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

PUBLIC MEETING MINUTES
August 24, 2021

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

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) convened the virtual meeting on Tuesday, August 24, 2021 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:

Marc Kastner, BESAC Chair, Science Philanthropy Alliance
John Allison, University of Michigan
Stacey Bent, Stanford University
Joan Broderick, Montana State University
Lin Chen, Argonne National Laboratory (ANL), Northwestern University
Beatriz Roldan Cuenya, Fritz-Haber Institute of the Max Planck Society
Helmut Dosch, Deutsches Elektronen-Synchrotron (DESY)
Thomas Epps, University of Delaware
Cynthia Friend, Kavli Foundation
Yan Gao, General Electric Company (GE), retired
Laura Gagliardi, University of Chicago
Jeanette Garcia, IBM
Murray Gibson, Florida Agricultural and Mechanical University-Florida State University (FAMU-FSU)
Javier Guzman, ExxonMobil
Francis Hellman, University of California, Berkeley, Lawrence Berkeley National Laboratory (LBNL)
Marsha Lester, University of Pennsylvania
Shirley Meng, University of California, San Diego
Allan McDonald, University of Texas, Austin
Pietro Musumeci, University of California, Los Angeles
Monica Olvera de la Cruz, Northwestern University
Abbas Ourmazd, University of Wisconsin, Milwaukee
Ian Robertson, University of Wisconsin, Madison
Andrew Stack, Oak Ridge National Laboratory (ORNL)
Esther Takeuchi, Stony Brook University, Brookhaven National Laboratory (BNL)
Matthew Tirrell, University of Chicago, ANL

BESAC Members Absent

Lynden Archer, Cornell University

Designated Federal Officer:

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

BES Management Participants:

Bruce Garrett, Director, BES Chemical Sciences, Geosciences and Biosciences (CSGB) Division
Andy Schwartz, Acting Director, BES Materials Sciences and Engineering (MSE) Division

BESAC Committee Manager:

Kerry Hochberger, BES Program Analyst

Tuesday, August 24, 2021

BESAC Vice-Chair, Cynthia Friend called the meeting to order at 11:00 a.m. Eastern Time to a virtual audience of approximately 428 people and requested all BESAC members introduce themselves.

International Benchmarking Subcommittee Report Presentation, Cynthia Friend, Harvard University, Kavli Foundation and Matthew Tirrell, University of Chicago

In February 2019, the SC charged BESAC to evaluate the status of BES's research, capabilities and workforce prospects in the context of intensifying globalization. The BESAC Subcommittee on International Benchmarking drafted a report titled *Can the U.S. Compete in Basic Energy Sciences?*, identifying key research and facility capabilities in which U.S. leadership is most threatened; advising on existing tradeoffs and new ways to leverage scarce resources; and recommending incentives to retain and attract scientific talent.

The Subcommittee deployed benchmarking methods recommended by the National Academy of Sciences (NAS), the American Academy of Arts and Sciences and Rice University's Baker Institute for Public Policy. The Scientific Areas subteam reviewed BES Basic Research Needs (BRN) studies, BES Roundtable reports, and BESAC reports dating from 2010 and identified five BES priority areas to delineate the report's topical scope: quantum information science (QIS); science for energy applications; matter for energy and information; industrially-relevant science for sustainability; and advanced research facilities. To evaluate these critical areas, the subteam engaged BRN chairs in deep-dive discussions to capture their perceptions of each area's global status. Based on these consultations, international publication and conference metrics were gathered for selected subareas and analyzed to complement expert opinion. Finally, this information was compiled with award records, community input from webinars promoted by professional societies, and other metrics. The Strategies subteam used a recursive interview process to identify U.S. strategies. The subteam generated hypotheses by consulting over 50 early career scientists and individuals representing leadership from U.S. National Laboratories, the National Science Foundation (NSF), private foundations, universities, U.S. and international industries, and international research facilities. Input was also sought from town hall sessions at professional meetings. Hypotheses were tested via additional consultations.

Findings indicate that while the U.S. has long been the global leader in research topics and large-scale facilities critical to BES, other nations are rapidly catching up with and overtaking the U.S. U.S. publication metrics have trended downwards since 2010, corresponding to a flattening in U.S. funding. Meanwhile, the European Union (EU) and China have made large research investments over the last decade. In particular, increases in Chinese publications correlate with increased funding. U.S. facilities benefit from long-range strategic planning and ongoing stewardship, but are no longer unique. Furthermore, U.S. support for mid- and small-scale instrumentation, which have historically led to breakthroughs, is increasingly hard to obtain. The U.S. is also falling behind in the important enabling fields of computation and data analysis and is losing ground in the global competition for talent. Without continued investments in basic science today, future U.S. discoveries and technological innovations will languish. To maintain leadership, the U.S. should pursue four broad strategies: 1) increase investment in BES research, including the development of advanced research facilities and instrumentation; 2) boost support for early-career and mid-career scientists to attract and retain talent; 3) enhance opportunities for staff scientists at advanced research facilities to foster creativity while supporting career development and talent retention; and 4) better integrate energy science research across the full spectrum of basic to applied to industrial research.

Additional recommendations include investment in computational and data analysis methods as well as computer hardware and architecture. Notably, enhanced international cooperation in select areas has the potential to increase U.S. competitiveness.

