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BASIC ENERGY SCIENCES ADVISORY COMMITTEE

to the
U.S. DEPARTMENT OF ENERGY

PUBLIC MEETING MINUTES
April 9-10, 2024

Hybrid Meeting

Gaithersburg Marriott Washingtonian Center
9751 Washingtonian Boulevard, Gaithersburg, MD

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**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, April 9-10, 2024, via Zoom and at Gaithersburg Marriott Washingtonian Center, 9751 Washingtonian Boulevard, Gaithersburg, MD. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act (FACA). Information about BESAC and this meeting can be found at https://science.osti.gov/bes/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
Stacey Bent, Stanford University
Joseph Berry, National Renewable Energy Laboratory (NREL), University of Colorado Boulder
Jennifer Brodbelt, University of Texas at Austin
Donna Chen, University of South Carolina
Lin Chen, Argonne National Laboratory (ANL), Northwestern University
Theda Daniels-Race, Louisiana State University
Abhaya Datye, University of New Mexico
James (Jim) De Yoreo, Pacific Northwest National Laboratory (PNNL), University of Washington
Serena DeBeer, Max Planck Institute
Tabbetha Dobbins, Rowan College
Thomas Epps, University of Delaware
Laura Gagliardi, University of Chicago
Jeanette (Jamie) Garcia, International Business Machines (IBM)
Murray Gibson, Florida Agricultural and Mechanical (A&M) University-Florida State University (FAMU-FSU)
Padmaja 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 (AMES)
Nadya Mason, University of Chicago
Gabriel Montaño, Northern Arizona University
Abbas Ourmazd, University of Wisconsin-Milwaukee
Daniel Resasco, University of Oklahoma
Jose Rodriguez, Stony Brook University, BNL
Rachel Segalman, University of California, Santa Barbara
Jinke Tang, University of Wyoming

BESAC Members Absent:

Ken Andersen, Institut Laue-Langevin
Valentino Cooper, Oak Ridge National Laboratory (ORNL)
Matthew Tirrell, University of Chicago, ANL

Designated Federal Officer:

Andrew (Andy) Schwartz, Acting Associate Director, 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

Office of Science Leadership:
Harriet Kung, Acting Director for the Office of Science, Deputy Director for Science Programs
Linda Horton, Associate Deputy Director for Science Programs, Acting Associate Director, Nuclear Physics

BESAC Committee Manager:
Kerry Hochberger, Management and Program Analyst

BESAC Subcommittee Members:
Helmut Dosch, Deutsches Elektronen-Synchrotron (DESY)
Eric Isaacs, Carnegie Institution for Science
Marc Kastner, Massachusetts Institute of Technology (MIT), emeritus; Stanford University, adjunct
Sakura Pascarelli, European X-ray Free Electron Laser (XFEL)

Invited Speakers:
Monica Olvera de la Cruz, Northwestern University
Rebecca Schulman, Johns Hopkins University
Akif Tezcan, University of California, San Diego

Tuesday, April 9, 2024

Friend, BESAC Chair, called the meeting to order at 10:00 a.m. Eastern Time (ET) to a virtual audience of approximately 229 people. BESAC members introduced themselves.

Update on Research Investment Strategies Subcommittee, Esther Takeuchi, Stony Brook University, BNL

SC charged BESAC to develop strategies for prioritizing research investments. Strategy proposals should be area-agnostic so BES management can apply them to specific topics. The Subcommittee considered how BES should determine high- and low-priority topical areas for investment, identify new topical areas and foster cross-cutting areas, balance research and instrumentation support for National Laboratories and academic grants, balance research modalities, weigh potential for technological impact and enable innovations, determine the "basic-applied boundary" sharpness/fuzziness, account for international competition, and consider frequency of re-evaluation. Additionally, demographics and appropriate inclusivity in funding distribution are core considerations of BES.

The Research Investment Strategies Subcommittee (RISS) analyzed how other organizations assess research portfolios and discussed methods used at DOE and BES. Four Subcommittee Subgroups were formed to address specific topics: Subgroup 1 adopted the DOE BES charge objectives into operational objectives, Subgroup 2 documented the DOE BES current practices used for portfolio analysis, Subgroup 3 summarized relevant aspects of prior reports, and Subgroup 4 conducted a test case of portfolio analysis for an area considered in the International Benchmarking Report.

Subgroup 1 translated questions in the charge letter into statements of BES's desired outcomes. Outcomes include: strengthening investments to advance foundational scientific knowledge and international competitiveness; becoming nimble in investing and disinvesting; optimizing portfolio balance related to university and national laboratory research; funding research and instrumentation across various funding modalities; addressing increasing costs of research; having effective tools for evaluating use-inspired basic research; and having effective approaches for investing in the workforce.

Subgroup 2 studied current BES strategic planning methods and found an effective balance of bottom-up and top-down planning. Strategic planning is critical to defining research directions and enabling BES to address cutting-edge, foundational science and long-standing energy science challenges. BES strategic planning involves the synthesis of multiple streams of input, namely: scientific communities; international trends; SC priorities; Administration and Congressional priorities; and other federal agency and non-governmental activities and priorities. BES employs self-evaluation of its research portfolio based on the following criteria: principal investigator (PI) performance; balance of supported institution type and location; progress in scientifically challenging areas; transition of discovery to applied research and development (R&D); awards and technology impacts; and quantitative and qualitative metrics obtained through formal reviews and informal discussions. BES has pursued strong community engagement for decades via reports, workshops, and other activities.

Subgroup 3 conducted a general review of domestic and international reports on research and portfolio assessment, summarized relevant aspects and recurring ideas, and extracted best practices to inform recommendations. Key themes include: the use of numerical metrics, such as publications or patents; the increasing role of artificial intelligence and machine learning

(AI/ML) tools in research assessment; the continued importance of expert input; and the inclusion of funded investigators in planning research directions.

Subgroup 4 conducted a portfolio analysis use-case. To ensure efficient and effective resource allocation in the evolving field of basic energy sciences, data-driven approaches aid in quickly identifying areas of improvement and potential disruptions to the fields. Risk assessment provides a complementary understanding of the consequences of a lack of sustained investment. Additionally, the cost of implementing advanced portfolio analysis and strategies for mitigating such costs are areas of consideration. Portfolio analysis should be field-specific due to the differences in research costs by level of maturity. Project managers (PMs) should have access to metrics including time-series data; growth trends; and leading indicators such as funding, citations, awards, and industry growth. Subgroup 4 tested a case of energy storage and included information sourced from multiple entities, including; the Joint Center for Energy Storage Research (JCESR), a DOE Energy Innovation Hub that operated for ten years; eight previous and active Energy Frontier Research Centers (EFRCs); multiple consortiums, including the Office of Energy Efficiency & Renewable Energy's (EERE) Battery500; and international reports, including the Volta Foundation Battery Report and the Faraday Report. Subgroup 4 analyzed metrics including publications, citations, patents, workforce development, industry interactions, funding, comparisons with international sources, and awards/fellowships. For the test case, time-resolved analysis of Web of Science data shows a steadily growing number of publications but a decreasing number of citations. The decreasing number of citations is likely due to evolving battery chemistry not captured in the analysis.

The RISS found BES's current strategic planning practices to be effective. BES strategic planning necessarily involves the synthesis of multiple streams of input, including engagement of scientific communities; consideration of SC, federal agency, non-governmental, administration and congressional priorities; and PM consideration of cutting-edge, foundational science and long-standing energy science challenges. Portfolio analysis is an important tool for strategic planning and defining BES research directions. The National Institute of Health (NIH) portfolio analysis report indicates using AI/ML approaches requires significant investment. When assessing the value of the portfolio, it is necessary to separate evaluation of the program or PI investigator from evaluation of the entire portfolio. Advances in portfolio analysis methodology could assist BES in addressing the specific desired outcomes identified by Subgroup 1.

The RISS' recommendations for BES include continuation of current practices; incorporation of appropriate metrics for success; use of qualitative measures; expansion of portfolio analysis; and adoption of innovative approaches for assessing emerging scientific trends. Recommendations for portfolio analysis include use of clearly outlined goals; assessment for investment balance; use of currently available tools; evaluation of new tools; development of training tools; consideration of cost of implementation; and collaboration across agencies. Possible approaches for identifying and assessing emerging scientific trends include analyzing topics proposed to early career programs and pursued by new postdoctoral scientists; encouraging BES PMs to drive new ideas through small-program awards, internal pitches for funding, and the broadening of strategic planning; using team research modalities; and using EFRCs to incubate new ideas.

Discussion

Mason appreciated the idea of using AI for portfolio analysis and pointed out the role and capabilities of scientific user facilities in directing research were not discussed. The report could incorporate lessons learned from the BESAC Report on New and Upgrade Facilities in BES report into how BES identifies new scientific areas. **Friend** elaborated that science should inform what the facilities might be and what they can contribute. **Takeuchi** agreed that the linkage between science and facilities is important, described the balance between funding PIs versus funding facilities, and noted the identification of a new scientific direction may drive the need for unique facility adaptation.

