BASIC ENERGY SCIENCES ADVISORY COMMITTEE
to the
U.S. DEPARTMENT OF ENERGY

PUBLIC MEETING MINUTES
September 24-25, 2024

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Hybrid Meeting

Hilton Washington, DC/Rockville Hotel and Executive Meeting Center
1750 Rockville Pike, Rockville, MD

DEPARTMENT OF ENERGY BASIC ENERGY SCIENCES ADVISORY COMMITTEE
SUMMARY OF HYBRID MEETING

The U.S. Department of Energy (DOE) Office of Science (SC) Basic Energy Sciences Advisory Committee (BESAC) convened a hybrid meeting on Tuesday and Wednesday, September 24-25, 2024, via Zoom and at the Hilton Washington, DC/Rockville Hotel and Executive Meeting Center, 1750 Rockville Pike, Rockville, MD. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act (FACA). Visit https://science.osti.gov/bes/besac for more information about BESAC.

BESAC Members Present:

Cynthia Friend, Chair, The Kavli Foundation
Esther Takeuchi, Vice Chair, Stony Brook University; Brookhaven National Laboratory (BNL)
Yohannes Abate, University of Georgia
John Allison, University of Michigan
Ken Andersen, Institut Laue-Langevin
Stacey Bent, Stanford University
Joseph Berry, National Renewable Energy Laboratory (NREL); University of Colorado, Boulder
Jennifer Brodbelt, University of Texas, Austin
Donna Chen, University of South Carolina
Lin Chen, Argonne National Laboratory (ANL); Northwestern University
Valentino Cooper, Oak Ridge National Laboratory (ORNL)
Theda Daniels-Race, Louisiana State University
Abhaya Datye, University of New Mexico
James (Jim) De Yoreo, Pacific Northwest National Laboratory (PNNL); University of Washington
Tabbetha Dobbins, Rowan University
Thomas Epps, University of Delaware
Jeanette (Jamie) Garcia, International Business Machines (IBM)
J. Murray Gibson, Florida Agricultural and Mechanical (A&M) University-Florida State University (FAMU-FSU)
Padmaja (Paddy) Guggilla, Alabama A&M University
Javier Guzman, ExxonMobil
Sossina Haile, Northwestern University
Ashfia Huq, Sandia National Laboratories (SNL)
Lia Krusin-Elbaum, The City College of New York-The City University of New York (CCNY-CUNY)
Surya Mallapragada, Iowa State University; Ames National Laboratory
Nadya Mason, University of Chicago
Gabriel Montaño, Northern Arizona University
Abbas Ourmazd, University of Wisconsin, Milwaukee
Jose Rodriguez, BNL
Jinke Tang, University of Wyoming
Matthew Tirrell, University of Chicago; ANL

BESAC Members Absent:

Serena DeBeer, Max Planck Institute
Laura Gagliardi, University of Chicago
Daniel Resasco, University of Oklahoma
Rachel Segalman, University of California, Santa Barbara

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Designated Federal Officer:
Andrew Schwartz, Acting Associate Director, Office of Basic Energy Sciences (BES); Director, Materials Sciences and Engineering (MSE) Division; Acting Director, Scientific User Facilities (SUF) Division

BES Management Participants:
Gail McLean, Director, Chemical Sciences, Geosciences, and Biosciences (CSGB) Division; Acting Director, Collaborative Research Division
Adam Kinney, Senior Technical Advisor, BES

BESAC Committee Manager:
Kerry Hochberger, Management and Program Analyst, BES

Office of Science Leadership:
Harriet Kung, Acting Director; Deputy Director for Science Programs

Invited Speakers:
Amy Clarke, Scientist, Los Alamos National Laboratory (LANL); Professor, Colorado School of Mines
Michael Cooke, Senior Technical Advisor, Office of the Deputy Director for Science Programs (DDSP)
Paul Dauenhauer, Professor, University of Minnesota; Director, Center for Programmable Energy Catalysis (CPEC)
Helena Fu, Director, Office of Critical and Emerging Technologies (CET), DOE
Oliver Gessner, Senior Scientist, LBNL
Alexander (Alex) Hexemer, Senior Scientist, LBNL
Johnpierre Paglione, Professor, University of Maryland; Director, Maryland Quantum Materials Center
Gabriela Schlau-Cohen, Professor, Massachusetts Institute of Technology (MIT)
Jenny Yang, Professor, University of California, Irvine

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Tuesday, September 24, 2024

Friend (BESAC Chair) called the meeting to order at 10:00 a.m. Eastern Time (ET) to a combined in-person and virtual audience of approximately 236 people and asked BESAC members to introduce themselves.

DOE Office of Science Update, Harriet Kung, Acting Director, SC

Kung presented SC staffing updates; starting in early October 2024, Sarah Staton will serve as the new Director of the Office of International Activities, Research Security, and Interagency Coordination (IRIC). Christopher Landers will serve as the new Director of the Office of Isotope Research & Development and Production (IRDP).

The SC FY 2025 budget request of ~$8.58B represents an increase of ~$343M (4.2%) over the FY 2024 appropriation. This increased funding targets the high priority areas of Artificial Intelligence (AI) (+$93M over FY24; $259M); Fusion Innovation Research Engine (FIRE) Collaboratives (+$15M; $60M); Reaching a New Energy Sciences Workforce (RENEW) (+$69M; $120M); Funding for Accelerated, Inclusive Research (FAIR) (+$32M; $64M); Microelectronics (+$22M; $95M); and SC Energy Earthshots (+$95M; $115M). Furthermore, a new Climate Initiative ($20M) seeks to augment the successful Urban Integrated Field Laboratories (IFLs), launched several years ago by the Biological and Environmental Research (BER) program, by broadening the program's scope to address rural areas across the U.S.

Regarding SC-stewarded national laboratories, the FY 2025 budget request aims to upgrade core lab infrastructure (*i.e.*, utilities and lab workspaces) through ongoing Scientific Laboratory Infrastructure (SLI) projects and General Plant Projects (+$32M over FY 2024; $50M); reduce the backlog of deferred maintenance and improve obsolete infrastructure; and continue the Laboratory Operations Apprentice Program (+$2M; $5M). The FY 2025 budget request will support facilities at ~88.3% optimal operation and will continue to support ongoing scientific user facility upgrade construction and infrastructure projects.

The FY 2025 House Energy and Water Development Appropriations Act (House mark) funds SC at ~$8.39B, which is $150M over the FY 2024 enacted budget and $193M below the FY 2025 SC request. The FY 2025 House mark supports Quantum Information Science (QIS) research at $245M, with $15M in support of the Quantum User Expansion for Science and Technology (QUEST) program and $20M for testbeds to integrate high-performance computing (HPC) and QIS, consistent with the FY 2025 SC request. Additionally, the FY 2025 House mark funds $20M for Energy Earthshots ($95M below request) and $40M for FIRE Collaboratives ($20M below request), as well as supports the expansion of microelectronics research, including the Microelectronics Science Research Centers (MSRCs), and directs the establishment of a Carbon Sequestration Research and Geologic Computational Science Initiative. Lastly, the FY 2025 House mark provides no funding for the Reaching a New Energy Sciences Workforce (RENEW) and Funding for Accelerated, Inclusive Research (FAIR) initiatives, but funds most construction projects at or near the SC request.

The FY 2025 Senate Energy and Water Development Appropriation Act (Senate mark) funds SC at ~$8.60B, which is $360M over the FY 2024 enacted budget and $17M over the FY 2025 SC request. The FY 2025 Senate mark supports Artificial Intelligence/Machine Learning (AI/ML) at $160M, with $100M for the Frontiers in Artificial Intelligence for Science, Security and Technology (FASST) initiative, consistent with the FY 2025 SC request. The FY 2025 Senate mark funds $265M for QIS research, including five National QIS Research Centers

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($15M below request); $60M for Energy Earthshots ($55M below request); $110M for microelectronics ($15M above request); $45M for Fusion Innovation Research Engine (FIRE) Collaboratives ($15M below request); $25M to the aforementioned Carbon Sequestration Research and Geologic Computational Science Initiative; and $10M for atmospheric methane removal research. Lastly, the FY 2025 Senate mark supports the RENEW and FAIR initiatives and funds most construction projects at or near the SC request.

Research security at DOE is an evolving landscape, with a long history in safeguarding and stewarding highly sensitive information. Risk is at the core of the Department's Office of Research, Technology, and Economic Security (RTES), including the development of policies and their implementation. Given DOE's broad mission space, RTES needs to address a wide range of risk levels. DOE and the national labs must cooperate to continue to attract and retain the best and brightest talent, as well as to promote principled international collaborations that: (1) are built upon openness, transparency, parity of intellectual and financial contributions, and mutual respect of intellectual property (IP) rights; (2) are driven by scientist-to-scientist ties and scientific community interest; and (3) advance U.S. competitiveness and discovery of the "best science." The SC is working closely with RTES in the development and implementation of research security policies and procedures.

