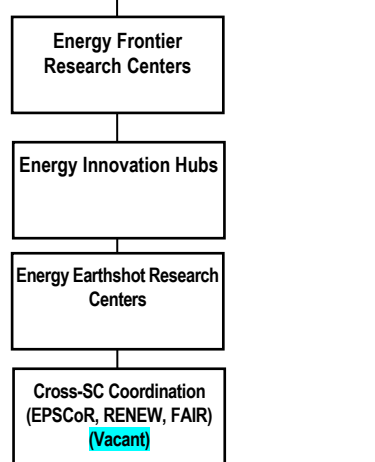
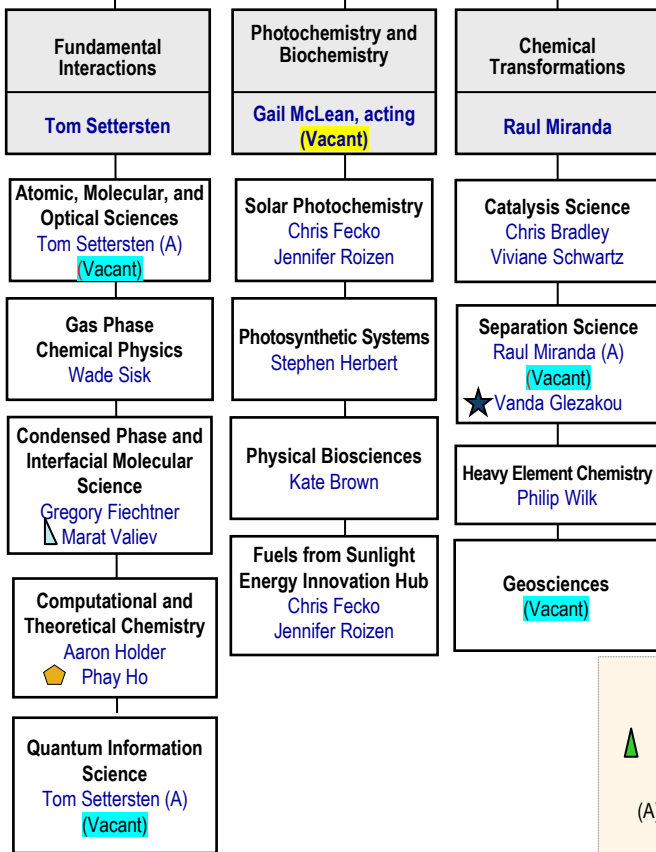
Andy Schwartz, Director

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

Scientific User Facilities Division

Linda Horton, Acting Director

Rocio Meneses, Program Support Specialist



LEGEND

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

Revised 12-06-2023

New Division Director

Chemical Sciences, Geosciences and Biosciences



Dr. Gail McLean

Expertise

- ◆ Plant biochemistry and molecular and cell biology
- ◆ Broad leadership in federal service, including previous service as the acting CSGB Division Director

Experience

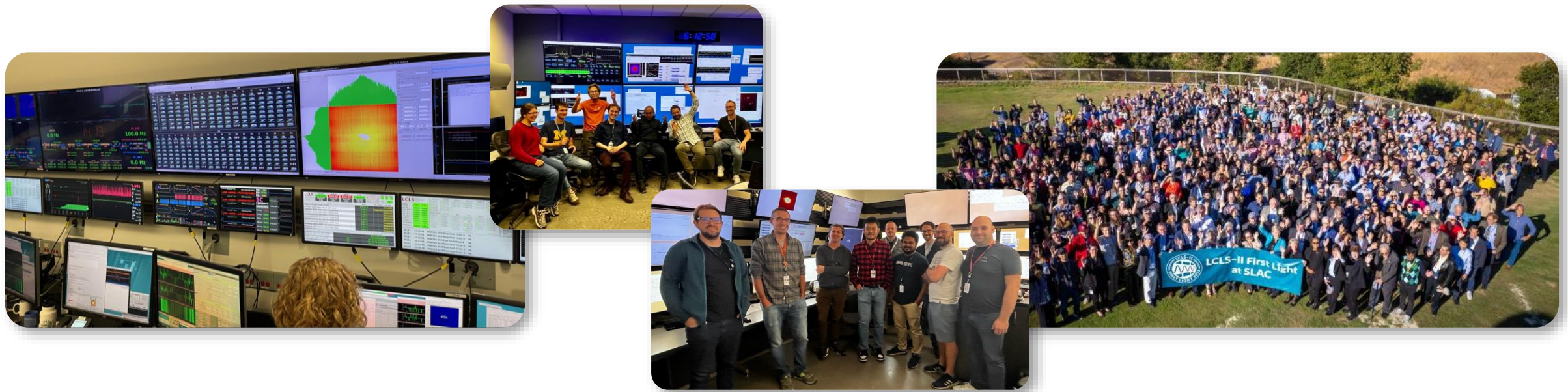
- ◆ Joined BES in 2008 as the program manager for Photosynthetic Systems, then Team Lead for Photochemistry and Biochemistry
- ◆ National Program Leader for Plant Biology, U.S. Department of Agriculture (USDA)
- ◆ American Association for the Advancement of Science (AAAS) Fellow
- ◆ Research in the Biochemistry Department at the University of Maryland-Baltimore Medical School and in the Plant & Microbial Biology Department at the University of California, Berkeley
- ◆ Ph.D., Molecular Genetics, University of Georgia