Dobbins appreciated how the RISS report builds upon prior BES reports and discusses the costs associated with AI/ML. AI/ML may usefully assess niche problems and workforce outcomes. **Takeuchi** clarified the role of the RISS was not to specify how AI/ML should be used but instead to encourage the consideration of AI/ML for future approaches. Starting small is important for developing methodology and highlighting value, and assessing workforce outcomes via a tracking mechanism can inform and improve effectiveness.

Friend noted there are commercial AI/ML products available and stressed the importance of dataset quality. AI/ML is a future direction but still needs development. **Berry** added that DOE and BES have different sets of user facility data that may serve as test beds. Additionally, the community may better appreciate data quality considering the impact of accurate reporting on portfolio analysis. **Takeuchi** agreed reporting is significant, and it may be worth communicating that value to the community.

Dobbins asked if the RISS report would clarify the distinctions between portfolio and program. AI/ML efforts may be more easily pursued with programs rather than portfolios. **Takeuchi** agreed clear definitions are useful and appropriate.

Gagliardi asked about the impact of the increasing cost of research. **Takeuchi** responded there are many drivers increasing the cost of research which may critically affect decisions regarding the size and number of grants. **Kastner** added increased costs constrain BES activities. Reduced funding frustrates allocation decisions.

Segalman cautioned that recent citation metrics may be misrepresentative due to delays associated with the publication process and the time it takes for ideas to spread. **Mason** added citations differ significantly by field. **Takeuchi** replied that quantitative metrics should not be used exclusively, but rather the insight these metrics provide should be cautiously understood in context with other relevant information to inform decisions. **Mallapragada** noted the NIH developed a citation-normalization ratio that could be employed.

Friend explained the importance of scrubbing data and noted data regarding BES-specific impacts would be useful for assessing parallels. The decrease in citations may be due to technological development and application, as potentially monetizable concepts would result in less publications. **Huq** said the Subcommittee investigated patents and focused on simple data collection processes. **Takeuchi** added there are a variety of possible explanations for the reduced citations phenomenon, which other data sources may help elucidate.

Friend asked if the chart of publication data referenced in the presentation is focused on BES-funded output or general, worldwide output. **Takeuchi** clarified the data is from Web of Science, which does not discriminate from BES outputs. The data could be filtered further with additional analysis. **Huq** noted the exercise used relatively available data, which comes with caveats. **Schwartz** explained publication data has been collected from a subset of EFRCs.

Epps commented that Subgroup 3 mentioned the need for expert input, which can help normalize metrics by field and by program. Regarding the battery test case, there may be limited metrics due to differences in field and program specific considerations.

Krusin-Elbaum asked if there was an investment research strategy and collaborative project between universities and industry, and whether this affects the gathering of statistics. **Takeuchi** discussed how the problems faced by industry can be enlightening for fundamental science and critically important for translational science. The RISS did not specify whether programs should be considered or created but instead commented on the value of industry involvement. **Kastner** added that to make the best decisions, BES staff must receive input from all relevant stakeholders, including academia, national laboratories, and industry. Stakeholders should not be prioritized before information is gathered.

Dosch questioned if there were lessons learned that could be added to the report. Based on the international benchmarking report and increasing cost of research, **Takeuchi** stated the current challenge is the need to refine the ability to make informed and effective decisions while considering new approaches given that not everything can be funded. **Kastner** explained the RISS examined BES's overall process, not specific decisions. BES considers broad input to inform decisions.

Haile commented on the importance of bringing in new ideas and outside stakeholders to evaluate the portfolio from a forward-thinking point of view. Creativity of unfunded postdoctoral researchers and bottom-up community participation should be encouraged. Additionally, the report could include information about how National Science Foundation (NSF) coordination connects to DOE priorities.

Report Out for the Nanoscale Science Research Centers (NSRC) Subcommittee, Murray Gibson, Florida A&M/Florida State University, Karl Mueller, Pacific Northwest National Laboratory (PNNL)

Gibson presented the NSRC Subcommittee charge to provide strategies for selecting high-impact future directions for NSRCs. Relevant considerations included historical impact; synergies in collective NSRCs and other user facilities; best practices for diversifying the user community; and how NSRCs should evolve to better serve the nation and user research. The five NSRCs have overlapping capabilities as well as a diversity of specialized capabilities and unique instrumentation which facilitates strategic direction.

In terms of measuring impact, NSRC-related publications, citations, and users have all steadily increased over the past two decades, although publications may have plateaued due to reaching saturation of support. NSRC intellectual property (IP) production has been impressive, although the level of patents has been decreasing from a recent peak. Highlights demonstrating innovative instrumentation included the Quantum Materials Press at the Center for Functional Nanomaterials (CFN) and the 4-D scanning transmission electron microscope at the Molecular Foundry (MF). The latter example has resulted in several discoveries and is a product of collaboration between the NSRCs. NSRCs also offer expertise and instrument-savvy personnel, which is critical to innovate instruments and collaborate with users. Three recent examples of impactful science were shared: borophane, a new stable 2D material; ultrafast light steering with metamaterials; and better supercapacitors manufactured using ML.

Understanding that the NSRCs already work together, the NSRC Subcommittee recommends increasing collaboration to bolster impact. The transmission electron microscopy project is a successful example of prior collaboration, and current collaborative efforts include a digital twin project to simulate instrument usage in advance of development. Every NSRC is co-located in a National Laboratory with unique capabilities that can be leveraged. For example, the capabilities of the Center for Nanoscale Materials (CNM) and the Advanced Photon Source were employed to chemically characterize a single atom using X-ray spectroscopy for the first time.

Although institutional diversity is broad, industry and non-R1 university user bases could increase engagement with NSRCs. The NSRCs are successfully working with small companies and instrument manufacturers to expand access to scientific capabilities. However, more attention should be dedicated to fostering mutually beneficial relationships with large industrial users.

Mueller acknowledged the history of the five NSRCs, the first of which opened in 2006 and now collectively serve more than 4,000 users annually at six locations across a broad range of research topics. The NSRCs have positively impacted materials and nanoscience research in the US and beyond. Foundational capabilities for scientific and commercial technologies have expanded to include electron microscopy user facilities, quantum information sciences, and innovation in techniques for nanoscale research. Additionally, NSRCs are distinctive sources of trained scientists and engineers, provide critical tools for advancing science and technology grand challenges, complement investments from other agencies, and build expertise of DOE user facilities.

The NSRC Subcommittee recommends sustaining and strengthening NSRCs. These centers have become a key element for US competitiveness, research on high priority scientific problems, and instrumentation development. The NSRCs are playing increasingly important roles throughout national priority areas, and the success of these centers lies in the combination of instrumentation and in-house expertise made available to thousands of users.

NSRCs have provided individual, sustained impacts in fields allied with nanotechnology, and these strengths could be combined for greater impact. The NSRC Subcommittee recommends the five NSRCs develop a singular strategic plan focused on national science priorities and grand challenge areas. The broad expertise of the NSRCs can help the US regain international leadership in instrumentation-enabled science. Details of the recommendation include ensuring engagement with the broader community of scientists; prioritizing the development of science-driven novel instrumentation and data infrastructure; advancing remote access capabilities; simplifying the user proposal portal to a single portal; and encouraging multi-facility utilization.

The NSRC Subcommittee recommends an increase in the training of instrument-knowledgeable scientists and engineers through expanded postdoctoral programs at the NSRCs. As NSRC staff and postdoctoral researchers move into research and academic positions, the user community expands, and the US science and technology enterprise is duly impacted. Training for the capabilities at these centers will increase the availability of expertise, which is currently needed to realize future strategic science directions and enable staff scientists to expand user collaborations.

The decision to co-locate NSRCs with other DOE capabilities was a prescient strategy resulting in complementary capabilities. NSRCs should take advantage of increased capabilities afforded by the current planned large facility upgrade projects, including X-ray light and neutron sources; high performance computing; networking; beamlines (BLs); and other co-developed capabilities.

Continued emphasis on broad outreach is critical for increasing impact and elevating science and technology from historically under-represented groups. The Subcommittee recommends the NSRCs expand proactive efforts to increase the diversity of user groups and staff. While recent outreach efforts have been successful, these efforts should increase the emphasis on training to reduce the barrier to entry for new users and develop a workforce pipeline for the NSRCs.

Lastly, the NSRCs have experienced positive but limited success in industrial interactions. Industry presents opportunities to expand in areas such as microelectronics and quantum information science. The NSRC Subcommittee recommends furthering efforts to lower barriers to industry participation and enhance industrial interactions with NSRC staff. Although there is a history of excellent collaboration with instrumentation development companies and small-technology spinoff companies, the NSRCs' engagement with larger companies has been limited. Efforts should continue to encourage meaningful engagement with industry on relevant science challenges through the user program and beyond.

In summary, NSRCs have positively impacted materials and nanoscience research, and the NSRC Subcommittee's recommendations chart a pathway to accelerate impact and strengthen US competitiveness.