Regarding the evolution of RTES, in 2016, early working groups were established to safeguard intellectual property and prevent foreign influence, focusing on DOE national labs. In 2019, a DOE policy was established to prohibit participation in foreign talent programs, but the restrictions only applied to federal employees and DOE lab contractors. In 2019, the Science and Technology (S&T) Risk Matrix was also developed and issued. In January 2021, National Security Presidential Memorandum 33 (NSPM-33) established national security policy for U.S. government-supported R&D and served as a foundation for research security policy. In January 2022, the NSPM-33 Implementation Guidance was established, followed by the creation of the Department-wide RTES Policy Working Group (PWG). PWG currently functions to address RTES policy development and consistency with interagency processes, including financial assistance (FA) and laboratory policies.

In 2023, the RTES office was established to provide consistency and support for due diligence reviews and risk mitigation in DOE FA and loan activities. Specifically, the RTES office functions in three main areas: (1) Due Diligence, Liaison, & Assessment; (2) Internal Information Sharing; and (3) External Communications & Outreach. Due diligence review consists of three phases. First, the RTES office will review Funding Opportunity Announcements (FOAs) prior to their release to ensure proper language and allow the community to understand the role of due diligence review in the solicitation process. Second, after a proposal has completed peer review, it is reviewed by the RTES office for potential risk factors and risk mitigation. Third, throughout the life cycle of projects, additional risk mitigation may be warranted if changes occur in foreign access.

The RTES PWG is in the process of updating DOE FA policies, recently discussing the adoption of a single common National Science Foundation (NSF)-stewarded disclosure form across agencies, as well as releasing a Conflict of Interest (COI)/Conflict of Commitment (COC) Notice of Proposed Rulemaking (NOPR) in the Federal Register, which closed on August 19, 2024. SC is working closely with the RTES Office to ensure due diligence reviews maintain transparency and do not create undue burden on the community. SC continues to recommend to the community universal disclosure of sources of support, positions, and appointments, as well as the use of the Science Experts Network Curriculum Vitae (SciENcv) to reduce administrative

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burden through the adoption of persistent identifiers (PIDs). SC has announced the acceptance of interagency common formats for current and pending support and bio-sketches. SC supports recent actions emerging from interagency partners, such as the Department of Defense (DoD) and National Institutes of Health (NIH) Decision Matrices, the NSF Trusted Research Using Safeguards and Transparency (TRUST) Framework, and the continued development of the NSF Safeguarding the Entire Community of the U.S. Research Ecosystem (SECURE) Center.

The DOE uses the S&T Risk Matrix to manage risks at national labs associated with critical and emerging technologies that otherwise do not have control mechanisms. The Risk Matrix only applies to countries of concern (*e.g.*, China, Russia, Iran, North Korea) and to the guidance and management of certain activities at national labs (*e.g.*, foreign engagements, official travel, foreign national access). The Risk Matrix is divided into three categories: Green (emerging technology topics with no sensitivities to economic or national security); Yellow (emerging technology topics with potential for sensitivities, potentially requiring additional protective measures); and Red (economic or national security sensitive technology topics requiring additional protective measures). The DOE updated the Risk Matrix in 2023 and will continue annual updates to ensure consistency with scientific and technological developments. An unlimited distribution S&T Risk Matrix has been developed and disseminated to the national labs, university partners, and sister science funding agencies. In addition, the DOE is working to update implementing orders related to RTES policy to meet statutory requirements.

Regarding interagency and community engagement, the DOE must coordinate its research security policy with partners, as well as increase public-facing engagements with leaders and membership of organizations such as the Federal Demonstration Partnership (FDP), the Council on Governmental Relations (COGR), the Association of American Universities (AAU), the Association of Public & Land-Grant Universities (APLU), and the Asian American and Native Hawaiian/Pacific Islander (AANHPI) research community.

Discussion

Dobbins asked whether the RTES policy will include explicit statements to show support for and protection of foreign researchers working in the U.S. who originate from the sensitive countries of risk, as a way to ensure RTES is not targeting foreigners. **Kung** replied the RTES policy and approach process is not directed at individuals, but rather portfolios. The RTES office seeks to avoid singling out or compromising individuals with potential foreign connections. Although it is uncertain whether such language has explicitly been included in the RTES policy, the general principle will be captured. The RTES office has not yet released a public-facing document but will soon release something akin to the DoD and NIH decision matrices. SC will not support any form of bias against individuals, regardless of their country of origin.

De Yoreo asked whether the source of expertise and the overall process that informed the determination of green, yellow, and red categories in the S&T Risk Matrix would be made available in a public document. **Kung** responded that the Risk Matrix was developed and finetuned through workshops with the S&T deputy lab directors from the DOE national labs and various subject matter experts (SMEs). National labs vet the green, yellow, and red categories of the Risk Matrix. Each national lab should ensure discussions are held among the effective individuals and research projects, so no confusion exists over how the Risk Matrix was developed. The Risk Matrix is not a prohibition but rather a tool to identify topics where additional vetting is required to ensure certain engagements are appropriate to move forward.

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Guzman inquired whether the budget dollars presented for FY 2024 and FY 2025 have been adjusted for inflation. While the budget appears to have increased for FY 2025, due to inflation, its actual value might be lower than the FY 2024 budget. **Kung** replied budget dollars were not adjusted for inflation; there is decreasing purchasing power. With the current debt ceiling, it was difficult to achieve the small budget increase for FY 2025, which is the result of heroic efforts from advocacy groups within the community and BESAC. Advocacy for the importance of robust growth in science must continue, particularly within our globally competitive landscape.

Haile inquired whether the RTES policy applies to all of DOE or just BES. Further, does DOE, through the RTES policy, have the power to remove foreign individuals from DOE-funded projects at any time or for any reason, without input from the PI? This was recently experienced with an award. **Kung** responded that the RTES policy applies across DOE and to all six science programs in the SC. All FOAs must undergo the three phases of review; this also applies to other DOE programs. Haile's award experience is not consistent with RTES policy and implementation. The forthcoming decision matrices will provide finalized implementation processes, including risk mitigation strategies. The BES leadership team is committed to providing as much clarity and support as needed; the community is advised to reach out to SC if questionable actions, directions, or information are experienced.

Daniels-Race wondered how restrictive the RENEW and FAIR programs are with respect to gender and race/ethnicity in the context of outreach. **Kung** replied that the goal for RENEW and FAIR is to broaden overall participation; awardees are not selected based on gender or race/ethnicity. The programs do not restrict specific demographic groups and aim to generate a diverse and inclusive group of awardees.

Mason was surprised the Energy Earthshots initiative seemed to fare poorly in both the House and Senate marks, while other initiatives such as QIS garnered greater support, and wondered how this trend may impact future DOE priorities. **Kung** replied that Earthshots is a Department-wide initiative with topical areas already embedded in BES research. One potential solution is institutionalizing the goals of Earthshots without creating a separate initiative that would otherwise be vulnerable in this funding climate.

Office of Basic Energy Sciences Update, Andrew Schwartz, Acting Associate Director, BES; Gail McLean, CSGB Division Director, BES

Schwartz presented BES staffing updates and current vacancies.

In Spring 2023, a fourth Division was established within BES, known as the Collaborative Research Division. The Division supports multidisciplinary, multi-institutional team research, such as the Energy Frontier Research Centers (EFRCs), the Energy Innovation Hub programs, and the Energy Earthshot Research Centers (EERCs), as well as cross-SC diversity and technology coordination activities through EPSCoR, RENEW, and FAIR.

The Director position for the Collaborative Research Division is vacant and will soon be officially posted, with a request for nominations ongoing until October 4, 2024. The Collaborative Research Division Director will be responsible for overall division management, including strategic planning; budget formulation and execution; program integration with SC activities and other DOE offices; interagency and international liaison; and management of the Division staff.