Discussion

Roldan Cuenya remarked that late U.S. budgets are a recurrent problem that interfere with long-term planning. Is there potential to extend grants beyond the typical three- to five-year award period? **Friend** advised that solutions to federal budget issues are unlikely. New funding cycles are possible but will still require approval of the federal budget. Some projects have longer funding windows: EFRC awards are four years and DOE Energy Innovation Hubs are five years in duration. Locking in funding long-term trades off with the ability to respond to new opportunities. **Eric Isaacs** (Carnegie Institution for Science) observed that the EU engages in longer-term planning relative to the U.S., and China pursues an intermediate strategy. Planning affects early career scientists who cannot be sure that the U.S. will maintain a leading position in their research field. BES has done a good job with long-term planning through BRNs and other reports within the limitations set by the political system. To keep international pace, however, the U.S. must consider plans on a 10-20 year scale. **Horton** relayed that Congressional scrutiny of SC research mortgages recently increased, and the SC is now required to fully fund research awards of ≤$1M out of the current year's appropriations. These regulations are unlikely to change in the near term. BES activities commit a subset of funds to multi-year awards: Computational Materials and Chemical Sciences awards are 4 years; Hubs are 5 years; EFRCs are 4 years; and Early Career Awards are 5 years in duration. BES tries to preserve core program areas across administration transitions. **Isaacs** clarified earlier statements, commenting that core programs are generally in good shape. In contrast, feedback from major facilities like DESY indicate the desire for 20-year horizons. This is the timescale for realizing next-generation light or neutron sources. **Horton** noted that for facilities, all strategic activities identified as high priority in the BES long-term plan are in progress. The initial mission need decision has been made for the High Flux Isotope Reactor Pressure Vessel Replacement (HFIR-PVR), though the funding profile activity has not been undertaken. BES is prepared to consider the next generation of light sources with near-term activities underway to keep U.S. facilities world leading. The 10-year horizon is a subject for future workshops. **Isaacs** reemphasized the need to consider the 10-year horizon.

Robertson called attention to how increased support has produced more PhD students in some disciplines than the job market can employ. **Friend** agreed that career trajectories are important. The Subcommittee did not explicitly review post-graduate employment prospects but did examine career paths within the national laboratories and academics. Many people are retiring, and there will be a need for technically trained scientists, not necessarily in academia. The report highlights a need to transition from fundamental research to other applications. Historically, the U.S. has relied on foreign talent to fill jobs, and these individuals have made important contributions. Further talent influx is needed to drive U.S. innovation. **Tirrell** echoed Friend's comments, adding that an academic appointment is usually considered the pinnacle of professional achievement in the biological sciences. Industry, however, is more likely to bring QIS, energy storage and sustainable materials research to fruition. **Zhi-Xun Shen** (Stanford University) concurred. There is no systematic study of this topic. Anecdotally, there is evidence that graduate students with strong quantitative skills are valued by industry, even if these students were trained in unrelated areas.

Bent commented that while the relationship between funding and scientific impact is likely more complex than dollars spent, the correlation found in the report is interesting. Did the report examine factors contributing to the U.S.'s poor competitiveness for global talent and whether these factors primarily affect talent attraction or retention? **Tirrell** cited anecdotal evidence that a U.S. post-doc experience no longer appears required for European students to successfully pursue research careers in Europe. Thus, the U.S. is not receiving the benefits of such post-docs' intellectual talent, regardless of where they ultimately end up. **Isaacs** agreed, referencing declines in foreign student applications to universities, even prior to the advent of the coronavirus (COVID-19) pandemic. While many factors contribute, there is a weak correlation between impact and dollars, and this affects choices. Anecdotally and alarmingly, young scientists are choosing other locations, not because the U.S. is a bad place, but because other places are getting better through investments. One could argue that others learned from the U.S. model set decades ago. The U.S. must continue be a science melting pot. **Friend** concurred.

Friend dismissed the meeting at 12:15 pm for a break and reconvened the meeting at 12:20 pm.

Dosch praised the recommendation advising more international cooperation and encouraged the SC to take this strategy seriously. Europe is ready to cooperate. The U.S. has always had world-leading infrastructure. Some places have become more scientifically competitive, and some U.S. politics are counterproductive. At the end of the day, however, it is the people that ultimately attract talent. Historically, the U.S. had unclassified and classified work, but now there appears to be a diffuse intermediate state that is not classified but not fully accessible. In some research areas, young scientists have the perception that scientific exchange is restricted, and they will not be allowed to communicate with all the researchers worldwide that they would like to if they work in the U.S. Granted, the world is more complicated today. Also, there is more and better support of users at European user facilities. European researchers form competence teams and apply as a group to gain long-term access to selected infrastructures. The U.S. should consider investigating this approach. **Friend** agreed. The strength of Europe's user support emerged in the report. **Tirrell** added that the report calls for a different relationship between the facility staff and user community. **Issacs** elaborated: user facility staff are overextended. Amongst facilities, there is variation in what staff have permission to do. Ideally, staff should strike a balance between science and instrument innovation. The nanoscience centers have done a good job with this. The challenge of how to recruit the best scientists and give them time to innovate came up repeatedly. It is time to consider whether U.S. facilities have the right model.