Discussion

Bent asked if the report assessed other synergies in the network. **Gibson** confirmed but explained the NSF nanocenters had different operational procedures, such as user access based on fees instead of the merit of proposals. **Mueller** commented that Table 1 of the report effectively compares NSF Nanotechnology Coordinated Infrastructure (NNCI) facilities and NSRCs. **Segalman** suggested studying NSF materials innovation platforms (MIPs), which are on a proposal basis and exhibit synergy. **Gibson** agreed and explained the NRSC Subcommittee assessed the National Nanotechnology Initiative (NNI) report on nanoscience, and the MIPs are relatively recent investments.

Dobbins noted the strong case for the NSRCs and the respective partnerships, asked whether value to the partners was assessed, and asked why a proposal was not made for a sixth NSRC. **Gibson** explained value was not directly addressed, but the meetings included representatives from relevant stakeholders. The proposal for another NSRC is outside of this assessment's scope, which is to determine whether NSRCs were successful, and to consider the current investment's role in the future of the NSRCs.

De Yoreo commented the value of NSRCs are found more in staff expertise than instrumentation. Collaboration across NSRCs is a challenge that will depend on the coordination of research programs. Research programs allow staff to develop capabilities. **L. Chen** appreciated the role of NSRCs in training young career scientists interested in instrument development, but not leading studies.

De Yoreo found a second challenge to collaboration is that access to the NSRCs is restricted to geographic regions, although the regional nature better suits projects requiring longer instrumentation time. Further, the NSF NNCI facilities have strong outreach efforts and online teaching modules, which NSRCs could adopt and apply to other areas. **Gibson** agreed, expressing the importance of incentivizing collaborations. Regarding outreach, NSRCs have recently started tracking PI diversity rather than institutional diversity, which is an important correction.

Takeuchi cited the financial and logistical challenges of travel to regional facilities and asked if submission of a proposal to a single facility would grant access to others. **Gibson** explained the NSRC Subcommittee understood the implications of regionality. Joint proposals may be challenging but possible. Awareness of the capabilities of peer NSRCs would facilitate joint proposals. **Haile** explained the intention of a joint proposal is not to use all five facilities. A single online portal could guide users towards the most suitable location considering relevant parameters such as distance or capability. Such a system would help raise awareness of each facility's competencies. Regional facilities provide value, and duplication of capabilities is appropriate where cutting edge science is not necessary.

Krusin-Elbaum commented that universities are at times more troublesome than industry during negotiations. **Haile** acknowledged that each NSRC is governed by a different legal document, and one of the intentions of the universal portal was to produce a universal legal framework for industry involvement.

L. Chen questioned whether the name "nanocenter" was obsolete when NSRCs are not limited to nanoscale materials and can perform quantum- and single-atom studies. **Gibson** explained the topic was discussed in the NNI report, which concluded the term "nanoscale" should incorporate all science on the very small scale. Routine instrument development is as important as novel instrumentation.

Guzman asked for clarification on the report's wording regarding outreach and lowering barriers to industrial participation. **Mueller** emphasized the recommendation is to continue the high level of outreach already in practice and consider all options for further outreach. Lowering barriers to entry includes increasing the interface between industrial scientists and staff at NSRCs and consolidating the various facility user agreements required for industrial use.

Segalman questioned whether industrial users would have an alternate pay structure as no user fees currently exist. **Mueller** explained users must currently pay for proprietary research.

Gibson commented that lowering industrial barriers must expand beyond facilitating instrument use. Using NSRCs as locations for industrial workshops and discussions on techniques should also be a goal.

Huq explained industrial start-ups are more interested in nascent technologies than larger corporations. The latter are more rigid in operation and protective of IP. **Gibson** agreed but found interaction could still be increased, as NSRCs can provide expertise not found in industry. **Mueller** commented that industry problems may drive instrumentation development. **Haile** suggested NSRCs should not be evaluated or penalized in terms of attracting industry.

Epps asked whether the reduction in facility users during COVID-19 was uniform across NSRCs or whether location-specific data could be utilized to inform improvements in remote accessibility. **Gibson** noted that while the NSRCs worked collaboratively to address the reduction in users, the NSRC subcommittee report avoided assessing centers individually. **Horton** noted varying regional requirements dictated whether staff could be on-site and cautioned against drawing conclusions from analyzing changes in levels of facility users by facility.

Krusin-Elbaum asked for clarification on remote access to user facilities and whether such access is still available. **Mueller** explained COVID-19 encouraged remote experimentation due to a lack of on-site staff. Remote access enables a wider user base and is still available at some facilities. [*Ed. Note*: Currently, all 5 of the NSRCs have remote capabilities and remote users. Not all instruments at each Center are necessarily available to remote users.]

Abate questioned the exclusion of graduate students in the efforts to expand the NSRC user base through training and expressed support for inter-NSRC collaboration. Establishing infrastructure for sharing data would be fruitful, but mandates may be required. **Gibson** explained graduate students are under consideration and will be reflected in the report. **Mueller**

acknowledged the problems with data sharing and suggested the ecosystem formed by NSRCs could be a model for building a PuRe Data resource. **Haile** explained graduate students are included in the term "early career scientists." However, post-doctoral opportunities are lacking.

Mallapragada asked about NSRCs' interfaces with currently funded DOE efforts such as EFRCs. **Gibson** explained these were not assessed in a portfolio analysis. **Mueller** commented that the consideration of user facilities is currently ongoing. **Schwartz** noted NSRCs and all BES facilities are tasked with providing services to the stakeholder community as a whole and not solely DOE programs.

Berry asked if the 6% industry participation referenced in the report is due to instrumentation development due to its potential to increase overall interaction. Industry impact may be a better metric than engagement. **Gibson** explained the goal is rather increasing interaction with larger industries. Most instrumentation development occurs without user proposals and with collaborations with small companies.

Friend continued by asking if all concerns raised through discussion were adequately addressed in the report.

Friend asked if the report should be accepted. Attendees unanimously agreed.

Welcome, Dr. Geraldine Richmond, DOE Under Secretary for Science and Innovation (pre-recorded remarks)

Richmond expressed appreciation for BESAC members' service and for answering the Facilities, Research Investment Strategies, and NSRC charges.

Recent highlights showcasing contributions of the BES program, lab scientists, and user facilities to major breakthroughs include the 2023 Gordon Bell Prize winner for materials simulations with quantum accuracy at scale, and the ANL-led utilization of X-rays to characterize a single atom as featured on the June 2023 cover of *Nature*. The research program focuses on strengthening the link between basic and applied research, including crosscutting initiatives such as the Energy Earthshots Initiative, for which BES has been a key contributor. In terms of upgraded facilities, the Linac Coherent Light Source II (LCLS-II) project achieved first light in August 2023 and will equip scientists with new capabilities to tackle challenges across a range of disciplines.

Richmond thanked former SC Director Dr. Asmeret Berhe for her leadership and expressed confidence in Dr. Kung's ability to provide strong leadership.

Office of Basic Energy Sciences Update, Andy Schwartz, Acting Associate Director, BES, Director, MSE, Acting Director, SUF Division; and Gail McLean, Director, CSGB Division, Acting Director, Collaborative Research Division

Schwartz reviewed changes in SC and BES leadership, vacancies, and posted positions. Andrew Schwartz is serving as Acting Associate Director of BES, Acting Director of the SUF Division, and Director of the MSE Division. Gail McLean is serving as Director of the CSGB Division and Acting Director of the Collaborative Research Division. Finalizing placement of BES leadership and filling vacancies are near-term priorities. Schwartz expressed gratitude for Horton's work and leadership in BES.

McLean introduced Dr. Amanda Haes as the new Separation Science Program Manager, CSGB, as of January 2024.

Schwartz presented an *In Memoriam* for the December 2023 passing of Mike (Michael) Markowitz, who led the Biomolecular Materials program from 2008-2022 and served as Team Lead for the Materials Discovery, Design, and Synthesis program from 2019-2023.

The Enacted Fiscal Year (FY) 2023 BES Budget was ~$2.5B, consisting of $1.1B in Research, $1.1M for Facility Operations, and $362.7M for Projects, including construction and major items of equipment (MIEs). In FY23, BES supported research spanning 16 national laboratories; 224 academic, nonprofit, and industrial institutions; and 46 states, plus Puerto Rico, District of Columbia, and Guam. The twelve BES user facilities collectively supported over 13,000 users, with 73% of users onsite and 27% remote. The average success rate for new grant awards was ~30%. BES continues to support 51 EFRCs, two Energy Innovation Hubs, and 25 core research areas.

