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

PUBLIC MEETING MINUTES
December 12, 2023

Virtual Meeting

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

The U.S. Department of Energy (DOE) Office of Science (SC) Basic Energy Sciences Advisory Committee (BESAC) convened a virtual meeting on Tuesday, December 12, 2023, via Zoom. 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)
John Allison, University of Michigan
Lynden Archer, Cornell University
Stacey Bent, Stanford University
Joseph Berry, National Renewable Energy Laboratory
Joan Broderick, Montana State University
Donna Chen, University of South Carolina
Lin Chen, Argonne National Laboratory (ANL), Northwestern University
Valentino Cooper, Oak Ridge National Laboratory
Theda Daniels-Race, Louisiana State University
Tabbetha Dobbins, Rowan University
Helmut Dosch, Deutsches Elektronen-Synchrotron
Thomas Epps, University of Delaware
Laura Gagliardi, University of Chicago
Jeanette (Jamie) Garcia, International Business Machines (IBM)
Murray Gibson, Florida Agricultural and Mechanical University-Florida State University
Padmaja Guggilla, Alabama A&M University
Javier Guzman, ExxonMobil
Sossina Haile, Northwestern University
Ashfia Huq, Sandia National Laboratories
Marc Kastner, Massachusetts Institute of Technology, retired; Stanford University, adjunct
Lia Krusin-Elbaum, The City College of New York-The City University of New York
Surya Mallapragada, Iowa State University, Ames National Laboratory
Nadya Mason, University of Chicago
Shirley Meng, University of Chicago, ANL
Gabriel Montaño, Northern Arizona University
Abbas Ourmazd, University of Wisconsin, Milwaukee
Jose Rodriguez, BNL
Rachel Segalman, University of California, Santa Barbara
Cathy Tway, Johnson Matthey

BESAC Members Absent:

Abhaya Datye, University of New Mexico
Serena DeBeer, Max Planck Institute for Chemical Energy Conversion
Marsha Lester, University of Pennsylvania

Designated Federal Officer:

Linda Horton, Associate Director, Office of Basic Energy Sciences (BES)

BES Management Participants:
Gail McLean, Director, Chemical Sciences, Geosciences, and Biosciences (CSGB) Division
Andy Schwartz, Director, Materials Sciences and Engineering (MSE) Division

BESAC Committee Manager:
Kerry Hochberger, Management and Program Analyst

Tuesday, December 12, 2023

Cynthia Friend, BESAC Chair, called the meeting to order at 11:00 a.m. Eastern Time (ET) to a virtual audience of approximately 330 people. BESAC members introduced themselves and **Friend** gave a brief overview of the agenda.

UPDATE ON BESAC CHARGES

Research Strategies Subcommittee Status Update

Esther Takeuchi, Chair, Stony Brook University, BNL; and Marc Kastner, Co-Chair, Massachusetts Institute of Technology, retired and Stanford University, adjunct

DOE SC issued a charge to BESAC to form a subcommittee to prioritize research investment strategies addressing recommendations given in the 2021 BES international benchmarking report. The charge spans a broad spectrum of research areas, such as emerging topics where sustained support is needed to fulfill the core mission of BES, as well as research areas beginning to wane. The subcommittee aims to submit the report for BESAC's approval at the spring or summer 2024 meeting. [Ed. note: Subsequently, this date was postponed to Fall 2024.]

The subcommittee has reviewed reports and documents from similar organizations – including the National Institutes of Health (NIH), National Aeronautics and Space Administration (NASA), and organizations from the United Kingdom and the Netherlands – to discover, analyze, and build upon existing research portfolio analysis tools that align with BES objectives. The analyzed documents provide a framework for the evaluation of research portfolios and the allocation of future resources.

Four subgroups were developed with distinct assignments within the subcommittee: Subgroup 1 is documenting the relevant DOE BES objectives; Subgroup 2 is documenting current BES practices used for portfolio analysis; Subgroup 3 is summarizing relevant aspects of prior reports compiled by the subcommittee; and Subgroup 4 is conducting a test case of the portfolio analysis for an area considered by the international benchmarking report. Subgroup 1 has provided an update to the subcommittee. Subgroups 2, 3, and 4 will provide progress updates in the next 1-2 months. The findings from the subgroups will be synthesized into the final report and presented to BESAC in 2024.

Discussion

Friend asked about the use of artificial intelligence (AI) and whether it would yield effective results. **Takeuchi** noted the NIH has invested in and investigated the use of AI and machine learning (ML) in portfolio analysis. While there is a significant amount of information available, data quality and variable data formats are a major obstacle to the use of AI/ ML. As an ever-changing industry, AI/ ML will undeniably have a role in the future of portfolio analysis.

Nanoscale Science Research Centers Subcommittee Update

Murray Gibson, Chair, Florida Agricultural and Mechanical University-Florida State University; and Karl Mueller, Vice Chair, Pacific Northwest National Laboratory

Stemming from findings of the 2021 BES international benchmarking report, DOE SC charged BESAC to form a subcommittee "to examine the impact of the Nanoscale Science

Research Centers (NSRCs) and to provide strategies for selecting high-impact future directions." The resulting 16-member subcommittee is considering instrumentation, synergies among and unique capabilities within the NSRCs, synergies with other facilities, best practices to diversify the user community, and how NSRCs can evolve to better serve the Nation and user research. A final report will be presented in the spring of 2024.