Celebration of First Light for the LCLS-II Project

The LCLS-II project – a 10-year, >\$1.1B effort funded by BES and led by SLAC National Accelerator Laboratory – achieved first light in August, offering beam to users in early October.

With the upgrade, the LCLS superconducting linac will provide X-ray pulses 10,000 times brighter (than the copper linac) at up to one million pulses per second.

The LCLS-II project adds capacity AND capability to LCLS and sets the stage for even more dramatic advances across science – from batteries to catalysis to medicine.



New BESAC Charge Focuses on Large Construction Projects for User Facilities



5 X-ray Light Sources
5 Nanoscale Science Research Centers
2 Neutron Sources

Facilities Charge Sent to All SC Advisory Committees

The Department of Energy's Office of Science (SC) has envisioned, designed, constructed, and operated many of the premiere scientific research facilities in the world. More than 38,000 researchers from universities, other government agencies, and private industry use SC User Facilities each year—and this number continues to grow.

Stewarding these facilities for the benefit of science is at the core of our mission and is part of our unique contribution to our Nation's scientific strength. It is important that we continue to do what we do best: build facilities that create institutional capacity for strengthening multidisciplinary science, provide world class research tools that attract the best minds, create new capabilities for exploring the frontiers of the natural and physical sciences, and stimulate scientific discovery through computer simulation of complex systems.

To this end, I am asking the SC advisory committees to look toward the scientific horizon and **identify what new or upgraded facilities will best serve our needs in the next ten years (2024-2034)**. More specifically, I am charging each advisory committee to establish a subcommittee to:

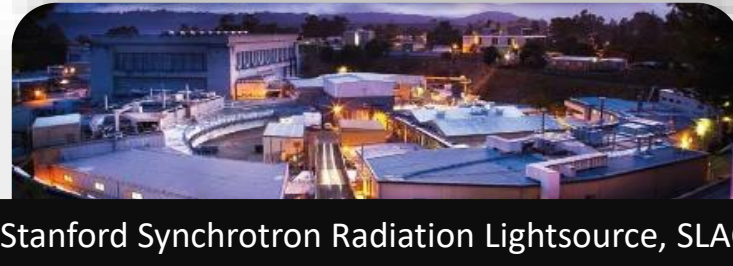
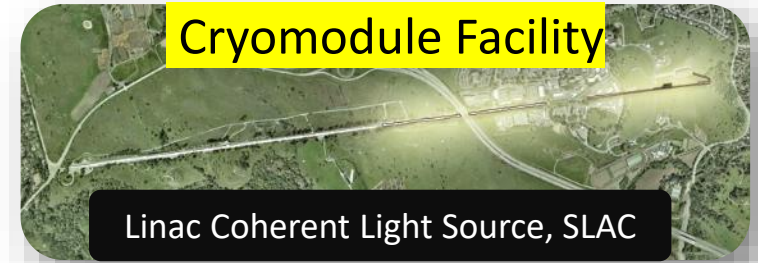
1. Consider what new or upgraded facilities in your disciplines will be necessary to position the Office of Science at the forefront of scientific discovery. **The Office of Science Associate Directors have prepared a list of proposed projects** that could contribute to world leading science in their respective programs in the next ten years. The Designated Federal Officer (DFO) will transmit this material to their respective advisory committee chairs. The subcommittee may revise the list in consultation with their DFO and Committee Chair. If you wish to add projects, please consider only those that **require a minimum investment of \$100 million**. In its deliberations, the subcommittee should reference relevant strategic planning documents and decadal studies.