The Enacted FY24 BES Budget of ~$2.6B represents a 3.6% (+$91.6M) increase over the FY23 budget. Research programs are funded at $1.075B in FY24, a decrease of $25M from FY23. Investments in clean energy, manufacturing, critical materials, the Funding for Accelerated, Inclusive Research (FAIR) program, and the Reaching a New Energy Sciences Workforce (RENEW) program continued at the same level. Furthermore, $119.7M is allocated for Computational Materials and Chemical Sciences, Energy Innovation Hubs (Hubs), and the National Quantum Information Science Research Centers (NQISRCs). The budget for microelectronics increased $10M, and BES has planned investments in multiple team awards to comprise a network of Microelectronic Science Research Centers as authorized by the CHIPS and Science Act of 2022. EFRC's budget is $130M. The SC Energy Earthshots Initiative budget decreased by $40M, and BES is working to maintain continuity of the program despite the decrease in funding. The Scientific User Facilities' budget increased by $179.7M, with ~$1.2B allocated for operation of 12 facilities at 93% full-normal operations. Facilities Research received $63.8M for AI/ML, Biopreparedness Research Virtual Environment (BRaVE), and preliminary planning for future MIEs. Funding for construction projects and MIE decreased by $63.1M, with $120M for the Linac Coherent Light Source II High Energy (LCLS-II-HE) project, $57.3M for the Advanced Light Source Upgrade (ALS-U) project, $15.8M for the Proton Power Upgrade (PPU) project, $52M for the Second Target Station (STS) project, and $10M for the Cryomodule Repair and Maintenance Facility (CRMF) project. Funding is designated for two new project starts: $13M for the High Flux Isotope Reactor (HFIR) Pressure Vessel Replacement, and $6.6M for the suite of BLs comprising the National Synchrotron Light Source-II (NSLS-II) Experimental Tools III (NEXT-III) project. MIEs include $5M for the NSRCs Recapitalization and $20M for the NSLS-II Experimental Tools-II (NEXT-II) project.

SC is engaged in a coordinated effort to support multidisciplinary research and innovation in advanced microelectronic technologies through co-design awards and EFRCs. Building on established capabilities at SC user facilities for computation, fabrication, and characterization, the research provides foundational knowledge for development of next-generation technologies in computing, communications, sensing, and power. Planning is underway for the establishment of SC Microelectronics Science Research Centers focused on common research goals. SC's basic research will complement later-stage CHIPS and Science Act investments of other agencies including the Department of Commerce and the Department of Defense.

McLean discussed FY24 BES funding opportunities. The Annual Open Solicitation accepts applications continuously. Proposals are under review for the Established Program to Stimulate Competitive Research (EPSCoR)-State/National Laboratory Partnerships, and for

Computational Materials Sciences – Exploratory Research at the Exascale. Proposals are encouraged for the Early Career Funding Opportunity Announcement (FOA) and for the EFRCs. The FY24 EFRC FOA emphasizes proposals related to quantum information science (QIS), microelectronics, transformative manufacturing, and environmental management. Pre-applications are solicited for FAIR and RENEW, due April 24th and 30th respectively.

SC launched the Energy Earthshots Initiative in FY23 to address key scientific challenges that underpin stretch goals for the first six DOE Energy Earthshots. SC announced 29 awards in FY23 consisting of 18 scientific foundation grants and 11 Energy Earthshot Research Centers (EERCs). BES supported nine of the foundational science, small group awards and eight EERCs. The EERCs received funding late in FY23 and early in FY24 to initiate the projects, and pending Congressional appropriation, will receive additional funding in FY25.

FY24 Small Business Innovation Research (SBIR)/Small Business Technology Transfer (STTR) awards have been issued, totaling $38.3M. Available BES award funding is reduced by ~50% from previous years due to SC facilities being made exempt from SBIR/STTR taxes in FY23. The FY25 FOA will be released July 15, 2024, with topics to be determined.

Recent scientific highlights include closed-loop cathode recycling in solid-state batteries enabled by supramolecular electrolytes and the first “freeze-frame” of water using an XFEL.

Schwartz presented facilities project updates and major milestones. The Advanced Photon Source Upgrade at ANL is underway with completion estimated for June 2024 and users returning in July 2024. The Proton Power Upgrade at ORNL is nearing completion in January 2025 and is scheduled to deliver neutrons for the user program in July 2024. The LCLS-II-HE project at the SLAC National Accelerator Laboratory (SLAC) is underway with a combined Critical Decision (CD) 2/3 anticipated by the end of FY24. Recapitalization across the five NSRCs is ongoing, with 16 of 18 instrument awards made and three instruments delivered.

The FY25 BES Budget Request of ~$2.6B is 1.65% (-$43.3M) less than the FY24 Enacted Budget. Under the FY25 Budget Request, funding for Research Programs decreases by $18.1M, Scientific User Facilities increases by $81.4M, and Construction and MIE decreases by $106.6M. Within Research Programs, there is increased funding for clean energy, critical materials, FAIR, and RENEW (+$13M); increased investments in the SC Energy Earthshots Initiative (+$45M); increased support for AI/ML (+$8M); continued investments in microelectronics research and the Microelectronics Science Research Centers; and flat funding for EFRCs, NQISRCs, CMS/CCS, Fuels from Sunlight and Batteries and Energy Storage Energy Innovation Hub awards, and EPSCoR. Operation of the 12 BES facilities are supported at 90% funding required for normal operations (~$1.3B). In the Scientific User Facilities portion of the Budget, funding for facilities research ($60.9M) includes increased funding for AI/ML (+$9M) and continued investment in accelerators & detectors, BRaVE, and preliminary planning for future MIEs. Funding for construction includes $100M for the LCLS-II-HE project, $52M for the STS project, $20M for the CRMF project, $11M for the HFIR Pressure Vessel Replacement project, and $10M for the NEXT-III project. No MIEs are included in the FY25 Budget Request. During each FY from FY23-25, BES has maintained a budgetary balance of at least 40% allocated to research and approximately 60% allocated to facility operations and projects. In total, the FY25 Budget Request allocates a 60% increase (+$17.4M) for AI/ML above the FY24 Enacted Budget. The funding is split between AI for Science and AI for User Facilities.

The October 2023 *Basic Research Needs for Accelerator-Based Instrumentation* Workshop resulted in a summary brochure and a forthcoming full report. The report outlined five priority research directions to revolutionize accelerator-based instrumentation.

Led by the Offices of Scientific Workforce Diversity, Equity, and Inclusion and Deputy Director for Science Program, SC established a coordinated outreach strategy to reach general and targeted audiences through participation in public events and major professional society meetings. BES has started to hold virtual "office hours" events as another mechanism to engage with the community and answer questions.

BESAC currently has three charges: i. the NSRC charge and ii. the Facilities charge, both reported during the present April BESAC meeting, and iii. a Research Investment Strategies charge, to be reported at the Fall 2024 BESAC meeting.

Discussion

Montaño applauded the outreach efforts to diverse communities and encouraged engagement with organizations such as the Society for the Advancement of Chicanos/Hispanics and Native Americans in Science (SACNAS) and the American Indian Society for Engineers and Scientists (AISES) to reach historically marginalized students. Regarding RENEW and FAIR, the upcoming reorganization of the Carnegie Institution for Science will impact the reclassification of Hispanic-Serving Institutions (HSIs) and Historically Black Colleges and Universities (HBCUs) as R1-status universities, which may result in widening the diversity gap. **Schwartz** appreciated the suggestion to expand outreach. BES has tried to normalize eligibility and continues to discuss optimal classification methods to encourage participation. If there is a change in Carnegie Institution classifications, BES will have a dialog regarding if and how requirements should be adjusted. **Horton** noted recent SC restructuring resulted in Dr. Tim Hallman serving as Senior Advisor on Equity, Inclusion, and Accessibility to address these concerns.

Mason identified a lack of AI training in the materials community and pondered how to ensure AI-trained personnel are available to help with material science research projects. Funding workforce development at the junior faculty or post-doctoral level could help to bridge the divide and create a cohort of expertise. **Schwartz** agreed that bridging domain science expertise with AI-relevant expertise is a challenge. Close coordination and partnerships with communities investing in computing, such as the Advanced Scientific Computing Research (ASCR) program, are important. **L. Chen** asked how scientists could best engage or collaborate with AI/ML experts. **Schwartz** noted the need for a dialog to connect the computing element with advancing science. BES should understand the opportunities where AI/ML can enhance science. **Horton** noted facilities have invested in AI, data, and digital twins, which are important for BLs. BES hosted data/AI calls and workshops, but the quickly evolving nature of the field is a challenge to identifying optimal applications. BES is assessing the merits of a research workshop to address AI/ML developments.

Dobbins asked for clarification regarding the FY25 funding allocation of $17.4M split between AI for Science and AI for Facilities. **Horton** confirmed it is split roughly 50/50.

Friend asked how priorities are set in response to adjustments to the FY25 Budget. **Schwartz** replied that the RISS will assist with priority setting. BES receives bottom-up guidance from community and researcher engagement while working to maximize scientific impact within top-down SC and DOE priorities and BES purviews.

Epps inquired about strategies for liaising with NSF to promote opportunities related to digital twins. **Schwartz** indicated BES regularly engages with NSF and noted ASCR is leading a significant effort on digital twins. BES should seek to leverage and integrate the work of these other programs. BES and the Department of Commerce are considering a new Manufacturing

USA Institute focused on digital twins, including when appropriate and possible coordinated investments are made. **Horton** explained SC executed a new Memorandum of Understanding (MOU) with NSF to expand the basis for collaborations.

Takeuchi asked if the intent for FY25 is to return the EERCs to their intended funding levels after the constrained EERC funding in FY24. **Schwartz** confirmed the intention is to regain and increase funding for this initiative and noted funding for EERCs and foundational awards increased ~15% from FY23 (~$100M) to FY25 (~$115M).