The subcommittee has gathered input from BES and the NSRCs, including through a two-day meeting with center directors in August 2023. Select science highlights from this meeting and ongoing work featured the creation of sequence-defined hierarchical peptoids from the Molecular Foundry; the quantum materials press from the BNL Center for Functional Nanomaterials; the characterization of a single atom using a combined synchrotron x-ray nanoprobe and scanning tunneling microscope at the ANL Advanced Photon Source and Center for Nanoscale Materials; a digital twin for *in silico* experiments developed across centers and user facilities; and transmission electron microscopy capabilities leveraging distinctive and complementary capabilities across centers and laboratories.

Four preliminary recommendations are to 1) sustain and strengthen the NSRC ecosystem, which has become a key element of U.S. competitiveness in instrumentation development and application to high priority scientific problems; 2) develop a singular strategic plan involving all five centers, focusing on national science priorities and grand challenge ideas; 3) strengthen postdoc programs; and 4) take advantage of large facility upgrades with new beamlines and capabilities.

Additional preliminary recommendations are to develop a single portal for all NSRCs and challenge the user community to generate proposals that use multiple facilities; to encourage the centers to expand efforts to diversify their community and staff; and to lower barriers to industry participation and identify tangible incentives for NSRC staff. Regarding industry, NSRC interactions with small companies are significant, but the impact on larger companies has thus far been modest.

Discussion

Takeuchi asked for comment on the approaches to coordination—in terms of proposals, submissions, planning, instrumentation, and complementary expertise— that have been considered by the NSRCs. **Gibson** replied that the centers have already undertaken significant collaboration, including on the development of responses to the five charge questions, but that collaboration may not be enough of a focus. Communication among the centers is central to the recommendation on strategic planning. If each center knows what the others are doing, planned upgrades to center instrumentation can be more synergistic. Enhanced communication among the NSRCs with continued guidance from BES would assist in ensuring these goals are met. **Takeuchi** further commented that the findings of the NSRC subcommittee may inform the broader context within which the Research Investment Prioritization subcommittee is working.

Montano wondered whether the proposed universal portal could help expand the user base by facilitating formation of new connections between users and NSRC staff, thereby reducing the need to have pre-existing relationships. Could a universal portal be used to match proposals with individuals from the five NSRCs with relevant expertise? **Gibson** agreed and emphasized that the NSRCs and DOE recognize the opportunity of a universal portal to support the user community and are moving in this direction. Having the right equipment and instrumentation is essential and knowing where to find capabilities can be a challenge.

Rodriguez asked about the lack of collaboration between large industry and the NSRCs. **Gibson** said this was not a huge subcommittee focus; the centers have fantastic collaboration with small companies but far fewer collaborations with large industries. However, the centers have expertise valuable to large industries and could benefit from learning what scientific areas large industries are interested in. More communication between the centers and large industries is the purpose of this recommendation.

Bent asked whether a report-out on access, the number of applications, and the proportion of successful applications is planned. **Gibson** replied in the affirmative. A report-out is planned, but there are additional considerations such as staffing and collaboration.

Dosch suggested that the next step for the NSRCs to increase center impact is to go to a universal portal with common strategic planning. This is a long-term goal; a first step could be center agreement on three to five strategic goals with clear deliverables and the integration of the user community. **Gibson** concurred.

Guzman asked if there is any benefit in comparing benchmarking and collaboration on an international scale. **Gibson** replied that the subcommittee has considered that question. All the centers have international users, and the nature of NSRCs differs from those in Europe according to some committee members. The NSRCs have a lot of leadership in some areas and that could expand with a more synergistic approach.

Chen thanked the subcommittee for providing a global view. Have strategies for the centers to acquire top-line instrumentation been discussed? Some specialized instrumentation is already available, but more common instrumentation may serve regional needs. **Gibson** agreed. In addition to unique instrumentation, additional routine, overlapping instrumentation is central to success and has been considered. The current NSRC Recapitalization project has allowed the centers to focus on unique instrumentation and to do so collaboratively. However, struggles for staff funding have hampered routine instrumentation maintenance and replacement. One of the recommendations includes resources to meet routine instrumentation needs and perform updates. **Haile** noted there will be overlap because of regional values. Centers need staff that can travel and appropriate travel resources. The subcommittee recognizes the need to balance those two aspects.

Mallapragada asked if users have opportunities to suggest instrument needs. **Gibson** said the subcommittee agrees the user community should have a role in developing plans and should have a way to communicate needs. **Dosch** noted that the broader community includes people who are not familiar with techniques but have important scientific questions to solve. These users need to be drawn in to use center equipment, and analysis can be collaborative. Data analysis capabilities are essential to keeping user communities engaged, especially considering the large amounts of data and whether the user community is equipped for analysis. Data analysis itself needs funding. **Horton** added that the user executive committees will discuss communication of instrumentation needs with the subcommittee in January. The portal may address this concern. The Advanced Scientific Computing Research (ASCR) program is focused on data-related user resource needs across SC. Turning the data into science is an opportunity to ensure the instrumentation, computers, and software required for data analysis are available. The digital twin activity discussed previously is an example from a user facility-centered funding program that was established based upon that same point.

Friend asked if there are plans for workshops and training for those who do not know how to use or analyze data. **Gibson** replied that the subcommittee conversations with the centers addressed this topic and pointed to examples of how diversity could be increased by helping to

overcome the barriers to joining the user community. **Horton,** extrapolating from a committee recommendation, advised that general trainings and a summer school could be developed, especially around some of the more complex instruments and techniques.