Facilities Charge (continued)

2. **Deliver a short letter report that discusses each of these facilities in terms of the two criteria below and provide a short justification for the categorization, but do not rank order them:**
 - a. The **potential to contribute to world-leading science in the next decade.** For each proposed facility/upgrade consider, for example, the extent to which it would answer the most important scientific questions; whether there are other ways or other facilities that would be able to answer these questions; whether the facility would contribute to many or few areas of research and especially whether the facility will address needs of the broad community of users including those whose research is supported by other Federal agencies; whether construction of the facility will create new synergies within a field or among fields of research; and what level of demand exists within the (sometimes many) scientific communities that use the facility. Please place each facility or upgrade in one of four categories: **(a) absolutely central; (b) important; (c) lower priority; or (d) don't know enough yet.**
 - b. The **readiness for construction.** For proposed facilities and major upgrades, please consider, for example, whether the concept of the facility has been formally studied; the level of confidence that the technical challenges involved in building the facility can be met; the sufficiency of R&D performed to date to assure technical feasibility of the facility; the extent to which the cost to build and operate the facility is understood; and site infrastructure readiness. Please place each facility in one of three categories: **(a) ready to initiate construction; (b) significant scientific/engineering challenges to resolve before initiating construction; or (c) mission and technical requirements not yet fully defined.**

Many additional criteria, such as expected funding levels, are important when considering a possible portfolio of future facilities, however, for this assessment I ask that **you focus your report on the two criteria discussed above.** I look forward to hearing your findings and thank you for your help with this important task. I appreciate receiving **your final report by May 2024.**

Projects NOT included in the Charge (>CD-2 or <\$100M): ALS-U, APS-U, PPU, Cryomodule Facility (CRMF), NEXT II, and NSRC Recapitalization MIEs*

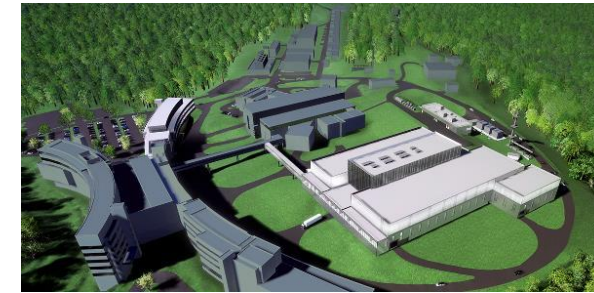


Current Line-item Projects and those prior to CD-0

Pre CD-2 Line-Item Projects; >\$100M

Linac Coherent Light Source-II-High Energy (LCLS-II-HE) at SLAC

Incr. linac energy to 8 GeV at 1 MHz and X-ray brightness by 1000x (5-12 keV); Under construction (CD-2/3: FY 2024); Est. TPC: \$710M