Regarding FY 2024 BES funding outcomes, the EPSCoR-State/National Laboratory Partnerships awards support collaborations between EPSCoR-eligible institutions and DOE

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national labs on fundamental, early-stage energy science research. The awards were announced on August 22, 2024, with $36M for 39 awards. The Computational Materials Sciences–Exploratory Research at the Exascale program focuses on computational codes and associated databases for materials design with advanced functionalities. The awards were announced on August 28, 2024, with $14M for 4 awards. The EFRC program supports multidisciplinary, multi-institutional centers to enable transformative advances in energy-relevant basic science. The FY 2024 solicitation emphasized QIS, microelectronics, transformative manufacturing, and environmental management. Awards were announced on September 4, 2024, with $118M for 10 centers. The Early Career Research Program (ECRP) was started in 2010 to fund early-career scientists in SC-supported research areas. Awards were announced on September 10, 2024, with $58M for 46 BES awards. Lastly, the RENEW and FAIR programs support efforts to broaden participation through training opportunities that leverage the DOE complex and direct research support at non-Research 1 (R1) Minority-Serving Institutions (MSIs) and Emerging Research Institutions (ERIs). Proposals are under review and award announcements are anticipated in early FY 2025.

Regarding upcoming awards, the annual open solicitation accepts applications continuously, providing research grants for all topical areas supported by the SC. The Batteries and Energy Storage Hub Awards were announced in September 2024 and include the Energy Storage Research Alliance (ESRA) and the Aqueous Battery Consortium (ABC). The ESRA is led by ANL and seeks to establish the scientific foundation to achieve unprecedented molecular-level control of reactivity, ion selectivity, and directional transport for long-duration grid storage and heavy-duty transportation. The ABC is led by Stanford University and seeks to establish the scientific foundation for large-scale deployment of aqueous earth-abundant (Zinc, Iron, Manganese) batteries for long-duration energy storage for the grid. Both the ESRA and ABC have five-year budgets of up to $62.5M (pending appropriations).

The MSRCs were authorized in the Creating Helpful Incentives to Produce Semiconductors (CHIPS) and Science Act of 2022. Each MSRC will comprised of several multi-disciplinary team awards with support from across the SC that will perform mission-driven research to address foundational challenges in the design, development, characterization, prototyping, demonstration, and fabrication of microelectronics. A lab call was released on May 8, 2024, and awards will be announced in early FY 2025.

The EPSCoR Implementation Program seeks to enhance S&T capabilities of designated jurisdictions to conduct nationally competitive research relevant to DOE's missions, as well as to promote geographic and institutional diversity, such as the training of scientists and engineers in geographically underserved jurisdictions. In FY 2025, the EPSCoR Implementation Program will award a total of ≤$35M, pending appropriation, with $25M allocated for BES. As a program coordinated across DOE, participating offices match ~10% of award funds. The EPSCoR FOA was issued on September 12, 2024.

The Energy Earthshots Initiative funds fundamental research to accelerate breakthroughs in more abundant, affordable, and reliable clean energy solutions. The first Earthshots awards were announced in FY 2023 and established the Energy Earthshot Research Centers (EERCs). Led by the national labs, the EERCs are multidisciplinary, multi-investigator teams that aim to advance foundational knowledge and state-of-the-art capabilities in the experimental, theoretical, and computational sciences, closely coordinating with the energy technology offices. The Science Summit for Energy Earthshot Innovation was held on September 4-5, 2024 and served as an opportunity for teams funded through BES, the Advanced Scientific Computing Research

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(ASCR) program, and the BER program to discuss foundational research needed to support the DOE Energy Earthshot portfolio. Over 200 attendees participated in plenary talks, poster sessions, and breakout discussions.

Regarding project updates and major milestones of the user facilities, the Advanced Photon Source Upgrade (APS-U) at ANL completed installation of the new multi-bend achromat storage ring in March 2024, achieving first light in June 2024 and a return of users in July 2024. Beamline installation and commissioning is ongoing. The Proton Power Upgrade for the Spallation Neutron Source (SNS) at ORNL delivered neutrons for the user program in July 2024 and is operating at 1.7 megawatts (MW) and 1.3 gigaelectron volts (GeV). Planning is underway for the Critical Decision (CD)-4 review in January 2025, with an early project finish expected in April 2025. The Linac Coherent Light Source II–High Energy (LCLS-II-HE) project at the SLAC National Accelerator Laboratory achieved a combined CD-2/3 approval for the start of installation on September 18, 2024. The Nanoscale Science Research Centers (NSRC) recapitalization project, which is taking place across the five labs hosting NSRCs, have issued 16 of the 18 total instrument awards. Five instruments have been delivered to date, of which with two installed. Finally, the National Synchrotron Light Source (NSLS)-II Experimental Tools-III (NEXT-III) project, which will see the development and installation of up to 12 new beamlines at BNL, achieved CD-1 approval on September 13, 2024.

The FY 2025 BES budget request of ~$2.58B is 1.65% (-$43.3M) less than the FY 2024 enacted budget. Under the FY 2025 budget request, research program funding decreased by $18.1M, SUF funding increased by $81.4M, and construction and MIE funding decreased by $106.6M. Within research programs, there is increased funding for clean energy and critical materials; microelectronics and the MSRCs; FAIR and RENEW (+$13M); Energy Earthshots (+$45M); and AI/ML (+$8M). Meanwhile, funding is unchanged for the EFRCs, the National Quantum Information Science Research Centers (NQISRCs), the Computational Materials and Chemical Sciences (CMS/CCS) programs, the Fuels from Sunlight Energy Innovation Hub program, the Batteries and Energy Storage Energy Innovation Hub program, and EPSCoR.

The 12 BES facilities are supported at 90% of optimal operations (~$1.3B). In the SUF portion of the budget, funding for facilities research ($60.9M) includes increased funding for AI/ML (+$9M) and continued investment in accelerators and detectors, the Biopreparedness Research Virtual Environment (BRaVE) initiative, and preliminary planning for future MIEs. Funding for construction includes $100M for the LCLS-II-HE project, $52M for the Second Target Station (STS) project, $20M for the Cryomodule Repair and Maintenance Facility (CRMF) project, $11M for the High Flux Isotope Reactor (HFIR) Pressure Vessel Replacement project, and $10M for the NEXT-III project. No MIEs are included in the FY 2025 budget request. During each FY from FY 2023-2025, BES has maintained a budgetary balance of at least 40% of funding allocated to research and approximately 60% allocated to facility operations and projects. In total, the FY 2025 budget request allocates a 60% increase (+$17.4M) for AI/ML above the FY 2024 enacted budget. This funding is split between AI for Science and AI for User Facilities.

Compared to the FY 2025 BES budget request, the House mark ($2.62B) is 1.3% above (+$34.3M) the FY 2025 request and 0.3% below (-$9M) the FY 2024 appropriation. The Senate mark ($2.56B) is 0.8% below (-$19.8M) the FY 2025 request and 2.4% below (-$63.1M) the FY 2024 appropriation, including $100M for AI across SC. Compared to the FY 2025 BES budget requests for research ($1.08B), facility operations ($1.32B), and projects ($183.5M), the House and Senate marks present decreased funding for research ($1.07B and $1B, respectively),

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increased funding for facility operations ($1.37B and $1.38B, respectively), and equivalent funding for projects ($183.5M).

The DOE SC Roundtables on Transformational Science Enabled by AI will take place on October 28-31 and November 7-8, 2024. The roundtables complement the focus of the ASCR program's AI workshops and will identify Priority Research Opportunities (PROs) to use AI to address the challenges faced within six scientific categories, all of which BES takes part in: (1) high energy & nuclear physics; (2) biosciences & environmental sciences; (3) materials & chemical sciences; (4) fabrication science; (5) fundamental energy research; and (6) user facility science and operations. A public report will be created from each roundtable.

Starting in September 2024, instead of the individual program offices hosting separate office hours, the SC will transition to hosting a single, comprehensive virtual office hour every month to share information about opportunities and answer questions. The SC office hours are open to all and will focus on a different topic every month, offering breakout discussions for each program office. Annual open solicitations will be the topic of the October 2024 office hour.

Discussion

Epps questioned how uncertainties associated with the Collaborative Research Division will impact staffing plans, full realization of the Division, and the future of initiatives such as Earthshots, RENEW, and FAIR. **Schwartz** replied these initiatives are not restricted to BES and involve interactions across SC. While uncertainty exists and change is expected, the foundational concept of the Division will remain the same. For each initiative, the boundaries between different program offices must be delineated, while advocating for the role of BES.

Bent asked how BES is considering workforce development in the funding strategies for microelectronics. **Schwartz** responded the CHIPS and Science Act has specific appropriations for the Department of Commerce (DOC) and NSF to work jointly on workforce development; research supported by SC will complement the progress in workforce development from DOC and NSF. Although SC has not released specific calls for workforce development, the MSRCs will serve as locations where early-career researchers can learn skills and gain experience. This has been and continues to be communicated between SC, DOC, and NSF.