Guzman inquired about strategies to translate fundamental research into applied technologies. **Friend** weighed in on funding barriers at universities that inhibit rapid translation. It is difficult to have an industry agreement at Harvard; intellectual property issues inhibit information flow. **Tirrell** highlighted the Fraunhofer-Gesellschaft Institutes model and the possibility of adopting select elements. **Isaacs** called attention to industry interviews addressing facets of technology transfer and communication, noting that GE provided a clear statement of things that BES could do. **Gao** remarked that there are good examples to follow, and the benchmarking report is the first step in changing direction. Rolls-Royce in England has set up laboratories at universities and engaged with a synchrotron user facility. This is a successful model. The U.S. Transformative Manufacturing BRN report suggests working in this direction. Historically, BES has focused on fundamental research only, but could change. Congress is

trying to pass legislation to support industry. In Europe, synchrotron facilities have a better relationship with industry. Also, Japan's Super Photon ring-8 gives 10% of operating time to industry with government support. **Maki Kawai** (Chemical Society of Japan) shared that the Japanese government's request that large facilities provide 10-20% of their time to industry has resulted in more mixing between academic and industry personnel. Though difficult to implement in the beginning, these policies have resulted in more inclusion of academics in industry. **Gibson** suggested further contemplation of legal barriers at facilities that are not imposed on industries. **Shen** stressed that the entire ecosystem, stretching from research to the marketplace, must be examined in order for translation to be successful.

Gibson emphasized large and diverse sources of funding for young individuals that do not necessarily have a proven track record as an important U.S. strength. However, this funding is decreasing. Many U.S. weaknesses, such as late budgets, are unlikely to change. Thus, to remain competitive, funding for this strength must increase. **Friend** said the study recommended increasing funds for Early Career Awards, though there is always a tension surrounding how limited funds are dispersed. **Gibson** reinforced the need to increase funding and broaden sources. **Isaacs** agreed. Scientists must have a way to naturally progress from early- to mid-career stages. There are questions surrounding content and funding continuity in the U.S., and early career scientists fear dropping off the cliff after 5-10 years. Both funding quantity and sources are important. Max Planck has a different model. **Anthony Cheetham** (University of California, Santa Barbara; National University Singapore) stressed the urgent need to improve funding for U.S. investigators. The European Research Council allocates roughly four times more funds for Early Career Awards than does the U.S. Following the five-year award period, researchers can apply for Consolidator awards and then Advanced Investigator awards. Researchers move to wherever funding is most generous.

Musumeci observed that some of the report's recommendations address affiliate science and technology (S&T) that is not funded by the BES program. The report's message should be transmitted across the SC and should call for joint actions in these areas.

Chen called attention to talent retention at U.S. user facilities. Many beamline scientists are from Europe, suggesting that the U.S. is doing something right to attract this talent. However, the pipeline for young U.S. scientists to become facility staff members is broken. There are not enough training opportunities, and this could be fixed by creating a training program. There are many talented PhDs, and not all are ready or want to enter academia. National labs used to retain such individuals as scientific associates, and their expertise was relied upon for experimental design. The DOE should consider talent retention across all talent levels.

Allison referenced earlier discussion of long-term funding and planning and personally credited a five-year award for the successful launch of a computational center. Though BES core program awards operate on a 3-year cycle, BES's renewal rate is higher than that of most U.S. organizations. This speaks to program managers' ability to nurture young investigators.

Gagliardi highlighted a lack of U.S. talent in Theoretical Chemistry and barriers faced by corresponding international talent. Recent events stress Diversity, Equity and Inclusion (DEI), but barriers do not stem solely from COVID-19 or a single administration. The majority of graduate students recruited to her program are international, and it is unclear what will happen to the field in 5-10 years. **Tirrell** reflected on the decline of domestic scientists, stressing the need to first develop and nurture talent in addition to recruiting. **Friend** acknowledged Tirrell's point, but added that getting people into the pipeline is beyond the report's scope. **Meng** (via chat) conceded that attracting young talent is beyond the report's scope. However, it seems only the

NSF emphasizes broader impacts, though some of the latest calls from DOE incorporate such requirements. This is a complex issue and principal investigators (PIs) are already overburdened. Nevertheless, DEI content and public outreach components must be added. The national labs could lead efforts.

While working for Ford, **Allison** said it was easier for non-U.S. academics to find basic research funding. Canada, England and Germany have excellent programs. The DOE could rectify this with policies. Did the Subcommittee review the NSF Grant Opportunities for Academic Liaison with Industry (GOALI) program when considering translation strategies? **Tirrell** explained that the report did not explicitly discuss GOALI but did consider national organizations like Fraunhofer-Gesellschaft. DOE can incorporate ideas from existing models. **Isaacs** said that connecting with industry used to be easier because industry had scientists to connect with. For example, Ford and Bell used to have their own beamlines. This gap in U.S. industry opened over the last two decades, and new ways to connect must be found. It is difficult for industry to work with DOE awards that can change every three years. Building relationships will require persistence and scientists that want to walk the value chain from research to product. **Roldan Cuenya** stated that it should be clear to the U.S. that great discoveries can emerge from basic science, as evidenced by Max Planck and Fraunhofer-Gesellschaft.

Roldan Cuenya compared strengths and weaknesses of European and U.S. research systems in academia. Europe lags behind the U.S. in creating tenure-track positions that allow early career researchers independence through startup packages. More U.S. positions like this should be created. Europe does a better job offering intermediate awards like the Consolidator award. Writing U.S. grants that have a poor success rate and reporting to funding agencies is time consuming. U.S. universities do not offer technical support and researchers that acquire instrumentation must pay for maintenance. This is difficult after startup funds are exhausted.

Ourmazd stated that disruptive events are accompanied by self-regulating processes that can reduce the importance of long-term planning. For example, structural biology may no longer be necessary with Alpha Fold. The best people will naturally be attracted to intellectually exciting areas, but there is a time lag. Therefore, the vital question to address is how to maintain an intellectually stimulating environment in order to retain talent.