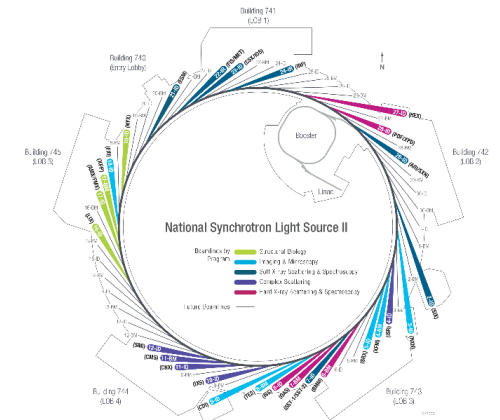


Second Target Station (STS) at ORNL

In planning with goal to reduce cost (CD-2: FY 2026); Est. TPC: \$2.1B

NSLS-II Experimental Tools-III (NEXT-III) at BNL

Additional beamlines; In planning (CD-1: FY 2024); Est. TPC: \$500M



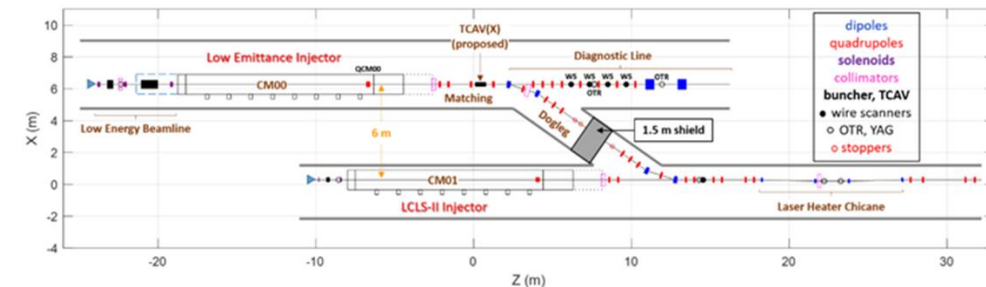
HFIR Pressure Vessel Replacement (HFIR PVR) at ORNL

In planning (CD-1/3A: FY 2026); Est. TPC: \$729M

Pre CD-0

Low Emittance Injector (LEI) at LCLS, SLAC

Adding SRF gun in a new tunnel to extend energy range to >20 keV; In planning (tentative CD-0 request: FY 2027); Pre-conceptual cost estimate: \$210M



Projects in Planning

NSLS-II Upgrade (NSLS-II-U) at BNL

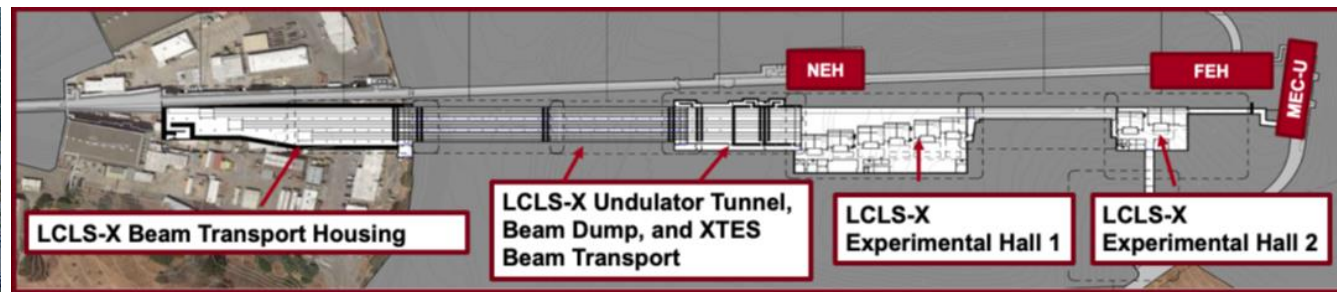
Planning underway for a 4th gen upgrade of NSLS-II based on a non-linear lattice design, increasing brightness and lowering emittance (tentative CD-0 request: FY 2030)

Linac Coherent Light Source – X (LCLS-X) at SLAC

Vision: New infrastructure to enable dozens of simultaneous instruments and significant facility performance improvements; requires additional community input and R&D to optimize upgrade (tentative CD-0 request: FY 2032)

Next Generation Light Source

Vision: Green field machine(s); requires strategic/community planning to determine the architecture for the machine(s) (tentative CD-0 request: FY 2033)



Not Included in the Facility Assessment Charge: BES Planning for MIEs and Projects <\$100M

Cryomodule Repair & Maintenance Facility (CRMF) at SLAC: West coast capability (CD-1: FY 2024); Estimated TPC: \$94.5M

MIE: Expanded X-ray Capabilities with Xtreme Light (EXCEL) at APS, ANL: In planning (CD-0 request: FY 2024)

MIE: Beamline Upgrades and Coherence-Enhanced Synchrotron Instrumentation (CESI) MIE at ALS, LBNL: In planning (CD-0 request: FY 2024)

MIE: Stanford Synchrotron Radiation Light Source Beamlines at SLAC: Proposal reviewed