Abate inquired whether a U.S. map showing the geographical distribution of EFRC awardees was available, akin to the map presented for ECRP awardees. **Schwartz** responded that an EFRC awardee map is available and demonstrates substantial geographic distribution across the country, due to many multi-institutional collaborations. **McLean** commented that the current (not historical) map is on the main EFRC webpage.

Guzman asked how BES plans to balance their funding portfolio, given the addition of new funding opportunities, and whether BES will de-emphasize certain topics by eliminating certain grants or reducing their funding. **Schwartz** responded this is an ongoing challenge within BES, which is one of the reasons for the charge to form the Research Investment Strategies Subcommittee. Programs evolve as program managers gather input from the scientific community and work to maintain alignment with DOE's priorities. Since the same topics are often funded through different modalities, it is important to understand how modalities complement one another. The strength of BES is in providing broad programmatic support to a wide spectrum of topics foundational to society. BES must maintain this strength.

Cooper asked about staffing challenges within BES, in particular, staffing plans for the Collaborative Research Division, given many vacancies in the current BES organizational chart. In the past, EFRCs were supported by program managers from divisions across DOE. **Schwartz**

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responded that staffing vacancies are a challenge, although not unique to BES. The Collaborative Research Division plans to hire a lead role to manage the EFRCs (and likely the EERCs, as well) but will continue to work closely with program managers in other divisions, since scientifically broad and diverse expertise is needed.

Research Investment Strategies Subcommittee Report Out, Cynthia Friend, BESAC Chair and Subcommittee Moderator; Esther Takeuchi, Professor, Stony Brook University, and Subcommittee Chair; Marc Kastner, Professor Emeritus, MIT, and Subcommittee Vice Chair

Takeuchi remarked that BESAC was charged to form a subcommittee in 2024 to follow up on the 2021 International Benchmarking Study Report and advise on strategies for prioritizing BES research investments. The subcommittee members are comprised of a mix of current and former BESAC members, as well as individuals from academia, national labs, and industry.

With respect to investments, the subcommittee considered how BES should (1) determine low vs. high priority of topical areas; (2) identify new topical areas; (3) identify and foster cross-cutting areas in the face of converging disciplines; (4) balance research and instrumentation support for national labs and universities; (5) balance research modalities (*e.g.*, team research versus single-investigator); (6) enable innovations to cross the "Valley of Death"; (7) delineate the boundary between basic and applied sciences; and (8) reckon with international competition, all while ensuring diversity and inclusion.

To meet the charge, the subcommittee compiled, analyzed, and discussed prior reports from other organizations relevant to the assessment of research portfolios, as well as discussed current approaches used across DOE. Four subgroups were established to address four distinct topic areas: (1) desired outcomes of the study; (2) opportunities to enhance research portfolio selection; (3) research assessment, provided through a summary of the existing literature; and (4) portfolio analysis via a case study.

The first subgroup determined six desired outcomes of the study to be: (1) BES strengthens investments to maintain and advance scientific knowledge and international competitiveness; (2) BES is nimble in investing and disinvesting in topical research areas; (3) BES optimizes balance in its portfolio; (4) BES addresses increasing costs of research; (5) BES has use-inspired tools for insight into evaluating basic research; and (6) BES has effective approaches for investing in and prioritizing workforce-enhancing measures relative to research, instrumentation, and facilities.

The second subgroup identified several opportunities to enhance research portfolio selection. First, BES may utilize big data analysis and ML to understand portfolio impact. Second, BES should remain inclusive of industry researchers throughout its efforts to convene the community across constituencies. Third, BES should better understand how and why various basic R&D activities have impacted U.S. industry, through potentially partnering with publishers. Lastly, BES should continue to broaden community engagement.

The third subgroup structured recommendations for research assessment into three components. First, quantitative metrics (*e.g.*, publication, patent, or citation rates; impact factors) should be normalized by field. Multiple indicators should be combined to provide a comprehensive assessment, but qualitative evidence, expert judgment, and the nuances across different academic fields must also be considered. Second, diverse methodologies, including AI/ML tools, should be considered for portfolio assessment. Currently, the NIH Office of Portfolio Analysis is developing and disseminating a multifaceted assessment approach to analyze portfolios using AI/ML, graph theory, and natural language processing. Portfolio

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analysis may help assess past impact and predict the likelihood of desired outcomes. Regardless, methodologies must use simple, transparent tools and establish clear criteria for research assessment. Third, expert input plays a key role in the assessment of research quality and impact. Expert panels should be comprised of SMEs who can address the gaps inherent in relying solely on quantitative metrics.

The fourth subgroup conducted a case study to understand portfolio analysis by investigating the impact of basic science funding on battery technology (specifically, lithium-ion batteries) and the scientific community at large, considering publications, citations, patents, awards, workforce development, and industry interactions. Multiple dimensions exist in portfolio analysis and must be considered comprehensively, such as the number of publications, citations, and patents. For instance, in recent years, the number of publications and citations on lithium-ion batteries has decreased, as research has not waned, but instead shifted to multiple, alternative battery chemistries. While the U.S. and Japan hold most of the original patents, China dominates in lithium-ion battery cell production. Workforce development and retention incentives are also critical, as are interactions with industry, which play a role in translating fundamental science to usable technology. The U.S. is home to the majority of startups and new companies willing to take risks in inventing new possibilities, thanks to the U.S.'s entrepreneurship core values and increasing support from national labs and universities.

To gain insight into new arenas of science, BES may consider "out of the box" approaches, such as: (1) conducting intermittent analysis to identify new fields pursued by postdoctoral researchers (postdocs); (2) surveying academic department chairs responsible for hiring young faculty members; (3) participating in multiple agency panels; (4) continuing to facilitate collaboration modes across DOE offices; (5) having program managers form small groups to pitch new areas to fund; (6) tracking news and media for emerging areas of interest; (7) using EFRCs to incubate new ideas, such as issuing Requests for Information (RFIs); and (8) leveraging the national labs' Laboratory Directed Research and Development (LDRD) programs for information about new ideas.

Overall, the subcommittee recommends several strategies for successful management of the future research portfolio. First, BES should continue to expand broad engagement with the research community to maintain and enhance technical excellence of the basic energy sciences in line with DOE's mission. In particular, BES engagement with industry may help to identify knowledge gaps or new opportunities. Second, BES should balance the funding portfolio across multiple axes, including support for research vs. facilities, single investigator vs. center or hub funding, and support for existing program areas vs. nascent fields of inquiry. Third, BES should facilitate seamless transitions from fundamental to applied research, which may involve cross-office interactions. Fourth, BES should consider the benefits of investing in and adopting new tools for portfolio analysis, coupling the use of quantitative methods with expert opinion.

Discussion

Kastner acknowledged Al Hammond's career and contributions as a science writer and editor, given the latter's upcoming retirement.

Ourmazd asked for more elaboration on the decision to include the subject of AI/ML in the report, since the subcommittee's earlier discussions were unresolved regarding this inclusion. **Epps** replied that the research assessment subgroup ultimately decided to include AI/ML, not as a specific recommendation, but as a potential opportunity to be appropriately vetted by BES. **D. Chen** expressed approval for the report's approach to addressing AI/ML.

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Andersen did not see the charge included in the report and asked about the intent of the report, specifically the actions that may result. **Schwartz** noted the report distributed to BESAC is not the final version, and that the charge is also available on the BESAC website. **Takeuchi** responded that the final report includes the charge at the beginning. The intent of the report is to provide BES with augmented tools and new approaches to consider for implementation while reinforcing existing successful strategies. The report reinforces the need for a balance of qualitative and quantitative metrics, as well as expert opinion, although focus is on quantitative analysis, given the extensive amount of data available now, which requires tools. As financial pressures continue, balance is critical between exploratory vs. application-inspired science, single-investigator vs. larger center grants, etc.

Tirrell noted the report reinforces BES's focus on use-inspired basic research and the desire to understand where inspiration for fundamental research comes from in more applied areas. **Takeuchi** responded that BES plays a pivotal role in facilitating the transition of ideas to innovation to actionable technologies, so that inspiration does not "die on the vine."

Dobbins praised the report, which dissected a big problem into actionable pieces. Regarding one of the "out of the box" approaches targeting postdoctoral research, postdocs are unsung heroes who are often not part of a larger community outside of their immediate research group. The National Postdoc Appreciation Week (NPAW) is held every third week of September. A large gathering could be held during NPAW for these types of discussions; opinions among postdocs could be documented and fed into a process that could be part of what gets implemented out of this report.