Chen suggested that the DOE offer different funding mechanisms for different types of staff, in order to help retain technical talent at national laboratories.

Stack inquired if DOE's decision to fold Early Career Award research areas at national laboratories into core research programs at the conclusion of the award has translated into better outcomes. **Tirrell** remarked that there is evidence of frustration among young scientists and failure to attain follow-on funding. The national laboratories probably have better support mechanisms than universities, and an organized way to get mid-career funding is needed.

Stack reiterated the need to reduce the proposal burden and inquired about use of white papers and preproposals. Low award rates are discouraging for young scientists. **Dosch** reinforced earlier comments about the need for the community to rethink interactions amongst facilities, universities and national labs to leverage full facility potential. The same systems have been in place for 40 years with no changes. Boosting proposal success rates is not enough. **Friend** clarified that Stack was referencing research proposals while Dosch was discussing beamline proposals. **Stack** acknowledged low success rates for both proposal types. **Friend** agreed. The report did not explicitly examine the effects of preproposals, but both preproposals and white papers have been helpful in downselecting for calls from programs like EFRC.

Gao reminded BESAC that industry does work with other parts of DOE as well as the U.S. Army and Navy. BES, however, focuses on basic science, and this can be isolating. To connect across the basic to applied to industry continuum and create a win-win outcome, BES needs to find ways to translate applied problems into fundamental research for university professors. User facilities offer industry valuable tools, but there is a lag before facilities are available. These points were outlined in the Transformative Manufacturing BRN report. **Tirrell** concurred. The report articulates that applied problems stimulate basic research.

Friend thanked the Subcommittee and the community before outlining next steps. BESAC should provide high-level feedback on the report by September 3, 2021 to herself or Jeff Miller. Committee members should review the scope of the charge before offering comments. Subcommittee team leads will incorporate edits and recirculate the report for final approval.

Friend dismissed the meeting at 1:20 pm for a break, and Kastner reconvened at 1:50 pm.

Office of Science Update, Steve Binkley, Acting Director, Office of Science

Binkley reviewed the status of political appointees, program organization and the FY22 budget. Binkley is currently serving as the SC Acting Director and will return to the SC Principal Deputy Director role when nominees are confirmed under the new administration. Secretary Jennifer Granholm and Deputy Secretary David Turk have been sworn in and are implementing the administration's vision. Geraldine Richmond and Asmeret Berhe are the nominees for Under Secretary for Science and SC Director, respectively. Both await confirmation by the full Senate. Richmond previously chaired BESAC. Tanya Das is new SC Chief of Staff and Natalie Tham is a new Special Assistant.

Under the Biden Administration, the DOE Applied Energy Programs have been returned to the purview of the Under Secretary of Energy for Science, as organized during the second term of the Obama Administration. Positioning SC programs in closer proximity to Applied Energy Programs will facilitate collaboration.

The FY22 President's Budget Request (PBR) seeks $7.44B for the SC, which is a 5.9% ($414M) increase over FY21's PBR. The House Energy and Water Development Subcommittee issued a lower mark of $7.32B. The Senate mark is slightly higher than the PBR at $7.49B. The SC anticipates a continuing resolution for some period of time. Notably, once the budget is finalized, the percentage funding increase will not be the same for every program within the SC.

Discussion

Referencing the difference between the House and Senate marks, **Kastner** asked about the anticipated budget level and requested an overview of how different SC programs will fare. **Binkley** expressed hope that the budget will ultimately come in close to the Senate mark. Biological and Environmental Research's (BER's) budget has increased the most of the six major programs; the Senate's mark is almost 10% above FY21 enacted levels. The Senate's mark raises ASCR's budget by ~2.5% and BES's budget by ~3.5%. The PBR increases the safeguards and security budget by nearly 40%, an increase of ~$50M, due to serious cyber problems.

Office of Basic Energy Sciences Update, Linda Horton, Associate Director; Bruce Garrett, CSGB Division Director; and Andrew Schwartz, MSE Acting Division Director

Horton discussed BES personnel and program statistics, highlighted FY20 efforts and summarized FY21 plans in the context of the FY22 budget. Schwartz and Garrett described FY21 funding opportunity announcements (FOAs) and coordinated activities across the SC.

Horton shared information about new personnel and retirements in BES, and noted that several BES program positions are acting.

New BES grants on average had a 25% success rate in 2020. The number of users at the 12 BES user facilities dropped from ~16,000 to ~12,500 in 2020, largely due to COVID-19. COVID-19 impacts on 2021 user statistics are expected.

The enacted FY21 BES budget appropriated ~$2.25B, including ~$910M for research programs, ~$923M for scientific user facilities operations and ~$418M for construction and major items of equipment (MIEs). BES continued to accommodate remote user operations due to COVID-19 at ~95% of optimal. Recognizing that remote operation is likely the "new normal," the SC User Facilities Roundtable produced a report titled *Lessons from the COVID Era and Visions for the Future*. Using funding from the Coronavirus Aid, Relief, and Economic Security (CARES) Act, the DOE National Virtual Biotechnology Laboratory (NVBL) leveraged DOE user facilities, high performance computing (HPC) capabilities, research expertise and partnerships to address COVID-19. BES's light and neutron sources were instrumental in characterizing viral structures for vaccine development in addition to supporting research for other medical therapeutics and materials. Both the National Synchrotron Light Source-II (NSLS-II) and the Advanced Photon Source (APS) operated ~10% more hours than planned for 2020. The Nanoscale Science Research Centers (NSRCs) generated novel viral detection methods; synthesized custom nanoparticles for vaccine encapsulation and delivery; improved effectiveness of personal protective equipment; and developed epidemiological models to predict virus spread.