Friend dismissed the meeting at 11:54 a.m. for a break until 12:00 p.m. ET.

Office of Science Welcome, Asmeret Asefaw Berhe, Director, Office of Science

Berhe thanked BESAC members for the contributions and guidance they offered to SC.

At the Falling Walls Science Summit in Germany, the value of U.S. engagement in international scientific partnerships was discussed, particularly the contributions these partnerships have made to the Linac Coherent Light Source-II (LCLS-II) project and DESY. Congratulations were offered to LCLS-II team members for achieving first light. Two new Nobel Laureates in the community were also recognized.

The eighth and final energy Earthshot, the Affordable Home Energy Shot, has been launched. SC has earmarked ~$260M for the fundamental science needed to close major gaps to achieve the ambitious goals of the Energy Earthshots. With the announcement of new Energy Earthshot Research Centers (EERCs) and the funding opportunity announcement (FOA) for Scientific Foundations for Energy Earthshots, basic science advances to meet Energy Earthshot goals are expected. Broadening participation efforts in Reaching a New Energy Sciences Workforce (RENEW), Funding for Accelerated, Inclusive Research (FAIR), and the Established Program to Stimulate Competitive Research (EPSCoR) are also making great strides. Together, these programs have awarded >$140M to historically underrepresented institutions.

Sustaining a portfolio requires balancing support for established research and new and emerging directions. The work of the current BESAC subcommittees ensures SC has a more robust toolbox in broadly maintaining this balance and managing portfolios. A new SC-wide charge asks BESAC to determine what new or upgraded facilities will best serve the BES mission and purpose over the next 10 years. Members are not expected to rank facilities or consider funding levels. Justification for each member's assessment is expected. The final report will provide SC with the information necessary to plan and execute many important projects across the portfolio.

Discussion

Referencing the new Supreme Court decision related to Diversity, Equity, Inclusion, and Accessibility (DEIA) initiatives, **Dobbins** asked if SC is partnering with other agencies or taking other measures to ensure the programs under RENEW and FAIR are fully realized. **Berhe** replied that, rather than seeking to fund a single group, SC strives to ensure public resources serve the public. This approach ensures SC efforts are not viewed as an exclusive effort. So far, there have not been significant challenges. Also, there has been interagency discussion of how the broadening participation efforts are communicated to make clear that the goal of DEIA is not exclusion, but quite the opposite. SC solicitations make the clear point that the goal is to support institutions that have not received an equal share of federal funding.

Office of Basic Energy Sciences Update & BESAC Charge, Linda Horton, Associate Director, BES; Gail McLean, Director, CSGB; and Andy Schwartz, Director, MSE

Presenters shared BES's organizational chart, noting vacancies and new hires. Dr. Gail McLean has been named the Division Director of Chemical Sciences, Geosciences and Biosciences.

A new, SC-wide charge focuses on large construction projects for user facilities. New construction projects must serve scientific needs from 2024 to 2034. BES has been asked to prepare a list of potential facilities requiring an investment of at least $100M. A subcommittee will be developed to identify which facilities should be considered and to compose a letter that evaluates the facilities based on two criteria: 1) potential to contribute to world-leading science in the next decade and 2) readiness for construction. This letter will be due in May 2024. The next BESAC meeting will be the forum for discussion and approval of the letter.

Several projects are not eligible for inclusion in the new charge due to their cost or stage of construction. Projects that may qualify are: LCLS-II-High Energy, Second Target Station (STS) at Oak Ridge National Laboratory (ORNL), National Synchrotron Light Source II (NSLS-II) Experimental Tools-III (NEXT-III), and High Flux Isotope Reactor (HFIR) Pressure Vessel Replacement at ORNL. Projects in planning include NSLS-II Upgrade, LCLS-X, and Next Generation Light Source [Ed. note: To avoid confusion with an earlier activity, this was subsequently rebranded as the Future Light Source]. For these facilities to be available in the next 20 years, planning must be underway now, and construction must begin in the next 10 years. New and upgraded beamlines for nearly every facility, as well as recapitalization projects for the NSRCs—among other smaller projects—are in planning but are not considered part of this charge as their individual costs are under the $100M threshold.

Several awards were funded late in fiscal year 2023 (FY 2023). BES supported 45 Early Career Awards, including four with the DOE EPSCoR program, totaling ~$56M at 32 universities and eight DOE labs representing 22 states. Broadening participation awards totaled $140M across SC programs and included RENEW, which supported six awards; FAIR, which supported 28 awards; and EPSCoR, which supported 14 awards. Two types of DOE-wide EPSCoR funding solicitations are issued in alternate years: larger implementation awards and smaller state/national laboratory partnerships. Fourteen implementation awards totaling $33M were announced for FY 2023, covering topics such as grid integration, renewable solar and wind energy, and advanced manufacturing. Accelerate, a funding solicitation for research to enhance the science foundations needed expedite the transition of discoveries to technologies, supported 11 awards totaling $73M to teams led by nine DOE labs. Biopreparedness Research Virtual Environment (BRaVe), which supports developing analytical capabilities foundational to future emergency response at DOE's laboratories, provided 10 awards totaling $113M to teams led by six DOE labs. Scientific Computing for BES User Facilities, which supports research developing advanced algorithms and software stacks for new and emerging techniques at DOE light and neutron user facilities to enable on-the fly data analysis and autonomous experimentation, provided three awards to teams led by three national labs totaling $30M.