MIE: LCLS Beamlines (post LCLS II-HE) at SLAC: In planning

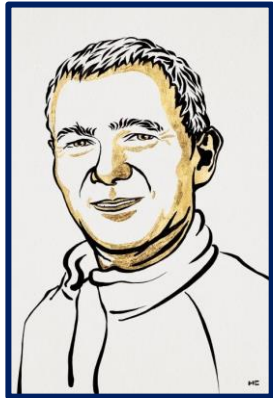
MIE: HFIR Beamlines Upgrade at ORNL: In planning

MIEs for Nanoscale Science Research Centers (NSRCs): Approach under discussion

2023 Nobel Prize Recipients Supported by Basic Energy Sciences

Nobel Prize in Chemistry 2023

“For the Discovery and Synthesis of Quantum Dots”



Mounji G. Bawendi (MIT)



Louis E. Brus (Columbia U.)



Aleksey Yekimov (Nanocrystals Tech., Inc.)

BES supported the research of Prof. Brus (photochemistry of carbon nanotubes, graphene, and nanoparticles) and Prof. Bawendi (quantum dot heterostructures, quantum optical materials) for twenty-five years, including through the Energy Frontier Research Center for Excitonics (Bawendi).

Nobel Prize in Physics 2023

“for experimental methods that generate attosecond pulses of light for the study of electron dynamics in matter”



Pierre Agostini (Ohio State U.)



Ferenc Krausz (MPI of Quantum Optics; LMU München)



Anne L'Huillier (Lund U.)

BES supported Prof. Agostini (correlated electron dynamics using attosecond pulses), including research at the Linac Coherent Light Source (right), where current capabilities were enabled by the Nobel-honored work.



FY 2023 Selected Scientific Accomplishments

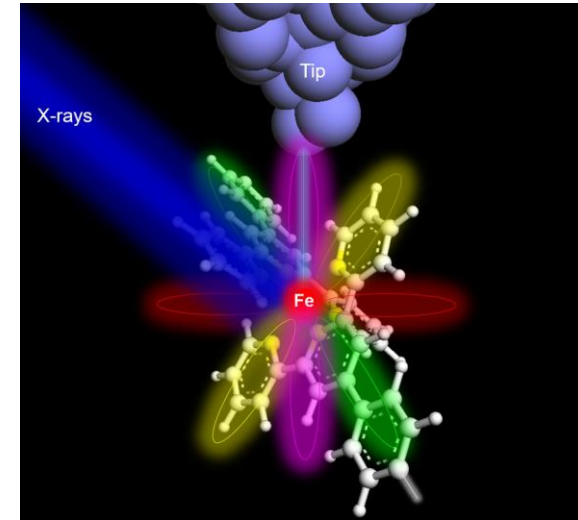


Rapidly accelerating materials discovery and synthesis with AI and automation

Using AI-guided robots and data available from the Materials Project and Google's DeepMind, researchers produced 41 new compounds out of 58 attempts over 17 days – a rate of more than 2 new materials per day.

Source: LBNL and Google

Ref.: [Nature, 624, 86–91 \(2023\)](#)



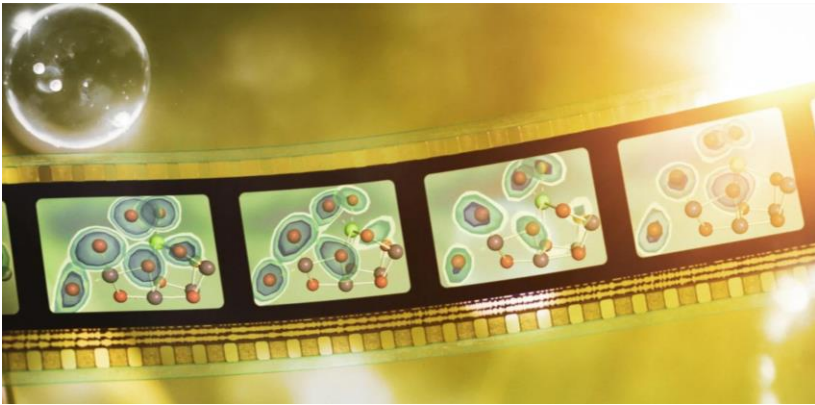
Characterization of a single atom with a novel X-ray synchrotron technique

The elemental type and chemical properties of a single atom (Fe, Tb) were measured for the first time using a novel beamline combining X-rays from APS with a scanning tunneling microscope.