Abate noted neuromorphic computing technology may increase energy efficiency of computing. Does BES consider energy efficiency when investing in AI? **Schwartz** answered energy efficiency is an important topic of discussion within DOE and is reflected in the BES budget. ASCR is interested in energy-efficient computing facilities, and the Advanced Materials Manufacturing Technologies Office (AMMTO) is developing an energy efficiency roadmap to increase efficiency via partnerships with academia, national laboratories, and industry.

Scientific Presentations, James De Yoreo, PNNL

De Yoreo introduced the invited speakers and presented an *in memoriam* in honor of Mike Markowitz, who influenced the Biomolecular Materials Program to emphasize function.

Scientific Progress in Biomolecular Materials, Monica Olvera de la Cruz, Northwestern University

Nature inspires the blueprint for materials that display complex yet well-coordinated collective behavior that are capable of functioning under harsh, non-biological environments and that coherently and actively manage multiple complex and simultaneous functions. Buckling in multicomponent membranes is an area of interest due to fluid-solid domain patterning. Nanoscale enzymatic crystalline membranes allow bacteria to exist in extreme environments and possess many surface proteins. Mutating the multiprotein surfaces enables the study of interactions with adjacent materials and the function of the multi-component shells. Most imaging reveals polyhedral shells, which have charges and different compositions. Interactions between assembled proteins differ from their components. Different parts of the microcompartment shells absorb and release reactants. Chemotaxis has been demonstrated, which is impressive given the small scale of the microcompartments. Current experiments are exploring chemotaxis behaviors as well as self-phoretic motion at the nanoscale. Directed motion is possible at the nanoscale due to patches of charge, and the velocity can be optimized to achieve micrometers per second. Reinforcement learning for non-equilibrium processes, such as active polymerization, is an exciting area where ML is being applied. An example of a non-equilibrium system is responsive enzymatic microcompartments with a functionalized membrane and a catalyst. In this context, a chemical reaction can be coupled with a mechanical response. Geometric feedback is used to model these behaviors and the mechanical pattern formation. The transient behavior of chemically responsive gels is affected by volumetric changes and the slow nature of water diffusion. Michael Hagan's research group is exploring ML approaches to understanding and controlling 3D active matter and are using light to modify activity. Electrostatics with membranes is an area of study that has explored mesoscale chirality. Mesoscale molecules with chirality have been assembled, and different types of chiral structures can be adjusted. Next steps include using proteins for functionalization and investigating whether the molecules can diffuse ions. Non-linear ionic transport can be used to create ionic machines which emulate neurons, enabled by confinement. Using an electric field for confinement shows strong non-linear effects in these systems.

Intelligent Chemistry to Guide a New Generation of Materials, Rebecca Schulman, Johns Hopkins University

A range of inspiring behaviors exist in natural biology that scientists have a strategic interest in emulating, such as the ability to harness energy and auto-repair complex structures. Understanding fundamental principles of nature enables the creation of technologies that emulate natural behaviors in ways that are more versatile and powerful. The Biomolecular Materials Program applies inspiration from biological functions to advance technology. Airplanes are an example of technology developed from humble origins to the point of full instrumentation. Biomolecular systems use biomolecular circuits to interpret stimuli and induce responses. Materials can use this active circuit control to create new functions, respond to a range of signals, and control self-assembly. Nucleic acids are ideal substrates for studying these phenomena and have been developed to create logic circuits and oscillators. Biomolecules can respond to the outputs of these circuits. However, there is a small range of biomaterials which interact in interesting ways. Newly created biomaterials can grow or shrink depending on the presence of DNA. Generally, a range of stimuli can be processed into a strand of DNA and subsequently cause predicted outcomes. For example, a molecular circuit can create a logic circuit, and integrating biomolecules can direct and power a macroscopic material change. Biomolecular circuits can guide complex pathways of assembly and disassembly through orchestration of different filaments. These actions present opportunities for dynamic materials pathways and development of programmed chemistry behaviors, such as maintaining the optimal conditions for crystallization. Recent exploration includes building additional types of circuits to develop new material dynamics. Creating analogs of complex biological systems can lead to sophisticated networks with well-predicted behavior. Future directions include using biomolecular circuits to program machines, create fields to control structure and shape materials, regulate material formation and behavior, and regulate synthesis.

Chemical Design of Functional Protein-Based Assemblies and Materials, Akif Tezcan, University of California, San Diego

Life's complexity is largely driven by supramolecular protein assemblies, which can take the form of biological machines and materials with unique properties. For example, microtubules are crystalline architectures yet are dissipative, dynamic, and exist in nonequilibrium, which allows them to be flexible and respond to stimuli. Research inspired by microtubule behavior aims to design artificial protein assemblies which combine the structural coherence of crystalline materials with the responsive behavior of biological/polymeric systems. Implications of this research include better understanding natural design principles of adaptive biomolecular materials and developing new structures and properties unencumbered by cellular or evolutionary constraints. A key chemical challenge is the existence of many complex non-covalent interfaces of the microtubule structure. To reduce chemical complexity, discrete bonding interactions were used to enable the self-assembly of proteins into larger structures. Disulfide-directed 2D protein assemblies engineered using controlled oxidation resulted in a 2D lattice of proteins arranged by alternating charges. The disulfide bonds are reversible and flexible. Mechanical shear can achieve a continuum of structures which rotate along the disulfide linkages, meaning the crystalline assembly can open and close. When the crystals shrink in one direction, the shrinkage in the orthogonal direction is equal, yielding a Poisson ration of -1. This characteristic is beneficial for impact reduction materials and adaptive filtration devices. When RhuA molecules arrange into 2D lattices through disulfide linkages, their dipoles align in an anti-parallel fashion. An external electrical field or a charged solid substrate can overcome the anti-parallel dipole alignment. For example, use of a positively charged mica template overcame the anti-parallel dipole alignment and forced the proteins into alignment. The functional consequence is a 2D material with permanent polarization. Because the crystals are coherently dynamic, these materials are expected to be piezoelectric. The flexibility of crystalline systems is limited due to the brittleness inherent to the high structural order and strength of crystalline materials. Soft, polymeric materials are highly flexible and adaptive due to low structural order and coherence at the atomic scale. Materials with high structural order and coherence as well as flexibility are desired, and porous 3D crystals can produce these characteristics. For example, Ferritin can be engineered to form polymer-integrated protein crystals. The porous crystals can be infused with polymer feedstocks to form a hydrogel network inside the crystal. If the polymer network interactions with the underlying crystal are sufficiently strong, an expansion of the network leads to an isotropic expansion of the underlying lattice, maintaining crystallinity. This phenomenon was successfully demonstrated at a small scale, with the added benefits of self-healing properties afforded by the underlying adaptive polymer network. Adaptive crystals can be used for controlled protein encapsulation and release. In summary, simple applications of chemistry can create complex biological assemblies with emergent properties. Additionally, higher structural order does not imply low structural flexibility. A future goal is to incorporate these types of materials into living systems.

Discussion

Friend asked the speakers to comment on the future of the scientific field. **De la Cruz** said ionic machines can be used to assemble intelligent materials that are more efficient and non-equilibrium phenomena. **Schulman** noted the emphasis on function and suggested leveraging biomolecular structure to explore multiple, coordinated, and efficient types of behaviors using many different types of biomolecules. **Tezcan** noted evolutionarily designed systems have been constrained by a cellular environment, and a future direction is to create assemblies that extend beyond evolutionary constraints to unconceived properties and functions.

Public Comment Session

No Comments.

Meeting adjourned at 4:17pm ET.

Wednesday, April 10, 2024

Friend called the meeting to order at 9:30 a.m. Eastern Time (ET) to a virtual audience of approximately 175 people.

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

Kung expressed gratitude to former SC Director Dr. Berhe, whose accomplishments include driving efforts related to Urban Integrated Field Labs, fusion energy sciences public-private partnerships, exascale computing, and SC Energy Earthshots. Dr. Berhe served as the Head of Delegation to the International Thermonuclear Experimental Reactor (ITER), deepened relationships with international partners, broadened community outreach efforts, strengthened participation in inclusive research and capacity building programs, and brought increased rigor and a robust diversity, equity, and inclusion (DEI) effort to SC.

Dr. Berhe led realignment efforts within SC and consolidated to two directorates: the Deputy Director for Science Programs (DDSP), and the Deputy Director for Operations. Leadership changes within the DDSP Office included: Dr. Linda Horton assumed the roles of Associate DDSP and Acting Associate Director for the Office of Nuclear Physics; Dr. Tim Hallman became Senior Advisor on Equity, Inclusion, and Accessibility; and Dr. Andrew Schwartz became Acting Associate Director for BES.

Dr. Berhe was a proponent of making SC accessible to the general public. To more intentionally and effectively communicate this effort, SC reaffirmed its mission into three pillars: Driving Discovery Science for the Nation, Fostering Great Minds and Great Ideas, and Providing Unique World-Class Facilities. SC connects people with tools to unleash discovery and advance scientific innovation to drive energy and national security priorities.