SC announced 29 awards totaling ~$264M for efforts under the SC Energy Earthshots Initiative that address key scientific challenges underpinning the stretch goals for the first six DOE Energy Earthshots. BES awards supported eight Energy Earthshot Research Centers (EERCs). EERCs are large multi-investigator, multi-disciplinary, and multi-institution teams with the capacity to advance foundational knowledge and enabling capabilities that address Earthshot goals. BES also supported nine foundational science small group awards. These are university-led projects that focus on use-inspired fundamental research to address knowledge

gaps that can be relevant to multiple Earthshots; thus, these projects did not need to focus on a single Earthshot goal.

The annual open solicitation for BES was updated and released for FY 2024. Several additional FOAs are in various stages of development and are not released. The Annual Early Career FOA, which supports outstanding early career scientists in all BES core research areas and to advance facilities capabilities, is expected to continue in FY 2024. The next solicitation for the Energy Frontier Research Centers (EFRC) program, which supports multi-disciplinary, multi-institutional centers to enable transformative advances in energy-relevant basic science, is also in development. The FY 2024 EFRC competition will recompete four-year awards from FY 2020, emphasizing DOE-priority topic areas, including quantum information science (QIS), microelectronics, transformative manufacturing, and environmental management. The next solicitation for the Computational Materials Sciences program, which funds the development of computational codes and associated databases for the design of materials with advanced functionalities, is expected in FY 2024 and will recompete funding associated with previous awards and will prioritize research with software from the Exascale Computing Project. The FY 2024 solicitations for RENEW and FAIR are still in development.

The FY 2024 EPSCoR program funding opportunity was announced December 8, 2023. This program aims to promote institutional diversity and enhance the research capabilities in EPSCoR jurisdictions, support competitive early-stage research in DOE science and technology areas, and develop science and engineering personnel to meet future DOE needs. The FY 2024 FOA focuses on support for EPSCoR institution partnerships with DOE National Laboratories.

The FY 2024 BES budget request was ~$2.7B, representing a 6.3% ($159M) increase over the FY 2023 enacted budget. The FY 2024 BES House Mark is ~$2.58B, which is 3.9% below the FY 2024 request but 2.1% above the FY 2023 appropriation. The Senate Mark is ~$2.68B, 0.5% below the FY 2024 request and 5.7% above the FY 2023 appropriation. There is no new budget information at this time; DOE is operating under a continuing resolution through January 19, 2024. [Ed. note: Funding for DOE was extended to March 1, 2024, under a third CR signed into law in January 2024.]

BES appreciates input for possible basic research needs (BRN) strategic planning workshops. Initial priority topics identified are AI/ML in materials sciences and chemistry; fabrication of next-generation microelectronics and quantum systems; and bioinspired chemical and materials sciences for sustainable energy and products. Possible topics for roundtable discussions include science foundations for critical materials sustainability and advancing subsurface science for energy.

Scientific accomplishments highlighted materials discovery at the autonomous lab at Lawrence Berkeley National Laboratory (LBNL), single-atom characterization using synchrotron x-rays and scanning tunneling microscopy at ANL, light-driven oxidation of water by photosystem II (PSII) at the SLAC National Accelerator Laboratory (SLAC), and the Gordon Bell Prize awarded for simulations of materials using Frontier, DOE's first exascale computer.

Discussion

Archer inquired about the Hubs competition. **Horton** replied award decisions are ongoing.

Takeuchi sought clarification on the FY 2024 timeline for EFRC and EERC calls. **Horton** replied that the FOAs presented are those known at this point. Continued uncertainty

regarding FY 2024 appropriations means it is not safe to assume that every FOA has been posted at this time.

Dobbins asked how the report resulting from the new infrastructure charge will be used and whether the charge is just an exercise. **Horton** replied the charge is not an exercise; SC will develop a strategic document based on the input received. The 20-year plan produced under former SC director Raymond Orbach offers an example of what the result of this work may ultimately be. However, whether the resulting strategic plan will be a public document has not been determined. Previous letters from BESAC are available on the website, and this one will be public as well.

Gagliardi noted that, based on previous solicitation, the FY 2024 EFRC funding call would be more targeted and asked whether this pattern would continue. **Schwartz** answered that there was more funding for the previous alternate year FOA; this year will have less funding and will therefore be more targeted to align with the available funds. **Horton** added that the words provided in the slides reflect the words used in the FY 2024 budget request.

Friend dismissed the meeting at 12:50 p.m. for a break and reconvened the meeting at 1:15 p.m.

SCIENCE OPPORTUNITIES WITH THE UPGRADED LCLS: PANEL DISCUSSION

Mike Dunne, SLAC National Accelerator Laboratory, Panel lead

LCLS provides the ability to study matter with atomic resolution for both lattice structures and disordered matter on timescales of picoseconds to sub-femtoseconds. Over the past ten years, advancements in LCLS capabilities have been significant. There are two key points for this discussion. First, the balance between active facility development and enabling capabilities (e.g., data science) and community-wide investments is essential to understanding what can be done and then executing on what's possible with a new capability. Second, though progress and impact of LCLS has been very impressive, there were major limitations to the original LCLS beam. The investment in LCLS through the LCLS-II project built upon existing capabilities and addressed key limitations in the original LCLS. The upgrade of LCLS was designed based upon broad user community needs spanning quantum materials, sustainability and material design, bioscience, nanoscience, and atomic molecular science. One substantial change is the increase in average spectral brightness. The new capabilities made possible by the LCLS-II project are not a replacement for the original LCLS. Rather, the capabilities of the original LCLS are preserved. Thomas Jefferson National Accelerator Facility (TJNAF), Fermi National Accelerator Laboratory (Fermilab), ANL, and LBNL contributed to the LCLS-II project. Over the course of the project, four instruments and 11 end stations were developed and are currently in use.