Commissioning activities and upgrades for construction projects and MIEs continued in FY21. The Linac Coherent Light Source-II (LCLS-II) was re-baselined in October 2020 with a new total project cost (TPC) of ~$1.14B. Accelerator and X-ray systems were installed, and both the soft and hard x-ray undulators are operational. Critical decision-4 (CD-4) is projected for FY24. COVID-19-related delays have moved dark time for the APS Upgrade (APS-U) installation to the third quarter of FY23, with CD-4 projected in FY26. Ongoing construction activities will double the Spallation Neutron Source (SNS) accelerator beam power to 2.8 MW via the Proton Power Upgrade (PPU); CD-4 is projected for FY28. The Advanced Light Source Upgrade (ALS-U) attained CD-2 in 2021 with CD-3 projected for FY22 and CD-4 anticipated in FY29. Long-lead procurements, design and prototyping activities are underway. New scope was added to the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project to provide additional instruments and a low emittance superconducting electron gun. The TPC estimate is $660M, with CD-2/3 projected for FY22 and CD-4 projected for FY30. The Second Target Station (STS) continued activities for a complementary pulsed source with an order of magnitude higher brightness cold neutrons at the SNS. The TPC is $1.8B-3.0B, with CD-2/3 projected for FY25 and CD-4 projected for FY37. The Cryomodule Repair and Maintenance Facility (CRMF) continued conceptual design and alternatives analysis. The TPC is $70M-$98M with CD-1 projected for FY23. ORNL has begun internal assessments for the HFIR-Pressure Vessel Replacement, pending funding, per the recommendations of the BESAC assessment and report. The cost range estimate is $300M-$550M.

The FY22 PBR requests ~$46B for the DOE, a 10.2% increase over enacted FY21 levels, to understand climate change; develop materials and concepts for clean energy; advance artificial intelligence (AI) and computing; support scientific facilities; and invest in Minority-Serving Institutions (MSIs) by enhancing research funding opportunities and augmenting workforce development programs. The FY22 PBR and House and Senate marks are similar to BES's request of ~$2.3B, which prioritizes clean energy stewardship, advanced manufacturing, the Reaching a New Energy Sciences Workforce (RENEW) program, computing and data, QIS, and facilities-related research and capabilities. Under this budget scenario, funding for research programs will increase by ~$109M to include funding for Core Research at ~$735M; Computational Materials and Chemical Sciences, Energy Innovation Hubs and National QIS Research Centers at ~$118M; EFRCs at ~$130M; and Established Program to Stimulate Competitive Research (EPSCoR) at $25M. Funding for scientific user facilities will increase by $15.7M, with $974.5M designated to support operations at 12 facilities at 97% of the optimum level and $38.4M to support facilities research in AI and Machine Learning (ML) and Accelerator Research and Development (R&D). Funding for construction and MIEs will decrease by $70M with $106M for APS-U; $32.4M for LCLS-II; $53M for LCLS-II-HE; $75.1M for ALS-U; $17M for PPU; $32M for STS; $3M for CRMF; $15M for NSRC Recapitalization; and $15M for NSLS-II Experimental Tools-II (NEXT-II).

Coordination across the DOE continues through joint FOAs, roundtables, BRN workshops and other mechanisms.

The Solicitation for the Office of Science Financial Assistance Program ("Open Call") is open for proposals. The Early Career Research program announced 83 awards in FY21, with 34 in BES. Thirty active Early Career awards since FY17 are to EPSCoR institutions, including seven awards in 2021. Fifteen active awards are to Hispanic-Serving Institutions (HSIs), four in FY21, and one FY21 award was to a Historically Black College or University (HBCU). The DOE announced nine EPSCoR Implementation Grants in FY21. The FY22 EPSCoR FOA will focus on partnerships between institutions and national laboratories. Applications for the DOE Office of Science Graduate Student Research (SCGSR) program are due November 10, 2021. Letters of intent for the FY22 Phase I Release I Small Business Innovation Research and Technology Transfer (SBIR/STTR) program are due August 30, 2021, and applications are due October 12, 2021. The FY22 Phase II Release I FOA will be issued October 18, 2021. Notably, FOAs released for FY22 will incorporate new collaborator, biosketch, and current and pending support templates.

Nominations for the 2021 E.O. Lawrence Awards are due September 21, 2021.

Five Scientific Discovery through Advanced Computing (SciDAC), 29 QIS Research, and eight QIS Infrastructure awards were announced in FY21. Awards for Microelectronics will be announced soon. Research highlights from these cross-disciplinary areas include new experimental evidence of anyons; identification and characterization of the correlated phase and bit-flip errors due to radiation impacts in superconducting multiqubit chips; and the first example of quantum-sensed nuclear magnetic resonance using nitrogen vacancy ensembles.

The five initial awardees for the National QIS Research Centers ramped up to full operations in FY21. The Quantum Systems Accelerator (QSA) center led by LBNL realized a sensor that uses quantum entanglement to achieve sensitivities that exceed the standard quantum limit.

BES and Fossil Energy and Carbon Management (FECM) are co-leading the Hydrogen Science & Energy Technology Team (SETT) with participation from Nuclear Energy (NE) and

Advanced Research Project Agency – Energy (ARPA-E) to advance the DOE's Hydrogen@Scale Initiative.

The BES virtual roundtable on Foundational Science for Carbon-Neutral Hydrogen Technologies, led by BES in partnership with Energy Efficiency and Renewable Energy (EERE), FECM and NE, identified priority research opportunities in August 2021.