SC stewards six core science programs and ten national laboratories, serves over 39,500 users across 28 facilities, and maintains ~24M ft^2 of facility space. BESAC is critical to ensuring BES and SC remain at the frontier of science and maintain a balanced portfolio.

The Enacted FY24 SC Budget of ~$8.24B represents an increase of ~$140M over that of FY23. The increased funding will be used to initiate the Microelectronics Science Research Centers (MSRCs) at $30M and the Fusion Innovation Research Engine (FIRE) Collaboratives at $45M. The Energy Earthshots Initiative was reduced to $20M, and SC is working to address challenges from the reduced funding. User facilities remain a high priority and will be funded at 89% of optimal operations. Congress enacted a requirement to start forward-funding research awards of $2.5M or less (raised from $1M), enabling SC to move nimbly if needed. Additionally, the FY24 FAIR and RENEW FOAs are currently open, with pre applications due April 23 and 30, respectively.

The FY25 Requested Budget is ~$8.6B and is balanced to provide support to cutting edge R&D for discovery, support for optimal operations, and upgrades to scientific user facilities and national laboratories' infrastructures. Budget highlights for research include funding AI research at $259M (+$93.1M); Microelectronics at $94.7M (+$22M), including $45M for MSRCs; U.S. Fusion Acceleration at an increase of +$18.8M; Climate initiative at $20M; SC Energy Earthshots at $115M (+$95M); RENEW at $120M (+$68.6M); and FAIR at $64M (+$31.6M). Operations and construction highlights include funding scientific user facility operations at 88% of operations (+$189.1M); core laboratory infrastructure upgrades at $50M (+$31.7M), including SLI infrastructure projects and General Plant Projects; line-item construction and MIE projects;

National Laboratories deferred maintenance and obsolete infrastructure backlog; Laboratory Operations Apprentice Program at $5M (+$2M); and Oak Ridge Nuclear Operations.

President Biden released an executive order of AI/ML requirements for federal agencies with the motivation to understand both the solutions and threats AI introduces. All six SC program offices will contribute to the Frontiers in Artificial Intelligence for Science, Security, and Technology (FASST) initiative. There are five main initiative directions: AI for Science, including scientific AI foundation models and models trained on supercomputers; AI Hardware Innovation, to improve energy efficiency by greater than 100-fold; AI for User Facilities and Advanced Instrumentation or Technology; AI Tools for Design and Evaluation of Trustworthy AI Systems; and a diverse AI workforce.

SC funded Energy Earthshots related activities for six shots, and two new shots were announced in 2023: Affordable Home Energy and Clean Fuels and Products. If additional funding is appropriated, SC will continue to expand the Energy Earthshots portfolio, as this initiative continues to be one of the highest priorities for DOE.

Current BESAC priorities include building on the impact and success of previous assessments. BESAC's current charges focus on three important BES priorities: assessment of BES facilities of the future; assessment of the impact and future directions for the NSCRs; and input on strategies for research prioritization.

Facilities for the Future of Science, published in 2003, established best practices of long-term planning and prioritization and drove 20 years of investment in US scientific excellence. Presently, many of the projects identified as priorities in the 2003 report have been completed or are near completion, including facilities such as ITER, Frontier, LCLS-II, NSLS-II, Majorana Demonstrator, and the Facility for Rare Isotope Beams. The facilities represent significant advances across many disciplines relevant to SC. The progress of upgrades has been adaptive and was tracked in a June 2016 BESAC report on BES facility upgrades. The BESAC facilities charge is critical to advancing U.S. science and innovation leadership for the next decade and beyond.

Discussion

Mason asked about private-public partnerships regarding AI, considering many private companies are buying up graphics processing units (GPUs). **Kung** replied there are emerging efforts to pool resources, such as NSF's National Artificial Intelligence Research Resource (NAIRR) initiative in which DOE participates. The queue for GPUs is lengthy, and SC may need industrial partners to meet this challenge. Private partners benefit by training the next generation of AI practitioners.

L. Chen asked for more information about the user facility workforce training internship program. **Kung** explained the program is for trade personnel, such as computer support, welders, etc. Laboratories have unique needs not widely covered in trade schools. The apprenticeship program is a partnership between the laboratories and local community colleges to engage in hands-on training in a lab-developed curriculum and is intended to grow a local workforce for the laboratories. **De Yoreo** recalled the National Ignition Facility's laser technician apprenticeship program was very effective.

Gagliardi asked about how to best allocate funding to DEI related initiatives. **Kung** noted, for the FY24 Budget, one of the Congressional chambers zeroed out funding for RENEW and FAIR, although this decision was ultimately reversed and RENEW and FAIR were kept at the FY23 Enacted levels. Although there is general support, it is difficult to predict if funding will grow for these efforts. Broadening participation efforts and implementing a DEI framework is practiced in all BES programs. SC will continue to advocate for dedicated programs while also ensuring DEI principles are adhered to in the greater portfolio.

Mason asked how SC balances supporting and maintaining current facilities versus pushing for new cutting-edge facilities. **Kung** acknowledged the difficulty of the task. The decision is made by weighing the continued viability of facilities versus starting new using factors such as cost-effectiveness and capacity.

Facilities Charge Report Out, Eric Isaacs, Carnegie Institution for Science & Serena DeBeer, Max Planck Institute for Chemical Energy Conversion

Friend noted the Future Scientific Facilities charge was issued December 1st, 2023. The report's timeline is abbreviated with the report due May 1st. The meeting objective is to discuss inclusions or modifications to the report and to obtain BESAC approval for the report with the discussed changes.

Isaacs presented the BES Facilities Subcommittee report which examined eight BES facilities and focused on topics including transformational science and future technologies, new opportunities for machines such as accelerators, new concepts for facilities, integration of AI/ML and robotics, and the new user modalities and facility operations.

The Future Scientific Facilities charge called for BESAC to consider new or upgraded facilities (projects with budgets exceeding $100M) that will provide the capability to deliver leading, transformative science and to assess the projects by level of priority. The charge also requested an assessment of the readiness of construction for new or upgraded facilities and a consideration of cross-directorate partnerships within SC and future science communities. New facilities and upgrades considered include neutron sources, synchrotron sources, XFELs, and a future light source (FLS).

BES Neutron and X-ray facilities have a substantial historical impact, including nine Nobel prizes, ~84,000 publications, and over 263,000 users. Additionally, BES facilities played a critical role in responding to SARS CoV-2.

Key BES Facility Subcommittee considerations included: enabling transformational science; seeking a distinctive science case that is highly compelling to Congress; providing new capabilities; including full digital integration of accelerator, source, sample environment, detectors, and data analysis; enhancing a geographically diverse user community; recruiting and training highly qualified facility staff; and identifying cross-cutting capabilities from other SC directorates and other cognizant agencies.

The approach to the report included a review of white papers and presentations prepared by each of the facilities. Four Subcommittee subgroups conducted assessment and writing for the facilities related to neutrons, synchrotrons, XFELs, and the FLS. The facilities have long laid the groundwork for these upgrades in consultation with BES, BESAC, and user facilities. The BES Facilities Subcommittee concluded the scientific mission for all the X-ray and neutron facilities considered was absolutely central to the future of U.S. science and technology. Each facility is in a different state of technological readiness, and more research may be encouraged to address challenges. Global competition is very strong, increasing urgency. For the U.S. to be a world leader, development and construction times must be considered.

The facilities were assessed according to the two primary charge elements of i. capability for science and ii. readiness for construction. The eight facilities reviewed were i. HFIR, ii.

Spallation Neutron Source (SNS) – Second Target Station (STS), iii. NSLS II NEXT III, iv. NSLS II U, v. LCLS-II-HE, vi. LCLS-X, vii. Low Emittance Injector (LEI), and viii. FLS. Additionally, the Subcommittee reviewed facility partnerships with other SC programs, EERE, and other agencies. All SC Federal Advisory Committees (FACs) are currently charged with assessing facilities. Now is an opportune time to develop partnerships and collaboration.

The SNS and HFIR at ORNL are core elements of the BES facility portfolio. ORNL proposed two facilities with three sources. The SNS STS would be globally unique and would result in the brightest cold neutron source in the world, which is important for quantum materials research. The STS has attained CD-1 with a well-developed machine concept; however, the BES Facilities Subcommittee would like to see better planning regarding the user community, initial key experiments, and training. The HFIR Pressure Vessel Replacement (PVR) is critical for U.S. isotope production. CD-0 has been achieved, and the PVR would likely take place in the late 2030s or early 2040s.

DeBeer discussed the two NSLS projects, which are necessary for U.S. leadership in synchrotron science. NSLS-II is the world's largest medium-energy storage ring, and NSLS II NEXT III will provide 8-12 additional BLs to expand capability and access. Driven by the need to enable multimodal and multiscale research, NSLS-II's management and the user community have planned the first four BLs. Increasingly, multiple BLs are required to better understand sample morphology, local structure, chemical and spin states of electrons, strain, charge/discharge, etc. Conducting this type of research requires having transferrable setups and an integrated approach to data analysis. NEXT III is absolutely essential for realizing the full vision of NSLS-II U, and the science case is both important and central depending on the BL. NEXT III has a clear plan to deliver the BLs and is ready to proceed to CD-1 in August 2024. The BES Facilities Subcommittee recommends engaging the domestic and global user community to quantitatively define the capabilities of the next four to eight proposed BLs.