Scientific Impact of LCLS Toni Taylor, Los Alamos National Laboratory, retired

Following DOE feedback on the 2022 SLAC Annual Lab Plan, a committee was assembled in 2023 to evaluate the overall scientific contributions of LCLS to key scientific disciplines and future opportunities. Charge considerations included accounting for gestation time for science results from novel XFEL technology; identifying seminal achievements in XFEL methods development over the last 10 years; and linking LCLS activities to key DOE mission elements (e.g., clean energy, environment, climate change, sustainability, and national security).

Based on a wide array of source materials, the committee concluded that the LCLS contributed to qualitative advances over a broad cross section of scientific fields, created new areas of science, and been credited with many scientific discoveries. The foundational knowledge contributed by LCLS should not be underestimated. Enabling steps taken by LCLS include sustained investment in R&D; scientific campaigns to address grand challenges; enhanced capabilities (e.g., multiplexing); nurturing and sustaining of staff; and close partnerships with Stanford. Findings from the assessment highlighted breakthroughs in atomic, molecular, and optical physics (AMO), gas-phase chemistry, condensed phase chemistry and catalysis, materials science and condensed matter physics, and enzyme catalysis for clean energy. Looking to the future, the upgraded LCLS will enable ultrafast and precise measurements to transform science to understand the dynamics of real-world materials and chemical science systems.

Atomic, Molecular, and Optical Science and Gas-Phase Chemistry Daniel Rolles, Kansas State University

AMO physics has several challenges, including probing of charge and energy flow at the molecular level, imaging molecular rearrangement during chemical reactions, and disentangling complex photochemical reaction landscapes. These challenges align with several BES-designated grand challenges: 1) How do we control matter at the level of electrons and atoms?; 2) How do we characterize and control matter away from equilibrium?; and 3) How do we design and synthesize matter with tailored properties?

The upgraded LCLS is equipped to address these challenges, as well as tackle new objectives. The upgraded LCLS can generate few-femtosecond to attosecond multicolor x-ray pulse pairs and visualize the charge flow on the attosecond time scale and is sensitive to electronic and atomic/nuclear structures and dynamics. Capabilities are further enhanced by the high repetition rate of the upgraded LCLS. Quantitative comparison to theory, advances in predictive theory, understanding of the coupling between electronic and nuclear degrees of freedom, and synthesis of molecules and materials with required functionality are among the AMO science objectives for the upgraded LCLS. A long-term goal is to influence and control charge and energy flow and chemical transformations at the level of atoms and electrons.

Condensed Phase Chemistry and Catalysis Junko Yano, Lawrence Berkeley National Laboratory

The BES grand challenges referenced previously apply to the chemical sciences and can be addressed with the capabilities of the upgraded LCLS. The chemical science objectives include achieving a deeper fundamental understanding of chemical reactivity, to exploit nonequilibrium dynamics to direct chemical outcomes, and to develop design principles for synthesis of molecules and materials with required functionality. The enhanced brightness and high repetition rate of LCLS will allow for the study of excited state chemistry and the development of novel modes of excitation in new molecular and materials systems to selectively drive chemical transformations. This instrumentation is also capable of mapping the evolution of frontier orbitals in transition metal photocatalysts with atom specificity. In the field of solar fuels generation, efficiently utilizing charges requires a fundamental understanding of the charge transfer cascade with element specificity, which can now be investigated with the upgraded LCLS, even in heterogenous systems.

Science highlights featured understanding the structure-function relationships in biological systems, like PSII, at the electronic structural level.

Quantum Materials Science at the LCLS-II Matteo Mitrano, Harvard University

Quantum materials are central to modern condensed matter physics, with energy, quantum information and materials science applications. There are several grand challenges in quantum materials science: 1) How to control complex correlations that give rise to remarkable properties of materials?; 2) How to master energy and information flow on the nanoscale to create new technologies?; 3) Beyond ideal materials: How do fluctuations, heterogeneity, interfaces, and disorder impact the functioning of real materials?; and 4) How to characterize and control matter away – especially very far away – from equilibrium?

These questions can all be addressed through the study of light-matter interactions. The upgraded LCLS offers new opportunities, with the quantitative increase in brightness offering a qualitative change in scientific opportunities – from X-ray diffraction towards quantitative spectroscopy. This leads to new opportunities to reveal emergent nonequilibrium quantum phases, to capture nanoscale fluctuations and heterogeneities, and to make high-precision measurements of quantum materials using methods such as time-resolved resonant inelastic x-ray scattering, dynamic coherent x-ray scattering, and time-resolved electron spectroscopy.

Discussion

Garcia noted the intersection between the discussed topics and quantum computing and asked the panel for thoughts on applying quantum computing and benchmarking with classical computing methods. **Dunne** noted that some of the speakers had touched on this topic when discussing materials and chemistry. It may be worthwhile to examine what stresses the measurement and calculation capabilities of AI/ML in simulations and models as well as those of quantum computing. Identifying how to stress test models most effectively may also be useful. **Rolles** noted that quantum computing for quantum chemistry is likely still a far future prospect, but the community is looking at applications of AI/ML and quantum computing to quantum chemical calculations, and AMO will likely be the community to implement quantum computing when that point is reached. However, the timeline is uncertain. **Yano** replied there is still a significant gap to fill before AI/ ML can be applied to these questions. **Mitrano** added that AI/ML may be useful in quantum transduction; once computation is complete, the information can be transferred immediately. Quantum simulators for ultrafast dynamics may not be sufficient due to the limitations of current computing power, especially in the area of quantum entanglement.