Source: Ohio U., ANL, USF, U. Strasbourg, Inst. le Bel, Shenzhen U.

Ref.: [Nature, 618, 69–73 \(2023\)](#)

FY 2023 Selected Scientific Accomplishments

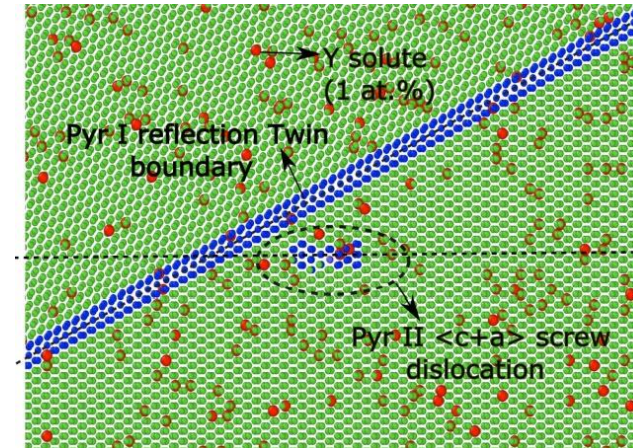


Closing the loop on photosystem II (PS II)

The room temperature structure of the final step in light-driven oxidation of water to oxygen by PS II was finally determined using two X-ray Free Electron Lasers. The result is the culmination of more than a decade of work on this complex biological reaction.

Source: SLAC, LBNL, U. Wisconsin (U.S.); Humboldt U. (Germany); Uppsala U. (Sweden); SACLA (Japan)

Ref.: [Nature 617, 629–636 \(2023\)](#)



Gordon Bell Prize: Simulating Materials at Scale with Quantum Accuracy

The 2023 ACM Gordon Bell Prize was awarded for breakthrough simulations of materials at large-scale with quantum accuracy, demonstrating a massive parallel electronic structure calculation of interacting defects in a material using Frontier, DOE's first exascale computer.

Source: U. Michigan, Indian Inst. of Sci. Bangalore, ORNL

Ref.: [Proc. of the Int. Conf. for High Performance Computing, Networking, Storage, and Analysis, Nov. 2023, 1-12.](#)

Awards Funded Late in FY 2023

- ◆ **Early Career Research Program:** Supporting development of individual research programs for outstanding scientists early in their career across all BES core research areas and facilities operations – BES supported 45 5-year awards (incl. 4 with the DOE EPSCoR program) totaling ~\$56M at 32 universities and 8 DOE labs representing 22 states.
- ◆ **Broadening Participation:** \$140M across SC programs
 - **RENEW:** Leveraging SC's national labs and user facilities to provide internships for students at academic institutions currently underrepresented in the portfolio; BES supported six 3-year awards, ~\$13M (including ~\$2M co-funding by OE)
 - **FAIR:** Research support at non-R1 MSIs and ERIs, incl. DOE lab and facility and R1 MSI partnering; BES supported 28 3-year awards, ~\$20M
 - **EPSCoR:** Promoting institutional diversity and enhancing energy science research capabilities at institutions in eligible jurisdictions; 14 implementation awards, 2-year awards totaling \$33M

Awards Funded Late in FY 2023: National Lab funding opportunities

- ◆ **Accelerate:** (Cross-SC) Research to enhance the science foundation needed accelerate the transition of discoveries to technologies; 11 2-year awards to teams led by 9 DOE labs totaling \$73M
- ◆ **Biopreparedness Research Virtual Environment:** (ASCR, BES, BER) Developing analytical capabilities foundational to future emergency response at DOE's laboratories; 10 3-year awards to teams led by 6 DOE labs totaling \$113M
- ◆ **Scientific Computing for BES User Facilities:** (ASCR, BES) Developing advanced algorithms and software stacks for new and emerging techniques at DOE light and neutron user facilities to enable on-the fly data analysis and autonomous experimentation; 3 4-year awards to teams led by 3 DOE labs totaling \$30M

SC Energy Earthshots FY 2023 Funded Award Announcements (BES, BER, ASCR)