The FY20 re-competition for the Fuels from Sunlight Hub issued awards to the Liquid Sunlight Alliance (LiSA) led by the California Institute of Technology, and the Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE) led by the University of North Carolina.

Research from the Biological Electron Transfer and Catalysis Center EFRC led by Washington State University provides a blueprint for engineering catalytic bias in synthetic oxidation-reduction catalysts, such as those used in hydrogen fuel cells.

The Carbon Management SETT, led by FECM with co-leads from BES and EERE's Bioenergy Technology Office (BETO), is addressing the NAS report on Negative Emissions Technologies (NET) and responding to Congressional direction to advance NET. Related research from ORNL demonstrates direct CO_2 air capture by crystallization of bis-iminoguanidine (BIG) carbonate salts. The Joint Center for Artificial Photosynthesis (JCAP) developed an efficient bipolar-membrane electrodialysis system to capture CO_2 from ocean water.

In FY21, Materials and Chemical Sciences Research for Direct Air Capture of Carbon Dioxide and Computational Chemical Sciences announced nine awards each. Awards will be announced soon for Data Science to Advance Chemical and Materials Sciences, Polymer Upcycling, and Critical Materials: Rare earth/platinum group.

The Energy Storage Grand Challenge, led by the Office of Electricity (OE) and EERE with participation from SC, FECM, ARPA-E and NE, launched the Long Duration Storage Energy Earthshot in July 2021.

The Joint Center for Energy Storage Research (JCESR), established in 2012, has made significant advances in research towards flow batteries and other innovative technologies.

The Materials Project is an important web-based database and analysis platform (sponsored by BES) that bridges basic materials science to applied research and R&D. It provides scientists information of known and predicted materials and chemistries and inspires the design of novel structures and processes.

The Public Reusable Research (PuRe) Data Resources aim to make DOE data publicly available in order to advance scientific or technical knowledge. Data sets from the Atmospheric Radiation Measurement Data Center; Joint Genome Institute; Materials Project (above); National Nuclear Data Center; Particle Data Group; and Systems Biology Knowledgebase are the initial recipients of the PuRe Data Resource designation.

Discussion

Epps asked about participation of HBCUs and MSIs from non-EPSCoR states. **Horton** stated that BES is considering revision of non-EPSCoR FOA program factors to encourage participation by MSIs and HBCUs from non-EPSCoR states.

Bent asked about opportunities for university participation in future microelectronics FOAs. **Schwartz** relayed that microelectronics was part of the EFRC FOA last year, and both awards are led by universities. This year's call was lab-focused. The FY22 budget increases

funding for microelectronics, and there is discussion about how to expand national laboratory efforts to include partnerships with universities and industry.

Stack asked if the various carbon sequestration roadmaps, including the NAS NET report and the Mission Innovation Carbon Capture, Utilization and Storage Experts' Workshop, are current enough to guide investments. **Garrett** noted that the NAS report was technology oriented with less attention given to infrastructure. Following Congressional direction, FECM is leading a committee with effort from SC-BES and BER to examine fundamental science opportunities relevant to carbon sequestration. BES has also been considering this topic itself.

Takeuchi asked about future EFRC calls. **Horton** confirmed that there will be an EFRC call in FY22 according to the budget request.

Kastner dismissed the meeting at 3:10 pm for a break and reconvened the meeting at 3:40 pm.

Roundtable Report: Office of Science User Facilities: Lessons from the COVID Era and Visions for the Future, Stephen Streiffer, ANL

The COVID-19 pandemic directly impacted the 28 SC user facilities, causing a shift to remote operations. An SC roundtable was chartered by the Office of the Deputy Director for Science Programs, in collaboration with the Science Programs Associate Directors and Office Directors across programs to capture lessons learned and to strengthen future operations.

The roundtable was held virtually from December 2-15, 2020. The ~50 participants, representing perspectives from different facilities and national laboratories, were divided into six panels based on themes derived from responses to a questionnaire that was circulated before the workshop: User research in virtual contexts; User research in physically distanced contexts; Facility operations in physically distanced or virtual contexts; User training/engagement; Computation, data, and network resources; and Crosscutting Issues. A letter report was delivered in January 2021 and a full report in July 2021.

During the pandemic, most facilities switched to full or predominantly remote operations with limited onsite users and functioned under new controls. In general, facility scientific productivity has been reduced, and early career researchers and staff have been significantly affected. Virtual collaboration tools have substituted for on-site presence, but gaps remain: new user training modalities have had to be implemented; user outreach has become limited; lack of onsite presence has impacted the concept of what " a user" means in some instances; higher-complexity, higher-payoff experiments have been deferred; staff have faced additional burdens to support remote users; creative interactions have been severely hampered; the loss of community built on physical presence has put mentoring, training, workforce development and other interpersonal activities at risk; and cyber security and cyber productivity issues have emerged.

On the other hand, remote operations have removed physical location and equity constraints leading to several opportunities to share lessons learned and best practices amongst facilities; develop new tools to engage and support broader user communities; federate data management tools and processes; reduce the environmental impact of travel and devote travel resources to other priorities; consider more efficient configurations for facilities and operations that confer better work/life balance; create and capture digital products from training sessions and other learning opportunities; free staff to focus on science by capitalizing on automation and virtualization; build and support more diverse and inclusive user communities and staffing paradigms; and support early career staff and users to ensure that they can succeed.