Archer mentioned that the Biodesign Center at Stanford University has shadowed medical doctors to establish needs and use that knowledge to identify science questions to address those needs. There is a similar opportunity here in that if a competitive industry is set on using certain materials and methods, tools like those available at LCLS provide an opportunity for those industries to gain new insights and advance their technologies. Are there ways to do this type of interaction better at the LCLS? **Dunne** noted that this type of interaction is currently happening, for example in the field of microelectronics, from fundamental materials development to the intelligent extraction of information from a next-generation chip-based detector system. Key partnerships are being explored to advance the co-design of systems, from materials discovery to device fabrication. There is fascinating information emerging about high-repetition rate, high-pulse rate detectors and coupling with real-time data analytics.

Dobbins asked about data storage challenges, especially with large amounts of data generated by the upgraded LCLS, and management of high costs. **Dunne** noted that there is an ongoing transition due to the sheer scale of the data in terms of rate and volume, which will be orders of magnitude greater than previous years. Following the memo from the Office of Science and Technology Policy (OSTP) last year, data accessibility has been a focus for both scientific reproducibility and data mining to teach ML models. The accessibility of this data will also broaden the aperture of who participates in this type of science and help to engage a broader cross-section of the community. There are no perfect answers to community participation at the moment, but the High-Performance Data Facility (HPDF) on the horizon will likely play a key part in the data ecosystem. **Yano** noted that depositing raw data may not be of use to most users. Depositing usable data would have more value, but there is the question of where this data is to be stored and what the data structure may look like with such a wide array of available experiments. **Dosch** added that storing this amount of raw data will not be possible, and that development of new data compression approaches is necessary. Investment in hardware and new data reduction concepts is going to be essential. There is no available solution at present. **Mitrano** noted that data needs vary widely across the user community. Perhaps in the future, the user community can establish what key definitions are, such as raw data, but all of these will be different across different fields as far as data needs and storage are concerned. **Friend** added this is something the BES community can look to other fields for guidance on as this is a global problem.

Huq inquired about the opportunity for synchronicity across BES facilities. **Dunne** replied by highlighting previous collaborative efforts. Balanced investment and balanced exploitation is the key to success. **Taylor** noted that many of the methods developed at LCLS were done collaboratively, particularly with the synchrotrons, so there is a history of coordination that has room for improvement. However, there is a base level of collaboration present. **Horton** added that the goal is to manage BES facilities as a system, rather than as individual facilities. There is a broader data discussion occurring across the entirety of SC. **Rolles** commented that, as the community is identifying new systems to study using LCLS, there is often a lack of high-resolution structures available in the literature. Collaboration with synchrotron facilities to provide the required high-resolution spectra may be essential. **Mitrano** commented that with the many upgrades to synchrotron facilities trending towards more coherent beams and shorter bunches, there is almost a convergence of capabilities between synchrotrons and FELs.

Haile asked whether LCLS capabilities are necessary to make the discussed scientific advancements, and whether the findings are scalable or achievable elsewhere. **Dunne** mentioned Haile's question ties in with the previous discussion about synchronicity across BES facilities and the related ecosystem. **Rolles** added that benchmarking quantum chemistry calculations is critical to making them scalable and applicable to more complex systems. **Taylor** noted that LCLS discoveries have provided fundamental understanding that will enable applications. Discoveries made with the upgraded facility, especially those leveraging enhanced operando capabilities, will bring the community close to applications. **Mitrano** mentioned while it is not necessarily possible to directly scale the fundamental knowledge gained from an LCLS experiment, the qualitative nature of the information that is generated is unique, not obtainable from other experiments, and informative for other areas of science. **Yano** stated that the ability to visualize changes is powerful and can enable changes to the system to enable new functionality.

Chen indicated that the discoveries made with ultrafast facilities like LCLS are significant but require interpretation, necessitating investments in theory to help push the field forward. This also requires investment in beamline scientists. **Rolles** agreed that LCLS has helped to reduce abstraction in fundamental concepts previously only understood through theory and computation. **Dunne** added this work will change how the scientific community looks at things, because some of the examined phenomena were only theoretical until the technology existed to see phenomena in practice. Investment in beamline scientists and in-house expertise is also necessary to fully exploit the investment that has been made in LCLS.

BRN Workshop on Accelerator-Based Instrumentation Laurent Chapon, ANL; Richard Ibberson, ORNL

The BRN Workshop on Accelerator-Based Instrumentation examined the pivotal role of light sources and pulsed neutron sources in supporting a rich science ecosystem. Particular focus was given to enabling instrumentation for accelerators, detectors, and optics and their transformative potential for BES user facilities. Previous BRNs did not take all facility instrumentation capabilities into account, which is a gap this BRN aims to fill.

The workshop included two sessions, held in October and December 2023. Workshop panels addressed electron accelerators, proton accelerators; neutron optics; x-ray detectors; x-ray optics; neutron detectors; and crosscutting topics. The workshop engaged 128 participants from DOE labs and universities. Twenty percent of participants were international. Observers from other SC offices also attended. Upstream of the workshops, the BRN gathered input through an online survey that contributed to refining the ideas and scope during later activities. The BRN chairs and panel co-leads met in a final December closeout meeting to review the proposed priority research directions (PRDs) and report structure.