- ◆ SC announced 29 awards totaling ~\$264M for 3- to 4-year awards under the SC Energy Earthshots Initiative that address key scientific challenges that underpin the stretch goals for the first 6 DOE Energy Earthshots.
 - Closely coordinated with the Energy Technology Offices.
- ◆ BES awards supported 8 Energy Earthshot Research Centers (EERCs).
 - Large multi-investigator, multi-disciplinary, and multi-institution (academic, national lab, industrial) teams to advance foundational knowledge and enabling capabilities to address Earthshot goals.
- ◆ BES supported 9 foundational science, small group awards.
 - Focus on use-inspired fundamental research to address knowledge gaps that limit achievement of the Energy 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

FY 2024 BES Funding Opportunities – Released and Pending

- ◆ **Annual Open Solicitation:** Supports grants for research in the topical areas supported by the Office of Science. **Accepts applications continuously. Released**
- ◆ **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.
- ◆ **Energy Frontier Research Centers:** Supports multi-disciplinary, multi-institutional centers to enable transformative advances in energy-relevant basic science. FY 2024 competition will re-compete four-year awards from FY 2020, emphasizing DOE-priority topic areas, including QIS, microelectronics, transformative manufacturing, and environmental management.
- ◆ **Computational Materials Sciences:** Computational codes and associated databases for the design of materials with advanced functionalities. FY 2024 competition will re-compete funding associated with previous awards and will prioritize research with software from the Exascale Computing Project.
- ◆ **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).

Established Program to Stimulate Competitive Research (EPSCoR)

◆ The DOE EPSCoR Program seeks to:

- Promote institutional diversity and enhance the research capabilities in EPSCoR jurisdictions
- Support competitive early-stage research in DOE science/technology areas
- Develop science/engineering personnel to meet current/future needs in DOE-related topics

◆ Coordination Across DOE – Office of Science and Technology Offices

◆ FY 2024 FOA announced December 8, 2023 (DE-FOA-0003201)

<https://science.osti.gov/-/media/grants/pdf/foas/2024/DE-FOA-0003201.pdf>

- EPSCoR institutional partnerships with DOE National Laboratories (State-Lab Partnerships)
- FOA Webinar – **December 18, 3-4pm EST**; Registration required:
https://science-doe.zoomgov.com/webinar/register/WN_nEE-wilaS_KEOUMSzyRcCg#/registration
- Pre-application due date: **January 17, 2024**, at 5:00 PM Eastern Time
 - Pre-applications are required and must be submitted to PAMS by an authorized institutional representative
 - Each institution limited to two submissions per program area listed in the FOA
- Application due date: **February 28, 2024**, at 11:59 PM Eastern Time

FY 2024 Budget Request – Status

- ◆ **FY 2024 Request: \$2,693M (+\$159M or 6.3% above FY 2023 Enacted)**
 - Continued investments in discovery science and research for clean energy (+\$31M above FY 2023)
 - Establish Microelectronics Science Research Centers (+\$25M) – CHIPS and Science Act
 - Operations of 12 facilities supported at ~90% of funding required for re-baselined, normal operations (\$1,228.2M, an increase of \$159M)
 - Construction: 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)
- ◆ **House Mark (June 14): \$2,587M** (-\$105.8M or 3.9% below FY 2024 Request and +\$53.1M or 2.1% above FY 2023 Appropriation).
- ◆ **Senate Mark (July 20): \$2,679M** (-\$13.5M or 0.5% below FY 2024 Request and +\$145.4M or 5.7% above FY 2023 Appropriation).
- ◆ **Under Continuing Resolution (CR) until January 19....**

Strategic Planning Update – Basic Research Needs Workshops

- ◆ Thank you for the input on possible topics for BES workshops for strategic planning.
- ◆ Initial priority topics under consideration for BES Basic Research Needs workshops:
 - Basic Research Needs for AI/ML in Materials Sciences and Chemistry
 - Basic Research Needs for Fabrication of Next-Generation Microelectronics and Quantum Systems
 - Basic Research Needs for Bioinspired Chemical and Materials Sciences for Sustainable Energy and Products
- ◆ Possible topics for Roundtables:
 - Science Foundations for Critical Materials Sustainability
 - Advancing Subsurface Science for Energy

Questions?