Virtual access is a double-edged sword, with costs and benefits differing for each facility. There are opportunities to capitalize on the rapid shifts necessitated by COVID-19 to move towards a new normal that might have been coming regardless.

Discussion

Chen asked about impacts to graduate students who need facility access to complete their research. **Streiffer** clarified that the report included graduate students with early career users.

Lester asked when user facilities will be considered essential travel for the national laboratories. **Horton** explained that the landscape is very complex. Central DOE coordination is incorporating feedback from across the system on this topic. **Streiffer** added that from the user facility and DOE perspective, the goal is to make sure everyone is safe. There will be dynamic adjustments at user facilities as circumstances change.

Roundtable Report: Research Opportunities in the Physical Sciences Enabled by Cryogenic Electron Microscopy, Amanda Petford-Long, ANL

CryoEM enables understanding of materials properties and chemical or biological processes at the atomic- to nano-scale when room temperature analysis is not appropriate. The CryoEM Roundtable Workshop was charged with identifying the key science drivers, research priorities, and research strategies for cryoEM in the physical sciences.

The workshop was held May 4-6, 2021, and participants were initially organized into four topical panels: Condensed phase chemical dynamics and reaction; Controls of structure and function in soft matter; Processes and chemical pathways in energy materials; and Low-temperature phenomena in quantum matter. Following discussion that included reconfiguration of the panels and crosscutting conversations, four Priority Research Opportunities (PROs) were developed: 1) Discover emergent behavior and coupled processes at interfaces; 2) Elucidate the role of heterogeneity in hierarchical systems; 3) Understand the evolution of matter in variable environments across length and time scales; and 4) Harness data analytics and automation to expand the role of cryoEM in enabling scientific discoveries. For PRO1, *in situ* experiments will link interface structure and chemistry to function by probing the frozen chemical states and physical behavior that only occur at low temperatures. For PRO2, cryoEM will lead to an understanding of how hierarchical systems form, how heterogeneity emerges, and how different system components interact. For PRO3, cryoEM will aid understanding of the energy landscape that controls assembly of matter, the subtleties of chemical transformations, and the dynamics of materials systems excited by an external stimulus. For PRO4, data science and data analytics offer exciting opportunities to revolutionize cryoEM use by capturing previously inaccessible phenomena.

To realize these opportunities, new capabilities are needed, including new approaches to sample preparation, storage, and transfer; high stability imaging and spectroscopy at cryogenic temperatures; *in situ* and *operando* experiments to track dynamic behavior; and integrating data science, theory, and correlative methods with cryoEM.

Discussion

Olvera de la Cruz asked how far away researchers are from developing the ability to track dynamics during experiments. **Petford-Long** said that some capabilities are already in

place, depending on the type of experiment. Following the dynamics of chemical processes, *in situ* will likely be the most challenging type of experiment because variable temperatures will be extremely important. Low temperature experiments in a magnetic field have already been enabled by use of the objective lens's magnetic field.

Gibson asked about varying temperatures for structural biology samples and whether instrumental developments are necessary. **Petford-Long** commented that getting to a fixed temperature and holding it is much easier than varying the temperature while simultaneously controlling other conditions like electric field. Though current detectors are faster and able to capture more processes than before, small instrumental developments will be necessary.

Ourmazd asked about thermal equilibrium and the impact of freezing or cooling on energy landscapes. **Petford-Long** mentioned that a number of nonequilibrium processes in quantum materials are important. Solid-state materials can be heated slowly and their processes examined under equilibrium conditions, but modeling and simulation are needed to ensure the correct operating conditions. Integration with theory, particularly for dynamics, will be critical to understanding operating and imaging regimes.

Diversity, Equity & Inclusion: Office of Science Activities, Julie Carruthers, Acting Director, Office of Diversity, Inclusion & Research Integrity

The SC has advanced several DEI initiatives by developing DEI plans at national laboratories; promoting DEI in SC's business practices; posting a SC statement of DEI commitment; increasing SC engagement with MSIs and underrepresented groups (URGs); facilitating DOE and interagency coordination; and establishing the Office of Diversity, Inclusion & Research Integrity.

In 2018, the SC called for a new SC working group on Diversity and Inclusion (D&I) to assess current DEI practices and to identify opportunities to further advance DEI in SC awards management and business practices. The working group systematically reviewed SC business processes related to research award activities, including award making policies; solicitation language; peer reviewer selection; peer review procedures; peer review of S&T research performance and SC facilities; workshops, roundtables and PI meetings; FACA committees and subcommittees; and implementation strategies. A broad spectrum of practices were documented, and the working group developed 15 recommendations that were further organized into seven action categories: DEI-supporting policies and practices; Standard review and selection criteria and protocols; Peer reviewers; Demographics tracking; SC-Sponsored meetings; Program manager guidance and supporting tools; and Community engagement. Recommended actions in these categories are geared towards being supportive and inclusive of women and URGs in Science, Technology Engineering and Mathematics (STEM) fields; allowing for more rigorous tracking of applicant, awardee, and reviewer diversity; limiting and mitigating potential implicit bias behaviors; and encouraging inclusive and professional behaviors in all SC-sponsored activities. The resulting report was unanimously approved.

To implement recommended actions, a reconstituted SC DEI Working Group is focusing on the development of a phased approach. Actions grouped within each phase will be implemented through a development process that involves pilot testing guidance or focus groups and regular check-ins with SC senior management.