Datye inquired about the desired outcomes of the report in terms of research investment strategies going forward for BES and the U.S. as a whole. **Takeuchi** replied that the challenge stems from the fact that this funding comes from taxpayer dollars. It is insufficient to fund research ideas solely on the basis of scientist interest; there must be compelling, real-world significance. Tradeoffs are inevitable. The work of [Acting Office of Science Director] Harriet Kung and [DOE Undersecretary for Science and Innovation] Geraldine Richmond is crucial.

L. Chen suggested minor modifications to the report including a table of contents and a diagram to link different sections together. In addition, Figure 2 may not be correctly positioned in the report. **Takeuchi** responded the final report includes a table of contents and is nicely formatted. The current report version distributed to BESAC is geared toward review of content only.

Montaño inquired if there is a plan to evaluate LDRD programs and their existing best practices, as mentioned in the "out of the box" approaches, since some national labs have LDRD programs to manage funding of aggressive, exploratory research. Such best practices can be adopted across other national labs as an effective way to manage exploratory ideas. **Takeuchi** responded the "out of the box" approaches do not provide specific recommendations, but rather ideas for BES's consideration. The challenge is to predict which ideas will be useful in the future, which is very difficult.

Dobbins suggested adding dates of the various reports referenced regarding AI/ML into the body of the text or as a footnote in the page. **Takeuchi** agreed, as such documentation referenced in the report may become updated in the future.

Huq commented that the fourth subgroup chose lithium-ion batteries as the topic for their case study to demonstrate a successful example of the impact of research investments. Scientists are custodians of these taxpayer dollars, which can be invested to achieve great benefits for

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society. **Friend** asked if the subgroup considered including examples of failed research investments. **Huq** replied the subgroup discussed this possibility, but decided it was too risky.

Tang remarked the report did not mention any NSF studies in the summary of existing literature. **Takeuchi** responded the subgroup was searching for portfolio assessments rather than individual principal investigator (PI) assessments. If NSF has portfolio assessments, please let the subgroup know. **Friend** reminded BESAC members the goal of this meeting is to discuss the content of the report and asked if aspects of the report warranted more discussion or needed editing.

Haile commented the report lacked a sense of urgency in the context of international competition, particularly the need for the U.S. to advance scientifically. The report needs to highlight the impossibility of the U.S. in maintaining its current rate of scientific advancement without additional investment. Additionally, more guidance would be valuable regarding the desired goals and outcomes of this report. **Takeuchi** responded that a meeting will be held with Kastner, Schwartz, and Friend to discuss and incorporate these comments into the report.

De Yoreo commented the case study on lithium-ion batteries lacked a paragraph retrospectively discussing lessons learned on strategic investment. Rather than evaluating whether a past investment was successful, the report should evaluate the process that led to the successful strategic investment, in this case, understanding the factors that led BES to initially decide to invest heavily in battery research. **Takeuchi** responded that funding was not the spark that initiated the development of lithium batteries. Instead, funding merely facilitated the battery's advancement once research was already initiated by Japan and Sony Corporation. Regarding strategic investment, the main lesson learned is the community cannot be fixated on a single metric such that other opportunities are missed.

Berry noted that the key to successful investment outcomes is convening the community, bringing together the appropriate stakeholders with a diverse, broad range of perspectives to identify how the relevant science may be applied to the real world. This notion was an integral part of the subcommittee's discussions and appears to be captured in the report. If this notion needs to be amplified, then it is of note.

Rodriguez suggested adding a sentence on pages 27-28 of the report to further support workforce development by communicating BES's commitment to coordinate with NSF and other agencies that prioritize undergraduate, graduate, and postdoctoral education and training. Thus far, the report does not mention such education or training. **Takeuchi** responded education is explicitly written into NSF's mission but not DOE's, although workforce development is part of DOE's mission. Coordination with agencies such as NSF is a good way to blend the missions of education and workforce development.

Mason commented the report seemed generic, such that it could be applied to any agency. More details could be added regarding the relevance of the report's recommendations to DOE and BES, as well as highlighting the vision and individuality of DOE and BES. **Takeuchi** replied that these suggestions will be considered.

Tirrell noted the first subgroup examined an NIH study which sought to develop a method to ascertain, at an early stage, the characteristics of research that would lead to real clinical applications. Findings from that study may be applicable to DOE and this report.

Dobbins noted BES has been successfully convening teams to discuss and develop priorities for given topic areas for 20+ years. This foundation makes up the core of DOE and BES. The other ideas in this report serve as extra recommendations to enhance this foundation. **Takeuchi** agreed BES executes many sound practices and is one of the best at gathering

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scientific participation and collecting expert opinions. Other augmentations and tools are worthy of consideration to add to an already solid foundation.

Mallapragada suggested the report could explicitly emphasize DOE's national lab complex as a unique strength not possessed by other agencies.

DOE PUBLIC ACCESS PLAN AND DATA MANAGEMENT PANEL, Adam Kinney, Senior Technical Advisor, BES, and Panel Moderator; Michael Cooke, Senior Technical Advisor, DDSP

Cooke remarked that the Public Access Memorandum was issued in 2013 by the White House Office of Science and Technology Policy (OSTP). The memo stated the results of federally funded scientific research, including peer-reviewed publications and digital research data, should be made publicly available, permitting a one-year embargo of peer-reviewed articles. This memo led to the 2014 DOE Public Access Plan (PAP), which required author submissions to DOE of accepted manuscripts (AMs) for peer-reviewed publications within 12 months of publication. A government-purpose license was used to share manuscripts through DOE's designated repository, DOE Public Access Gateway for Energy & Science (PAGES®), with voluntary participation of publishers. The Data Management Plan (DMP) provided requirements for public sharing of digital research data.

In August 2022, Dr. Alondra Nelson, former Director of the OSTP, released a new memorandum on public access to federally funded research, entitled: "Ensuring Free, Immediate, and Equitable Access to Federally Funded Research." Known as the Nelson Memo, this directive required all federal science agencies, including DOE, to develop new PAPs. The Nelson Memo emphasized use/re-use, machine readability, and equitable access, and required PAPs to provide immediate public access to publications, removing the 12-month embargo; immediate public access to data displayed in or underlying publications; and expanded use of PIDs.

In June 2023, the DOE's new PAP was released. This DOE PAP involved intra-agency coordination across DOE, led by SC. Input was provided through working groups on digital data and Scientific and Technical Information (STI) managers across DOE national labs. Interagency coordination efforts also helped to develop the PAP, through the OSTP Subcommittee on Open Science (SOS) and PID Services partners from 12 agencies. Lastly, external community engagement helped inform the PAP, through professional societies, publishers, and libraries.

According to the new PAP, publications will transition from a 12-month embargo to immediate access upon publication. Authors will continue to submit AMs via E-Link, but earlier, and provide access through DOE PAGES®. The Federal Purpose License allows DOE to provide immediate access to the AMs. Submission of AMs "upon acceptance" is encouraged, rather than "upon publication", and will allow a transition period to adjust workflow process. DOE allows authors to choose between publishing Green Open Access (OA), which is encouraged, or Gold OA. Green OA involves the author publishing their work in a journal or book and then self-archiving a copy in a free, publicly accessible repository. Gold OA involves the author directly publishing in an OA journal or book and may require article processing charges (APCs).

Under the new PAP, Data Management Plans (DMPs) have transitioned into Data Management and Sharing Plans (DMSPs). Scientific data management is founded upon three updated principles: (1) to increase the pace of scientific discovery; (2) to protect integrity and enhance the value of science; and (3) to maximize appropriate data sharing. The DMSP has five

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requirements updated from the DMP: (1) validation and replication of results; (2) timely and equitable access; (3) data repository selection; (4) data management and shared resources; and (5) data sharing limitations. All DOE-funded R&D awards and contracts will be subject to a DOE-approved DMSP and data reporting.

For the DMSP, data repository selection should align with the Desirable Characteristics guidance put forth by the National Science and Technology Council (NSTC) SOS. This guidance improves consistency in instructions to researchers about selecting data repositories and helps ensure research data are findable, accessible, interoperable, and reusable to the greatest extent possible, while integrating privacy, security, and other protections.

PIDs are long-lasting, managed, and registered unique digital references, often in the form of a Uniform Resource Locator (URL), to a research object (*e.g.*, a person, organization, research output, or award) that can be represented or described online. Under the Nelson Memo, metadata associated with publications and data should be collected and include author names, affiliations, and funding, referencing PIDs; metadata should also include the date of publication and a unique digital PID for the research output. PIDs must be used in publishing, when available, and when reporting R&D outputs. PIDs must meet the common standards of a PID service, as defined in the NSPM-33 Implementation Guidance.