The BRN identified five draft PRDs: 1) Realize next generation capabilities that approach theoretical performance limits; 2) Understand scientific mechanisms limiting system performance and utilization; 3) Tailor and control beams with unprecedented precision and speed to probe complexity in matter; 4) Lead innovation in materials, design, and fabrication as a foundation for integration of instrumentation for accelerator-based facilities; and 5) Accelerate progress with advanced modelling, real-time feedback, and physical-digital fusion.

The BRN outcome will be discussed at the Facility Directors' six-way meeting (a meeting of the Directors of the 5 light sources and the Director for the two neutron sources) in January 2024, and a final report will be submitted for publication in March 2024.

Discussion

Ourmazd discussed an iterative approach that works within AI/ML and physics-based data compression. While the physics are yet unknown, this is likely the best approach. **Chapon** agreed and noted there was a lot of discussion about the data storage and compression issue; the iterative approach is a solution that has multiple steps. Previous comments about data storage facilities were referenced; the amount of data that will be generated in the coming years is a growing and recognized concern.

Friend dismissed the meeting at 3:15 p.m. for a break and reconvened the meeting at 3:45 p.m.

Synthesizing Functional Materials for Energy Research, Sheng Dai, ORNL

Mesoporous carbon materials have applications in nuclear energy, the chemical industry, carbon capture, energy storage, and energy conversion. Mesoporous carbon materials are ordered, with pores from 2 nm to 50 nm in size. One important functionality of mesoporous carbons is transport. Compared to microporous structures, mesoporous structures provide channels that increase transport within the material.

Carbon materials were previously synthesized using a nanoscopic mold. Recent developments have resulted in soft-template synthesis, using a typical polymer and capitalizing on the solvent-driven assembly of high-fidelity hydrogen bond capabilities when hydrophobic and hydrophilic materials are combined, resulting in a carbon-yielding reaction. Improvements upon the soft-template synthesis methods utilize enhanced hydrogen bonding and local polymerization by mediated chromic interaction. These resultant structures are very stable. Very recently, solvent-free self-assembly synthesis of mesoporous polymers and carbons has been achieved using mechanochemistry—even when using biomass precursors.

Examples of recent research and application of mesoporous carbons include fast ion transport in capacitive desalination; capacitive energy storage; and the impact of mesopores on carbon dioxide absorption, as revealed by deep learning.

Research focused on the porosity associated with liquids has seen several advancements in recent years. Free volume is a result of the extrinsic porosity of liquids, with changing interstitial sites, as they are dynamic. Free volume is connected to fundamental processes, such as absorption (gas solubility) and transport (gas diffusion and ion conductivity). Research has focused on creating liquids with intrinsic porosity, rather than extrinsic porosity. One approach has been to synthesize nanoscopic ionic liquids through the control of inter-particle interactions of hollow nanoparticles through interfacial functionalization. Starting with a hollow silica nanoparticle, introducing a bulky charge on the surface, and inducing covalent interactions, a mesoporous liquid will result. In addition to silica, carbon, zeolites, and a metalloorganic framework can serve as the building block for formation of mesoporous liquids. Applications for micro- and mesoporous liquids include enhanced gas solubilities, enhanced gas transport, and antagonistic cascade catalysis.

Other examples include a supramolecular approach to cage-based porous ionic liquids for gas storage and separation and porous liquid zeolites using Zeolite Socony Mobil–5.

Synthetic graphite has traditionally relied on a high-temperature synthesis methodology that is not ideal. A novel approach to the synthesis of graphite is the use of molten salts as a mediator to graphitize carbon black, an amorphous carbon powder. This process is an electrochemically driven flux synthesis without the passage of current. One of the key applications of graphite is energy storage. Electrochemically driven flux synthesis also has other potential applications in the energy field. A presented example of this research is the electrochemical graphitization of activated coconut charcoals and coal chars.

Discussion

Rodriguez inquired about the statement that carbon mesopores can be used to trap carbon under high pressure and the mechanism by which that is achieved. **Dai** responded that at high pressure, the carbon dioxide is contained in the mesopore space.

Archer asked about free volume and mesoporous liquids. While the density may be diminished compared to expectations, it is not necessarily true that the glass transition temperature of the tethered ligands would undergo significant changes. Has the glass transition temperature been measured as a function of empty space for these materials? **Dai** replied that

when the temperature is high, above the gas-transition temperature, the pores remain accessible and the gas is stored within them. If gas is stored at high pressure and the temperature is lowered significantly, the gas will be essentially sealed, as though in a nanocylinder. Another dream of this research is the storage of gas without steel tanks.

UPDATE ON COMMITTEE OF VISITORS

Workforce Development for Teachers and Scientists (WDTS) Simon R. Bare, SLAC

The WDTS COV was asked to assess the efficacy and quality of the processes used to solicit, review, recommend, monitor, and document application, proposal, and award actions, as well as the quality of the resulting portfolio, including its breadth and depth and its national standing, benchmarked with other comparable federal Science, Technology, Engineering, and Math (STEM) programs. Additionally, the COV was asked to judge the efficacy of online WDTS components and outreach efforts to enhance Diversity, Equity, Inclusion, and Accessibility (DEIA). The 2023 COV charge had three additions with respect to previous evaluations: 1) pre-college programs; 2) the WDTS Application and Review System (WARS); and 3) the impact of COVID-19. The COV had full access to the WARS staging site. All information for the programs was available, and it was easy to navigate and find all necessary information.