In September 2020, SC began development of an SC-wide approach to increase engagement with MSIs and URGs. A formal working group was established in December 2020 to coordinate and implement a set of actions focused on increasing participation of MSIs and

URGs in SC-sponsored research; sharing outcomes and identifying lessons learned; and developing best practices. Near-term initiatives are aimed at identifying and developing opportunities to engage MSI faculty in increasing the number of applications (and proposal success rates) with MSIs as the lead institution; developing partnerships to attract and sponsor URGs; and increasing outreach, engagement, and recruitment of URGs at the national laboratories. The FY22 PBR includes funds to support the RENEW initiative geared towards providing undergraduate and graduate training opportunities for URGs to expand the SC workforce pipeline. To inform SC strategy, the working group launched a series of listening sessions seeking community input. A request for information to solicit broader community feedback is under development.

Discussion

Robertson asserted that universities need to be held accountable for adverse culture or climate. **Carruthers** agreed and invited suggestions on how federal agencies can hold universities accountable. Current award instruments offer limited leverage. Federal agencies are likely to be more effective acting as a whole with input from White House leadership. National laboratories are testing new ideas. For example, BNL created a one-week undergraduate opportunity during the winter semester for participants to tour the lab and meet staff. This program enables students to explore the lab environment and has been successful in increasing subsequent research applications from URGs. Other laboratories are adopting this program.

Robertson suggested that content from a prior workshop series held for academic and national laboratory leadership in chemistry, physics, and materials science could be useful. At the time, equity content relating to women and URGs impacted thinking of the leadership in attendance. **Carruthers** stated that content from that equity series was reviewed by the working group.

Bent expressed concern about the amount of effort placed on expanding the diversity of peer reviewers, claiming it is a diversity tax. As much or more emphasis should be placed on funding diverse recipients for research awards or symposia. **Carruthers** agreed. Many program managers recognize that by diversifying peer review panels, they are repeatedly asking the same people. This is why the SC wants to increase efforts to expand the reviewer pool and update the business system so that it is easy for program managers to track reviewer participation.

Takeuchi stated that bringing in and retaining diverse talent are equal challenges. If the culture and environment are not suitable, people will leave. Addressing individuals' sense of belonging and being able to succeed is critical. Individuals that repeatedly do not display welcoming behavior need to be held accountable, yet some are not. This requires community thought.

Gibson recommended providing resources to release faculty teaching loads at HBCUs and other MSIs that have been historically underfunded. Such institutions lack research infrastructure and need money to cover academic salaries in ways that Carnegie Research I (R1) institutions do not. **Carruthers** was unsure if SC financial assistance policies allow buying awardees out of teaching. The working group has heard about teaching load challenges and others. For example, Sponsored Research Offices at these schools may be small and unable to support applications for large solicitations. The amount of time a solicitation is open may also be limiting. **Kastner** remarked that SC policies previously allowed for buying out since he was required to do so by his university when working as a professor.

Chen asked about the demographics collected by the reviewer database. **Carruthers** said that the Portfolio Analysis Management System (PAMS) houses information from reviewers and applicants. Updates now require users to answer diversity questions, even if the answers are that the users decline to provide such information. These updates also make it clear that this information is protected by the U.S. Privacy Act of 1974 and can only be shared in aggregate. The system is imperfect because it requires individuals to already have an account for a program manager to identify reviewers. PAMS is an award management system and was never intended to serve as a reviewer database. Ongoing discussions are considering whether to increase PAMS functionality or to pursue options outside of PAMS. **Chen** emphasized that scientific expertise, not just demographic information, is necessary for selecting reviewers.

Olvera de la Cruz discussed challenges for finding peer reviewers for journal articles. In some cases, most reviewers are concentrated in a single country, necessitating a search for international reviewers. DOE might consider sending grants to certain countries when ethnicities are missing from the DOE review portfolio. **Carruthers** commented that the SC identifies experts from other countries. Indeed, all potential U.S. reviewers for a given solicitation are sometimes conflicted. Internal discussions about potential tools for identifying new reviewers are ongoing.

Public Comment Session

Benjamin Gilbert (chat) said there is a strong desire at national laboratories to collaborate on efforts to better include underrepresented researchers, but there are few structured opportunities and few incentives for scientists to participate. Internship programs are invaluable, but finding enough funding is challenging. Ideas and leadership from DOE are very helpful for ongoing laboratory networking efforts with MSIs.

Lemuel Patterson (chat) offered three suggestions: providing virtual lab tours; pre-recording Zoom meetings to introduce the lab setting and researchers; and supplying hyperlinks with a few engaging research questions for the undergraduates to explore, accompanied by dialogue opportunities with national laboratory graduate students.

Uta Ruett (chat, APS) asked if the 97% optimum funding level for facilities includes recommendations from the benchmarking report, such as better user support. **Horton** relayed that the calculation is based on the current funding level and does not include any major upgrades to user support. This will be evaluated moving forward. The RENEW program is part of the FY22 budget request and is being considered as part of current outreach activities.

Ruett (chat) asked about opportunities for facilities to improve outreach to and accessibility for industrial researchers. **Horton** stated that there are ongoing efforts to expand industrial access at user facilities, and every facility has industrial representatives on their advisory groups. There is still room for improvements.

Ruett (chat) remarked that opinions on remote access at user facilities may have changed since December 2020 when the Lessons Learned at User Facilities during the COVID-19 Era roundtable was held. People were initially excited about virtual opportunities, but many drawbacks have since emerged. **Horton** agreed that remote operations are difficult, and Streiffer's presentation discussed many drawbacks.

Kastner adjourned the meeting at 5:10 p.m.

Respectfully submitted, September 9, 2021

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ORISE/ ORAU