Regarding implementation of PIDs, new procedures exist, and interagency discussions continue to be held to discuss options and best practices. Agencies must assign unique digital PIDs to R&D awards and intramural research protocols. Federal and contract employees, as well as FA recipients conducting R&D, must obtain PIDs for themselves. E-Link 2.0, which is tentatively expected to be released in January 2025, will be used to collect and associate authenticated DOE contract and grant numbers with STI reports. This ensures connection from DOE funding identifiers to PIDs for people, organizations, and outputs; options are being explored to assign PIDs to awards. A new organization authority will be used to associate organization PIDs with various organization metadata fields in E-Link 2.0. The DOE Order 241.1C requires PIDs for R&D output records, consistent with current Digital Object Identifier (DOI) practices, and PIDs via Open Researcher and Contributor ID (ORCID) for DOE and DOE-funded authors. FA letters will require recipients to provide PIDs for themselves when reporting to the Office of Scientific and Technical Information (OSTI). The DOE PID working group is a federal integrated project team working on PID implementation strategies and coordinating their approach across DOE, focusing on PIDs for individuals and ensuring implementation of that aspect of the Nelson Memo and NSPM-33.

Regarding the implementation timeline for the 2023 PAP, the DOE must publish its related policies on Section 3: "Publications & Data" by December 31, 2024, which must then become effective by December 31, 2025. Similarly, the DOE must publish its related policies on Section 4: "PIDs to Ensure Research & Scientific Integrity" by December 31, 2026, which must then become effective by December 31, 2027.

Implementation requires a coordinated effort across DOE to update research funding and reporting mechanisms to reflect the new PAP, including updating DOE Orders (*e.g.*, 241.1B), contractor requirements documents, FA guidance, award terms and conditions, reporting requirements, and applicant guidance, among others. Targeted updates include STI reporting requirements and guidance; guidance, requirements, and suggested elements for the DMSPs; and guidance and requirements for researcher PID reporting. The Scientific and Technical Information Program (STIP) focus group will be formed to discuss publisher-related topics, such

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as APCs, OA fees, and Read-and-Publish agreements. Coordination with other federal agencies will continue, including through the OSTP SOS and participation in various working groups.

DOE envisions the Integrated Research Infrastructure (IRI) will serve as a revolutionary ecosystem to deliver seamless, secure interoperability across national lab facilities. The High Performance Data Facility (HPDF) will enable analysis, preservation, and accessibility to the staggering amounts of experimental data produced by SC facilities. A distributed operations model will be essential for long-term success and required performance levels. A hub and spoke architecture will provide seamless, tailored service to users worldwide.

Data Management in the Center for Programmable Energy Catalysis, Paul Dauenhauer, Professor, University of Minnesota

Dauenhauer remarked that the DOE Center for Programmable Energy Catalysis (CPEC), an EFRC, seeks to invent tomorrow's advanced catalysts through integration of the chemical sciences. CPEC is multidisciplinary and integrates expertise in electronic materials, surface science, catalysis, and computational chemistry to invent and understand dynamic, programmable heterogeneous catalysts. Programmable catalysts change with time at the frequency of surface reactions via a prescribed electronic "program" that accelerates and controls reactions. CPEC has created new methods, tools, and techniques for fundamental research, generating an abundance of data.

Regarding short-term data sharing and management, CPEC has several data and organization policies. The CPEC Portal, managed through Google Drive, is a hub comprehensively linking information together, such as the personnel directory, conference presentations, meeting content, manuscripts, references, and project descriptions. Each folder has different access permissions; some are read-only while others are editable. At CPEC, monthly team and all-center meetings are held, in addition to quarterly executive committee meetings. These meetings feature confidentiality policies, safety spot discussions, center updates, and research presentations. CPEC also holds annual Spring and Fall meetings, which serve as combined research, training, education, and strategy sessions.

Regarding long-term data sharing and management, CPEC data is shared through publications and associated methods. Preprints are promoted, and publications are made openly available, with data sets attached within supporting information files. All publications on the CPEC website are provided to OSTI. Simulation codes are shared via the CPEC GitHub site, while large data sets are made available through the CPEC Data Conservancy. Data tracking within the CPEC Portal allows for review and compliance. CPEC promotes the sharing of additional data beyond what is necessary or required, given that internal or external researchers may be able to re-use or re-interpret that data, particularly if inconclusive. CPEC seeks to preserve data, allowing its use internally and externally in the future, and establish strategies to educate students and faculty about data management processes.

The CPEC Chemical Catalysis Database (CatTestHub) is an open database of experimental catalysis data designed for benchmarking catalyst performance. Specifically, CatTestHub houses experimentally measured kinetic, thermodynamic, and characterization information relevant to chemical turnover on catalytic surfaces. CatTestHub is currently under beta testing; CPEC aims to submit the preprint on CatTestHub for peer review in November 2024.

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Office of Science Data Management and Sharing Plan Requirements, Alexander Hexemer, Senior Scientist, LBNL

Hexemer remarked that the recent advancements in BES light sources have led to massive, multimodal volumes of data. In five years, DOE light sources are projected to generate one exabyte of data per year, the analysis of which would require peak computing power of up to one exaflop per second. Thus, there is a pressing need to identify and classify features and patterns across modes; merge simulation and experiment data to drive experiments and new results; and execute experiments dynamically using real-time reduction and AI/ML.

These data and computational challenges are changing the landscape for users and facilities. Given the user community's diversity in scientific backgrounds and domains, expectations vary on the types and scales of computing capabilities and on the services provided by facilities. There is an increasing digital divide within the user community, as currently, few user groups have the ability to manage and process their data. Furthermore, there is increased interest towards open and findable, accessible, interoperable, and reusable data. The role of facilities is unclear, as facilities do not have the infrastructure in place to consistently collect, curate, archive, and disseminate data and metadata at the required scale.

From a SUF perspective, several challenges exist towards making data findable, accessible, interoperable, and reusable. The ontology in each scientific field must be defined precisely and agreed upon to ensure clear communication and data interoperability. Not all experimental metadata is available to user facilities (*e.g.*, material synthesis), and data/metadata of a single study may be spread across multiple facilities. Other challenges include authentication and authorization across facilities, as well as the difficulties in managing and analyzing large data sets; data deletion brings additional implications. However, implementation of findable, accessible, interoperable, and reusable data brings opportunities in data reusability, experimental reproducibility, improved cross-facility collaboration, development and testing of AI/ML models, and seamless integration of data with HPC resources.

The light source community has created data web portals to streamline data management and access across facilities. Data portals are available for the APS at ANL, the Advanced Light Source (ALS) at LBNL, the NSLS-II at BNL, and the LCLS at the SLAC National Accelerator Laboratory. Various data analytics, processing, reconstructions, and workflows are being implemented through a collaborative effort across BES and ASCR program facilities.

Across light sources, high priority computing developments include: (1) data management and workflow tools to integrate beamline instruments with computing and storage for use during and after experiments; (2) real-time data analysis capabilities to reduce data volumes and provide feedback during experiments, improving data quality and driving autonomous experiments; (3) on-demand utilization of computing environments to enable quasi-real-time data processing; (4) data storage and archival resources to house data in a common, smart data portal; and (5) an easy-to-use solution to provide an inclusive environment for researchers across user facilities.

Data Management in Research Groups, Gabriela Schlau-Cohen, Professor, MIT

Schlau-Cohen presented on data management in research groups, particularly in the context of research on the dynamics of solar energy conversion in biological and bioinspired systems. The life cycle of scientific data in a research group involves: (1) generation, (2) manipulation, (3) sharing, and (4) preservation; these four steps should be linked together and emphasize data standardization and protection.

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Cloud-based repositories enable integrated data management, bridging the steps of the data life cycle. The Protein Data Bank (PDB) is a mature database for data sharing, preservation, and standardization, supported by DOE since 1971. The PDB is well-integrated to support new methodology and is easy to coordinate with publishing; it offers a robust user interface (UI) for searching and visualization, with a streamlined deposition and a high level of quality control. GitHub is an emerging database on Microsoft servers that enables data generation and manipulation. In GitHub, code is stored with a versioning language and is easily linked within publications, enabling publicly accessible software packages and collaborative software development. Storage is limited to code or small data volumes, with quality control managed individually at the project-level. Zenodo is a catch-all repository enabling data sharing and preservation at scale across all disciplines, with no standardization or quality control and limited search functionality. Ultimately, repositories are best leveraged to advance scientific discovery when well-supported by federal funding agencies.