The major findings of the COV were that participation in WDTS programs is limited by mentor capacity, number of mentors, and space; the success rate of the Office of Science Graduate Student Research Program (SCGSR) program is excellent, and; the capabilities of WARS is impressive. Additionally, COVID-19 was found to have a significant impact on all WDTS programs.

Among the COV's major recommendations is for WDTS to work with ORISE to simplify and standardize application procedures. Major recommendations for the Science Undergraduate Laboratory Internship (SULI) program include collaboration between WDTS and hosting laboratories to develop and implement strategies to increase the number of mentors, implement mechanisms that include a greater emphasis on DEIA, and improve communications. Administrative recommendations emphasized the need for inclusion of mentoring and annual performance reviews, encouragement from lab management, and the implementation of awards for excellent mentors. Major recommendations for the Community College Internship (CCI) program include a strong encouragement for increased outreach efforts to reach schools and students and to make them aware of the outstanding opportunities for technical careers at the national laboratories, emphasizing the technician mentor model, and extending the acceptance of recently graduated community college students up to two years upon graduation. Recommendations for the SCGSR program include efforts to increase the number of applications to the program. The proposed effort could include encouragement for more female scientists to participate and capitalizing on RENEW recruitment from minority-serving institutions (MSIs). Broadening participation remains an overall challenge for the National Science Bowl, especially for underserved communities; the COV recommends that recruitment strategies be explored to expand the pool of participants. The recommendations for the Albert Einstein Distinguished Educator Fellowship are to increase the applicant pool. Thus, the COV recommends an increase in stipends commensurate with other competing fellowship opportunities. Overall, the COV fully supports increasing the WDTS budget.

Discussion

Gagliardi discussed the issues surrounding the diminished national laboratory involvement of international students and requested this topic be communicated up the chain of command. **Bare** is unable to comment on this topic. **Haile** similarly cannot comment.

Allison expressed gratitude for the exposure to the programs within the scope of the COV. Fewer, shorter trips for the graduate students is a great recommendation. **Bare** agreed that underserved communities have barriers that must be considered to facilitate participation.

Chen inquired about the four-year DOE graduate fellowship. **Horton** replied this fellowship was not in the mission space of DOE, per Congress.

Mallapragada mentioned that flexibility is essential for the community college program due to the many paths available. **Bare** remarked that it was the aim to highlight the various possibilities available to a community college student.

BESAC unanimously voted to accept the report.

Materials Sciences and Engineering (MSE) Division Frances Hellman, University of California, Berkeley/LBNL

BESAC formed a COV to evaluate the BES MSE Division. Specifically, the COV was charged to 1) assess the efficacy and quality of the processes used to solicit, review recommend, and document proposal actions and monitor active projects and programs, and 2) comment on how the award process affected the breadth and depth of portfolio elements and the national and international standing of the portfolio elements from FY 2018 to FY 2022. The program components examined were Materials Discovery, Design, and Synthesis; Condensed Matter and Materials Physics; Scattering and Instrumentation Sciences; EPSCoR; and topical FOAs spanning BES with a significant component within MSE.

To conduct the review, 19 COV panelists were organized into five panels.

Major findings touched on the impressive breadth and depth of the MSE portfolio, a fair and objective award process, excellent communication with the scientific community, a notable commitment to supporting diversity and inclusion, and a strikingly low number of proposals submitted to EPSCoR by MSIs.

The findings led to seven major recommendations from the COV. Balance the number and size of awards to reflect the rising personnel and other research costs and potential flat budgets. Collect the demographic and institutional statistics of submissions for all programs, beyond award demographics (this recommendation should be broadly considered by BES and DOE). Assess the workloads of MSE program managers to ensure the appropriate level of staffing support is provided and pay attention to the career development of MSE program managers. Explicitly include in instructions that reviewers should identify and assess the strengths and weaknesses in all review criteria, as well as focus on assessing the scientific importance and proposal strengths and weaknesses, avoiding simple metrics such as publication venue (i.e., impact factor) and number of papers published. Finally, for future COVs, MSE should highlight the role and responsibility of BES for National Laboratory stewardship, including setting programmatic directions with intention to produce great science, laboratory workforce development, and maintenance of scientific expertise.

Discussion

Takeuchi commended the panel for their work and mentioned the challenges of completing this work virtually. **Hellman** mentioned the decision to use virtual environments for this work was made in concert with leadership; the virtual environment worked well.

Haile asked about the balance of principal investigator age, the number and amount of the awards, and the perils of cutting the number of students to match available funds. **Hellman** replied that stipends must continue to increase, but the general logistics are difficult to answer at this time. The balance between early career, mid-career, and experienced categories is another consideration. Unfortunately, there is no statistical data available for inclusion in the current report.

Daniels-Race commended those who participated and encouraged reading the appendices for more detailed information. **Hellman** agreed, noting that there are several levels of detail available in the report. All five panel reports are available in the appendices.

BESAC unanimously voted to accept the report.

Public comment:

A participant (chat) requested information regarding EFRC awards and renewal**. Horton** replied there is no further information aside from what was presented in the budget. Release dates, award numbers, and renewals are unavailable at this time. Renewals are, of course, subject to peer review.

Friend adjourned the meeting at 5:15 p.m.

Respectfully submitted on January 4, 2024,
Natalia Travis
Science Writer for the Oak Ridge Institute for Science and Education (ORISE) and Oak Ridge Associated Universities (ORAU)