NSLS-II U would be the world's brightest multi-modal storage ring, especially in the 1- to 10-keV range. This is relevant to addressing challenges in microelectronics, clean energy, quantum materials, bio-preparedness, and beyond. A fully multimodal facility will enable the study of operando phenomena across time scales. Science driver highlights include enabling microelectronics beyond Moore's Law, enabling ghost x-ray imaging, and advancing multi-length and multi-time scale problems. In terms of readiness, NSLS-II plans to deliver the first beam to users eight years after CD-0. The upgrade will preserve the present source location to allow continuous use of existing BLs and reduce power use. The BES Facilities Subcommittee considered NSLS-II U to be absolutely central and recommended further evaluation of the accelerator concept by an expert panel and early engagement of the user community.

The BES Facilities Subcommittee evaluated three LCLS projects: LCLS II-HE, the world's first continuous-wave hard x-ray source; LEI, a high-energy extender for LCLS II-HE and LCLS-X; and LCLS-X, which brings XFEL science into an era akin to current storage ring facilities. LCLS II-HE is at the most advanced stage of development, and its high brightness, from 5- to 13-keV, is central to maintaining U.S. competitiveness in XFEL science. Without investment in U.S. facilities, European and Chinese XFEL capabilities may match or exceed U.S. capabilities by the late 2020s or early 2030s. Science drivers include transformative insights into the atomic-scale function of materials and devices, dynamics of chemical transformations, and complex biological systems. LCLS-II-HE will achieve CD-2 or 3 by May 2024. [*Ed. Note*: The LCLS-II-HE project is currently on track to achieve a combined CD-2/3 by the end of FY 2024.]

The LEI is a high-energy upgrade to LCLS-II-HE which extends coverage to sub-Å ultrafast X-rays at high repetition rates, provides operational redundancy, protects availability of superconducting radio frequency, and sustains US leadership. Science drivers include addressing questions related to model-free structural dynamics, complex energy systems, and quantum materials. The LEI benefits experiments requiring sub-atomic spatial scale, natural timescales, and penetration depth for tailored sample environments. The LEI is at an advanced stage of readiness with essential R&D underway and the design of the injector largely complete, although a more robust readiness assessment will occur after RF gun prototype tests planned for 2025.

LCLS-X would be the first “3rd-generation” XFEL and would potentially allow for 20-40 simultaneous experiments. Drivers include the ability to host new types of sources, such as cavity-based free electron lasers, which would increase brightness significantly. Additionally, multiple end stations would allow for dedicated, custom-designed instruments and tailored infrastructure. Higher brightness would enable investigating natural time scales, dilute systems, rare events, and QIS systems. Multimodal capabilities would enable user communities to conduct novel experiments. The BES Facilities Subcommittee considered LSLS-X to be absolutely central to U.S. leadership. Regarding readiness, LCLS-X is at an earlier stage of development, LCLS-II-HE should be sufficient to feed 10 XFEL undulators, and additional engineering assessments are required. Data science integration will be key to the facility design. Phased delivery of the end stations is recommended.

Isaacs presented on the FLS, which currently is in an early-stage of development for its science case. The BES Facilities Subcommittee gathered information via an FLS expert panel. The FLS represents an opportunity for source-to-sample integration, including extending the digitization of data to the control of the accelerator. Preliminary science drivers include precision data at the atomic or attosecond scale, bio- or soft materials and biomedical use cases, and attosecond chemistry. Facility options have not been determined yet, and considerations include XFELs combined with oscillators for increased brightness as well as plasma-driven X-ray sources. Considerations for facility layout include a distributed layout, compact XFELs, compact synchrotrons, distributed data centers, and embedding within a complementary facility. New facility modalities for accelerated discovery include full digital integration with ML, digital twins to support remote access, remote and hybrid access modes using virtual reality and precision robotics, fast access to multiple tools, and engagement of new communities. The BES Facilities Subcommittee notes that FLS is absolutely central for the future of US-based light source science and represents an opportunity to fully integrate digital instruments. Recommendations include considering the balance of capacity versus capability, initiating an expert panel and workshop process to anticipate science and user needs, and initiating pilot projects at existing facilities related to ghost imaging, autonomous operation, robotics, and AI/ML.

Isaacs presented overall facilities observations. The eight proposed facilities address the DOE BES mission, and facilities differ in states of developing science cases and layouts. It is essential for BES to continue to balance funding for core programs and facilities. While some scientific complementarity and overlap among the facilities is natural, the BES Facilities Subcommittee urged better distinction among the science cases. Recommendations include encouraging facilities to identify distinct, compelling targets for grand science challenges; requesting BES coordinate an effort with facilities to ensure a synergistic science case, an instrument portfolio optimized to serve U.S. science communities, and continuing BES' effective strategy of balancing funding for major user facilities and research. Maintaining readiness and urgency is key to remaining competitive globally. SC and BES should proactively consider their roles in partnership coordination and international collaboration. Lastly, users are central to facility design and modalities.

Discussion

Epps suggested partnering with the Department of Commerce and the National Institute of Standards and Technology (NIST), questioning if industry or start-up revenue derived by using DOE facilities can be measured. **Isaacs** noted metrics exist for IP generated. However, obtaining publicly shared financial data is often difficult. **Schwartz** expressed interest in pursuing such metrics or sharing examples of successes.

Gibson noted all facilities were graded as absolutely central and asked about strategies to effectively communicate the credibility of the report. **Isaacs** found true that all the facilities are absolutely central and transformational if they can be realized, due to either their capabilities or distinct science cases. The report attempts to stress the importance of the facilities while articulating nuances. **Friend** added it is important to consider the future when grading, such as in the case of the FLS. **Gibson** raised the idea of using novel categories for more clarity and to describe readiness. **Friend** noted the charge grades must be used; the report is not a prioritization exercise. **Kung** said a short description can accompany the grades. **Epps** asked if the caveats were included in the beginning of the report. **Friend** and **Isaacs** agreed the report could be revised to emphasize the nuances. **Mason** noted the grading system is not meant to be comparative. The caveats as written relate to readiness, not technical capabilities. It is unclear how funding a facility within a category would impact funding for other facilities in the same category. **Isaacs** saw a natural sequence to funding, especially with NSLS-II and LCLS, with some projects already underway. **Berry** added that capturing the state of the facility as context would be beneficial. **Isaacs** responded the charge called for assessing the value to scientific enterprise, and sequencing responsibilities lie with BES and SC.

Ourmazd noted the report lacked discussion of the roles and plans of DOE and NSF. Additionally, approaching the projects as hardware-software codesign projects would be fruitful. **Isaacs** replied that full integration is considered in the report.

Bent noticed a lack of justification for the three types of sources. The report is written with the assumption that the facilities are needed. To reach a broader audience it would be helpful to explain at a high level why the technologies and techniques are important for the Nation.

Mason suggested separating technical rationale, science case, and readiness. **Isaacs** believed leading the narrative with the science case to be ideal, but when science cases overlap between facilities, distinctions based on technical justifications are recommended. **Haile** commented that the report could note which scientific discoveries would have been accelerated with the new facilities.

Mallapragada asked if the PVR would extend the lifetime of the reactor and if the report should note the consequences of neglecting to replace the pressure vessel. **Horton** noted the intent is to plan well in advance due to the long lead time of the PVR to maintain isotope production. **Epps** mentioned the BES Facilities Subcommittee's neutron report notes 2060 as the decade the pressure vessel will experience issues and isotope production would stop. **Dobbins**

noted it would be useful to identify the science cases justifying why the facilities are absolutely central in the executive summary.

Gibson asked if the NEXT III upgrade would be affected by the performance of the 1-to10-keV BLs. **DeBeer** noted the initial four proposed BLs are designed with regards to NSLS-II U compatibility and future optics. **Isaacs** added the current proposal includes four BLs with the capacity for an additional four to eight BLs. Planning will be more advanced when additional BLs are considered.

D. Chen noted that discussion of beam coherence was lacking from the report and asked if NSLS-II would maintain capability over the entire the X-ray region. **DeBeer** agreed to clarify the benefit of beam coherence in the report and answered that NSLS-II would be world leading in the 1- to 10-keV range and globally competitive beyond 10 keV.

L. Chen asked about "multimodality" and provided descriptions of why certain benchmarks are impactful. **DeBeer** replied that multimodality can refer to BLs capable of both diffraction and spectroscopy as well as integrating the user experience of performing experiments at different BLs. **L. Chen** said multimodal also could imply a combined optical experiment; clarification may be beneficial. **DeBeer** noted the limited space of the report. Various aspects of multimodality were not exhaustively addressed. **Friend** added the report has appendices for detail.

Abate asked how the BES Facilities Subcommittee addressed the additional technologies required for ghost imaging. **Isaacs** said the report includes recommendations for beta-testing concepts such as ghost imaging; novel ideas for X-rays should be benchmarked and tested elsewhere.