Discussion

Takeuchi asked how the PAP will balance research security and confidentiality with public data sharing, particularly regarding the release of unpublished data. **Cooke** replied the DMSP encourages researchers to think and decide upfront about appropriate data to share. A long list of reasons exist in which data sharing could be limited, such as the protection of personal privacy, businesses, IP, or U.S. competitiveness. Discussions should be held early in the process, so the necessary tools are integrated into the workflow, and scientists can share the appropriate data at the appropriate time.

Mallapragada asked how long data needs to be stored and made publicly available, and whether the community of interest and the duration of usefulness will be considered, given the budget constraints and the Nelson Memo being an unfunded mandate. Another question is whether a system will be in place to ensure data shared (that are not directly linked to a publication) are of sufficient quality. **Cooke** responded the PAP allows flexibility in implementation. Across DOE, there is not a single answer regarding length of data preservation. The community will inform these aspects of the DMSP, including data quality standards. The DOE will support data resources long-term, if deemed mission critical.

Kinney asked whether specific DMSP requirements would be established in the future, as input on DMSPs is increasingly gathered from the different communities. **Cooke** replied the PAP was purposefully designed to enable flexibility for programs to define their own expectations, so that needs could be met across all scientific domains. However, as communities create and refine their own standards, this may become reflected in certain solicitations or in program guidance.

Epps asked whether the evolving data repositories are considering the inclusion of physical samples (*i.e.*, sample repositories). In the context of materials science, the use of data from repositories can be significantly enhanced if the actual experimental sample is also shared. **Dauenhauer** agreed on the importance of having benchmark materials available. In the field of catalysis, there is currently no standardized method of sample sharing, which occurs amongst the community on an individual basis. **Haile** noted discussions about sample sharing have occurred within the NSF Materials Innovation Platforms (MIP) program. **Friend** noted biological samples are commonly stored for follow-up research in the biotechnology realm. **Schlau-Cohen** noted a central database exists for *Chlamydomonas*, where researchers in the biotechnology industry can obtain specific types of high quality and standardized strains, although the cost is high.

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Cooper wondered whether a timeline exists for individual researchers to start implementing the new PAP into their own research groups, particularly those based in universities. Processes from the new PAP may require socialization and a different way of thinking. Currently, researchers are probably not thinking deeply about the PAP's implementation. Federal agencies may need to manage their expectations about how quickly individual researchers can ramp up to meet the new requirements. **Cooke** responded the federal agencies will inform the communities of the new PAP requirements by the end of 2024, completing implementation by the end of 2025. Existing awards will not be reevaluated; accepted DMPs under the current standards will persist. The new requirements will be announced in the FY26 solicitations at the beginning of the award cycles. National labs may see faster implementation, given their close coordination with DOE.

Guzman asked if the new PAP would make federally funded research data available globally, and whether other countries were implementing a similar approach. Another question is how DOE will measure success of the PAP. **Cooke** responded data sharing under the PAP is globally public with no restrictions; however, data sharing may be appropriately limited for the aforementioned reasons. In terms of measuring success, monitoring the network of data inputs and research outputs allows researchers to be recognized for sharing data and tools that resulted in impactful science. In turn, universities and institutions can translate that recognition into career advancement decisions.

Overview of the Office of Critical and Emerging Technologies, Helena Fu, Director, CET

Fu remarked the CET was launched in December 2023 with the goal of leveraging DOE's broad scientific and technical expertise to accelerate progress on critical technologies. The CET focuses on four areas: (1) AI; (2) biotechnology and biomanufacturing; (3) quantum science; and (4) semiconductors and microelectronics, all of which bring enormous potential to solve urgent problems and drive future economic development. The CET was developed in response to the White House's October 2023 Executive Order (EO): "Safe, Secure, and Trustworthy Development and Use of AI," which charged the DOE to "establish an office to coordinate development of AI and other critical and emerging technologies across DOE programs and the 17 national labs."

DOE and CET play a critical role in managing guidelines, standards, and best practices for AI safety and security, protecting privacy, promoting innovation and competition, and strengthening leadership abroad. Partnerships will be key to success, as DOE continues to promote the benefits of AI through establishing pilot training programs, identifying applications, developing agendas for best practices, and expanding access to computing resources. DOE also continues to manage AI risks through assessments, testing and model evaluations, and increasing testbed availability, as well as through the Research Coordination Network launched with NSF, which is dedicated to privacy enhancing technologies.

The FASST initiative leverages DOE's enabling infrastructure to advance safe, secure, and trustworthy AI for scientific discovery, applied energy, and national security. FASST will build the world's most powerful integrated scientific AI systems through four key interconnected pillars: (1) AI-ready data; (2) frontier-scale AI computing infrastructure and platforms; (3) safe, secure, and trustworthy AI models and systems; and (4) AI applications. A RFI has been issued to gather community input and new partnership ideas. It closes on November 11, 2024.

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Discussion

Bent asked for more information regarding CET's three other focus areas besides AI, and how SC is coordinating programs across different efforts. **Fu** replied CET is in startup mode, with many new endeavors in development in each of the focus areas. CET is focused on delivering their responsibilities from the AI EO. CET has established a cross-departmental working group to harness and leverage the activities across SC, the National Nuclear Security Administration (NNSA), and other DOE program offices. CET is actively working to develop partnerships internally and externally, coordinating across SC, EERE, and NNSA. CET has an active and ongoing effort in biotechnology and biomanufacturing and has begun a similar effort in quantum science. CET aims to bridge the gaps as needed, but not replicate existing efforts.

Haile inquired whether CET's focus areas will remain "emerging" into the future, in particular whether focus areas will remain static or transition in due time to the other DOE program offices. It is unclear how CET connects to the other program offices that conduct research in the four focus areas. **Fu** responded that the four focus areas have been critical for a significant period of time, due to their implications for U.S. economic prosperity and national security. DOE has been directed to focus on these areas as opposed to other technologies. CET's role is not to fund or conduct research, nor to provide guidance to other program offices on their R&D activities. CET will oversee policy discussions and strategize a "one-DOE" approach for these focus areas, leveraging all the program offices, as well as external entities, to bring expertise.

Huq asked how CET is engaging with industry, since the focus areas have significant industry investment and involvement. **Fu** replied that CET is meeting with many players in industry and is identifying the boundaries between DOE's work and that of industry. CET is focused on leveraging recent breakthroughs in the focus areas, both within DOE and among industry partnerships, to push advancements to the next step, particularly through FASST.

Berry asked if CET's goal is to technologically facilitate research projects across the "Valley of Death." **Fu** responded that the Office of Technology Transitions is tasked with managing circumstances related to the "Valley of Death." CET, however, seeks to bring together the best of DOE to create one concerted approach towards each focus area. For example, when industry partners engage with DOE, they will receive one unified voice.

Public Comment Session

No comments.

Meeting adjourned at 4:28 p.m. ET.

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Wednesday, September 25, 2024

Friend called the meeting to order at 10:00 a.m. ET to a combined in-person and virtual audience of approximately 140 people.

EARLY CAREER RESEARCH PROGRAM AWARDEE PANEL, Gail McLean, CSGB Division Director, BES, and Panel Moderator

McLean remarked the ECRP aims to develop the next generation of scientists who will make an impact in the energy sciences. Past ECRP awardees will give a brief presentation on their ECRP research and discuss how this award led to their current BES-supported research.

Solidification Science, Amy Clarke, Scientist, LANL; Professor, Colorado School of Mines

Clarke received the ECRP award in FY 2012 to investigate *in-situ* monitoring of dynamic phenomena during solidification, focusing on visualizing and modeling the melting and solidification processes of metal alloy materials at high temperatures. State-of-the-art imaging techniques at the APS and at LANL were used for *in-situ* characterization of evolving microstructure development under controlled processing. This project resulted in an enhanced understanding of multiscale prediction and control of metallic alloy solidification dynamics, critical for advanced manufacturing.

More recent work has shifted towards investigating rapid solidification conditions related to additive manufacturing, complemented by modeling. In particular, proton radiography (pRAD) of a tin-bismuth alloy provided real-time visualization of casting and informed solidification modeling. Dynamic Transmission Electron Microscopy (DTEM) was used to measure interface velocity during rapid solidification, providing quantitative data on melt pool dynamics. Grain refinement was demonstrated in a titanium-copper alloy during solid state phase transformation. Quantitative phase field models were developed to examine microstructural evolution under rapid solidification, incorporating latent heat and the prediction of velocity-dependent properties. Other modeling endeavors seek to better understand isotropic effects, grain competition and pattern selection under rapid solidification, and deviations from standard, predicted growth patterns, as well as improving models for microstructure selection to consider kinetic effects during additive manufacturing.