Berry commented that the challenge for NEXT III is identifying the critical next steps towards NSLS-II U. The notion of multimodality is ambiguous, and it may be more compelling to frame the approach as science across multiple length scales. In addition, the report lacked a discussion of the implications of neglecting investments in NEXT III. There are immediate needs for capacity, multimodality, and upgrading. **DeBeer** noted multiple length scales are captured by "multiscale." BLs are rated separately as important or central; more granular inference is difficult at this stage of development. **Friend** added the report addresses insufficient BL capacity and future science capabilities. **DeBeer** said NEXT III would address near- to mid-term science, while NSLS-II U has longer-term objectives.

De Yoreo stated the science cases for the LCLS upgrade projects should be emphasized, especially for LCLS-II-HE.

Gibson asked why LCLS-X's multiple BLs and undulators were necessary for certain experiments. **DeBeer** clarified that the increased brightness is required for biologically relevant science at micromolar concentrations.

Ourmazd asked about the use of autonomous observation in experiments. **Isaacs** said autonomous observation is essential for all the facilities' instruments. The report recommends fully digitally integrating facilities.

Haile thought short summaries of the proposals could help clarify technical capabilities, science cases, and proposal readiness. **Epps** noted describing the outcomes that upgrades would enable may be helpful. **Friend** felt this was ideal, noting that some upgrades have more robust details than others.

L. Chen asked if the report discusses pulse duration and resolution. **DeBeer** answered the Subcommittee has information regarding pulse duration and resolution but did not include it in the report. **L. Chen** asked about the continuous-wave hard X-ray source. **Pascarelli** clarified continuous-wave means the repetition rate is variable and can go up to 1 MHz without interruption.

Dosch commented that the proposal is not requesting a well-specified light source but rather the coordination of a process towards defining and designing such an FLS. Two drivers are relevant and important: i. the potential scientific driver and ii. the potential novel user modality driver. The scientific driver is well understood, but the unfamiliar user modality driver may involve new user facilities and machines. The FLS is complementary to existing light sources, and the BES Facilities Subcommittee recommends initiating an FLS process over the next decade involving monitoring scientific development, conducting pilot studies, and analyzing competing technologies.

De Yoreo stated the rationale for facility investments in the report overview needs to make three points: i. technical specialty, ii. scientific capability, and iii. impact. As the report stands, each facility has a partial rationale stated in the overview. Details on science cases would not be appropriate for a high-level overview. **Isaacs** committed to addressing insufficient rationales and strengthening the overview while being cautious to avoid attributing opinions to facilities. **Friend** noted that some science cases are better articulated than others, whereas the science cases lacking details would benefit from a discussion of their potential to be absolutely critical. **Isaacs** mentioned the challenge of balancing a high-level overview with details that make each facility distinctive.

Berry asked about the extent to which recommended facility upgrades were considered as a portfolio and the basis for the classification of "critical." **Isaacs** responded that the BES Facilities Subcommittee received recommended upgrades as a portfolio. **Friend** clarified facilities could be considered a portfolio with complementary capabilities.

Allison asked about the advanced user operation modes for FLS and whether the BES Facilities Subcommittee envisioned similar modes for all the facilities. The report did not prominently discuss the facilities delivering multimodal capabilities. **Isaacs** replied FLS should consider similar modes as a new facility, and other facilities should test and consider incorporating some of the resulting possibilities. For example, existing facilities should beta test ghost imaging. **Isaacs** explained the report's statement regarding multimodality is generic and suggested incorporating multimodal capabilities wherever reasonable. **Garcia** added there are several compelling options depending on different capabilities and use cases which create opportunities for engaging with people with varying skill sets. **Dosch** mentioned the modalities represent a challenge and required trained people. Pilots may suffice as a short-term strategy for implementation. In the long-term, it is necessary to train the next generation of scientists and collaborate with universities to train people both in science and informatics. **Friend** noted several of these aspects are described in the report.

Gibson recommended using language that communicates potential and the need for further development for the underdeveloped science cases. **Friend** suggested alternative language be considered in selective cases.

Abate discussed how AI will fundamentally impact the future of science. **Friend** agreed and noted the importance of the partnership with ASCR. **Isaacs** said the report could increase emphasis on such partnerships.

Huq asked for clarification on the report's intended audience. **Friend** said it was primarily the Director of SC. **Kung** noted the report should be compelling and credible because it will be used by the BES community, Office of Management and Budget (OMB), Congressional staffers, and SC. SC will review all six reports to formulate the future facilities strategy. The report should appeal to different stakeholders.

Ourmazd predicted AI/ML will bring a qualitative change in current methods and worried that BESAC may be overlooking important aspects of the potential impacts. For example, ML can advise on measurement in scientific experiments and aid in information extraction. **Isaacs** acknowledged the challenge of appropriately addressing AI/ML while not being overly specific or prescriptive given the rapid development of the field but agreed that certain aspects or examples could be emphasized in the report. **Dobbins** noted while AI/ML implications are not known, the potential for virtual platforms to expand access is exciting. **Epps** shared an example from chemical engineering illustrating how student interactions with simulations or example models develop interest and foster workforce development. **Garcia** added the development of interest lowers barriers to entry. **Isaacs** noted the remote connection ideas involving digital twins and virtual reality access to operate BLs are in the report and may be worth including in the summary.

Horton expressed excitement about the science cases discussed and suggested BES may combine the cases. Facility directors could develop a unified approach to collectively address the grand science challenges and articulate distinctive science cases and unique capabilities for each facility. **DeBeer** agreed. Facilities struggled to articulate their distinctions to the BES Facilities Subcommittee. **Friend** noted the possibility of a recommendation for a subsequent workshop on this topic.

Friend discussed key changes in the report in light of the discussions emphasizing the importance of specific facilities and adding more nuance about grades in the report. Given that the facilities are in different development stages, **Epps** wondered about tailoring the "absolutely critical" grading to specific circumstances. **Friend** answered BESAC must use the grading system outlined in the charge despite the lack of granularity, and **Isaacs** added that more details can be included to elaborate upon the grades. **Friend** shared the example of articulating the difference between developing BLs for capacity versus for unique capabilities. **Haile** suggested further developing the narrative and using the three categories of i. capabilities, ii. science outcomes, and iii. readiness. **Friend** stressed the importance of clearly describing the facilities and proposals. **Allison** asked if the report plans to change the language of the grading scale. **Friend** answered the language would remain the same, but caveats would add granularity. **Epps** said "absolutely central" could be incorporated into a sentence. **Friend** agreed and stated "potentially absolutely central" may be used to add nuance.

Dosch asked if this was the first time this grading scale has been used. **Friend** answered it was not. **Dobbins** added if the facilities have historically used the criteria of readiness and science along with the "A, B, C, D" grading scale. **Horton** responded this charge mimics the previous facilities charges from SC.

Dosch asked about the implications of a facility receiving a "B" or "C" grade. **Kung** noted the grade, narrative, and nuances are important considerations for the comparison SC will conduct across all six reports. Aspects that may warrant prioritization include capabilities with promising break-through potential.

Tang said the role of AI was well articulated in the report and asked about collaboration with ASCR. **Friend** responded there is enthusiasm for the collaboration with ASCR, and BES plays an essential role in providing the underlying science. **Isaacs** agreed ASCR will be an important collaborator and noted BES will need to develop data centers, tailor equipment, and become more educated on ML. ASCR is engaged in the conversation driven by SC-1. ASCR may assist with the ML aspects of BL digitization, but digitization will be ultimately up to BES.

Gibson noted the FLS is largely accelerator R&D and is unlikely to have an effect within 10 years. While important, its capabilities remain unknown. Preparatory work must continue. **Isaacs** agreed that planning is critical. **Berry** suggested the portfolio purview helps to demonstrate that grading the projects as absolutely critical is important to future science planning.

Friend asked if BESAC would prefer to raise the question of approving the report with caveats or schedule another public meeting. **Isaacs** asked members to review the report and provide feedback. The BES Facilities Subcommittee would consider separating out the science, technical aspects, and readiness of upgrades. **Horton** suggested editing the report draft to incorporate discussion feedback before sharing with BESAC.

Ourmazd and **Berry** motioned for approval, stating their trust that the Subcommittee will address the feedback. **Friend** called for approval of the report, considering said report will be revised and recirculated to BESAC. Members agreed unanimously.

Ourmazd proposed a motion thanking the leadership for authoring the report in a short timeframe. Members agreed unanimously.

Public Comment Session

Mike Martin (Senior Scientist, Advanced Light Source) noted slide 50 of the presentation stated BES partnerships with international facilities, especially transatlantic partnerships, are encouraged and asked whether the committee discussed the types of future partnerships, specifically whether they were advancing technical innovation or enabling remote scientific experiments. **Isaacs** replied that the BES Facilities Subcommittee had an international panel which discussed global competition and the importance of international collaboration, in particular transatlantic cooperation.

Meeting adjourned at 2:40 PM.

Respectfully submitted on May 7, 2024,
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