Fundamentals of Solar Light Harvesting: Ultrafast X-ray Insights into Interfacial Electron Dynamics, Oliver Gessner, Senior Scientist, LBNL

Gessner received the ECRP award in FY 2012 to examine the possibility of translating ultrafast dynamics in small molecules to more complex systems for applications in renewable energy technologies. In particular, this project aimed to use modern light sources (*i.e.*, LCLS) as ultrafast x-ray stroboscopes to understand interfacial electron dynamics through capturing snapshots of critical short-lived intermediates, using inner shell electrons as local reporters. Results from this project demonstrated support for the interfacial exciplex model regarding electron charge transfer, as opposed to the biphasic injection model.

Recent projects move beyond single snapshots of short-lived intermediates. Currently, an entire visualization of interfacial charge transfer dynamics was captured by the Free Electron Laser in Hamburg (FLASH) at the German Electron Synchrotron (DESY). At the ALS in LBNL, experiments have demonstrated picosecond time-resolved x-ray photoelectron spectroscopy (XPS) capabilities. Future research will continue to exploit the capabilities of light sources. In

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particular, the upgraded LCLS will provide increased pulse repetition rates to allow progression from the picosecond to the femtosecond domain, allowing closer examination of interfacial charge transfer dynamics as well as interfacial chemical processes, at accurate time scales and with atomic size specificity.

Superconductivity in Strong Spin-Orbit Materials, Johnpierre Paglione, Professor, University of Maryland

Paglione received the ECRP award in FY 2013 to study non-centrosymmetric superconductivity in candidate topological insulators. This project uncovered a new family of superconductors in ternary half-Heusler semimetals, yttrium platinum bismuth (YPtBi) and palladium-based rare earth-bismuthide (RPdBi), demonstrating the coexistence of superconductivity and magnetism in topological materials. Discovery of unconventional spin-3/2 superconductivity in YPtBi, thought to be the first "high-spin" superconductor, has led to sustained scientific investigation.

Recent research continues to explore superconductivity in strong spin-orbit materials, resulting in the discovery of nearly ferromagnetic spin-triplet superconductivity in uranium ditelluride (UTe_2). UTe_2 has demonstrated re-entrant superconductivity at high magnetic fields above 40 Tesla (T), with a continuous superconducting state achieved under fine-tuned systems. Collaborators continue to uncover exotic phases of UTe_2, including the detection of a pair density wave state. Future research will investigate the fundamental properties of UTe_2 to ascertain its potential role in quantum computing.

Design of Efficient Molecular Electrocatalysts for Water and Carbon Dioxide Reduction Using Predictive Models of Thermodynamic Properties, Jenny Yang, Professor, University of California, Irvine

Yang received the ECRP award in FY 2014 to design efficient molecular electrocatalysts for water and carbon dioxide (CO_2) reduction using predictive models of thermodynamic properties. This project synthesized water-soluble transition metal complexes as electrocatalysts to reduce water to hydrogen and CO_2 to formate, measuring thermochemical properties, such as hydride donor ability, to optimize catalyst performance. Predictive models were generated from this thermochemical data and other mechanistic and kinetic studies for the development of catalysts for other reductive reactions, particularly CO_2 reduction to methanol.

Current and future research focus on bridging hydrogenation and electrocatalysis. Minimal overlap exists between catalyst discovery research for homogeneous CO_2 hydrogenation catalysis and for CO_2 reduction electrocatalysis, despite both types of catalysts sharing mechanistic similarities. Current endeavors focus on applying these commonalities to advance research and unite the two respective fields, with an emphasis on translating hydrogenation chemistry to electrocatalytic systems.

Discussion

Friend asked about the kinds of developments or types of research support that would be most valuable in the future to the panelists and their advisees. **Gessner** replied that an infrastructure which promotes team science and multidisciplinary collaboration is most important. Cross-fertilization leverages the expertise and resources across different communities and institutions.

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Clarke noted that the advancements made by SUF have resulted in immense experimental progress. People development and the ability for experimentalists to collaborate with modelers and theorists as a team has been important. **Yang** responded that workshops, reports, and PI meetings connect scientists with potential collaborators and facilities, as well as provide a better understanding of: the current fundamental problems in science; the paths that will see the biggest impact; and the kinds of projects that would bridge the gaps between different research fields.

Paglione noted ECRP awardees may experience concerns regarding the continuity of funding support, particularly during the period after completing the ECRP but before starting a regular grant program. It would be helpful if DOE had a way to provide additional, longer-term support for ECRP awardees. **Epps** noted that discussions have occurred regarding the development of a mid-career award, given concerns from national lab researchers over funding continuity, although it is uncertain whether a solution had been determined. **Friend** noted the issues regarding support for mid-career scientists were identified in the 2021 International Benchmarking Study Report and have not yet been solved. **Gessner** agreed on the challenges of funding continuity and noted the ECRP previously covered the entire salary of the PI, in addition to salaries for some supporting team members. Now, the ECRP no longer covers the PI's salary, requiring supplementation from the PI's host institution. The ECRP appears to have transformed from a major funding opportunity to a supplemental grant.

Berry questioned how community engagement could be further facilitated and whether resource constraints are barriers to this engagement. **Yang** responded having national or society meetings which are problem-focused instead of discipline-focused would promote engagement across different communities. **Clarke** noted virtual meetings are a convenient way to unite researchers, as well as sessions or workshops tied to annual events like the APS user meetings. **Paglione** noted the Fundamentals of Quantum Materials Winter School held annually in Maryland unites graduate students and postdocs, often leading to deep discussions, new ideas, and future collaborations. Such events geared towards junior scientists, which exclude or lessen participation from PIs, can support these deeper interactions.

Epps noted the EFRCs have developed early career programming networks for senior graduate students and postdocs. Knowledge gained from those developments can be used to launch early career networks for the ECRP and other programs. **Schwartz** responded that DOE has established early career networks outside of the EFRCs, although each network is self-guided and self-driven by the program. Additional opportunities do exist and will be considered.

Haile asked if the absence of a Knight shift from the Nuclear Magnetic Resonance (NMR) measurements marks a sign of topological protection of the interior material. **Paglione** responded the Knight shift will drop upon entering the superconducting state in a typical superconductor. The absence of a Knight shift suggests a triplet rather than singlet pairing, where the electron pairs have spins oriented in the same direction. Some researchers argue all spin triplets of superconductors are topological; whether this phenomenon indicates topological protection is inconclusive.

Research Investment Strategies Subcommittee Updates and Approval Vote, Cynthia Friend, BESAC Chair and Subcommittee Moderator; Esther Takeuchi, Professor, Stony Brook University, and Subcommittee Chair; Marc Kastner, Professor Emeritus, MIT, and Subcommittee Vice Chair

Takeuchi presented updates to be made to the report based on BESAC's discussion on September 24, 2024. To make the report more specific to DOE and BES, the Executive

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Summary will incorporate language describing BES's mission and the roles of its program managers, as well as emphasize the need for research investment evaluation, highlighting escalating research costs and the urgency for scientific advancement.

For two of the report's recommendations, wording will be updated regarding: (1) balance of the funding portfolio across multiple axes (*i.e.*, research vs. facilities; single-investigator vs. group [center or hub] funding; established programs vs. emerging fields; and discovery-based vs. use-inspired research) to optimize the impact of DOE research, especially in times of constrained resources, and (2) balance of investment in and adoption of new assessment tools in conjunction with more traditional online methods (*e.g.*, publication and citation analysis) for making portfolio decisions, combining quantitative methods with expert opinion, while recognizing AI/ML models are still in their infancy.

The main text of the report will be updated to: (1) add language about coordination with other funding agencies in the context of workforce development; (2) clarify upfront the purpose of the case study (*i.e.*, to illustrate the capability of publicly available tools and information to provide a view on a topic or technology, such as lithium-ion batteries); (3) include dates and other needed information in the references; and (4) undergo copyediting and report formatting for the final version, which will include the charge, member list, and table of contents.

Discussion

Mallapragada suggested explicitly mentioning the balance between academia and national lab investments as one of the "multiple axes" in the report's recommendation on balance of the funding portfolio, to which **Takeuchi** agreed.

Epps questioned whether the report should include the exact DOE mission statement word-for-word, given this mission statement could change in the future. **Takeuchi** clarified the report refers to but does not include the exact mission statement, since DOE's goals evolve over time.

Friend asked if any BESAC member(s) would make a motion to accept the report, pending the aforementioned modifications. **Dobbins** and **Epps** motioned for approval. **Friend** called for approval of the report. BESAC unanimously voted to accept the report.

Public Comment Session

No comments.

Meeting adjourned at 11:39 a.m. ET.

Respectfully submitted on October 9, 2024,
Lily Gu, MS
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