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

PUBLIC MEETING MINUTES
July 14, 2022

Virtual Meeting

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 a virtual meeting on Thursday, July 14, 2022, 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, Kavli Foundation
Esther Takeuchi, Vice Chair, Stony Brook University, Brookhaven National Laboratory (BNL)
John Allison, University of Michigan
Stacey Bent, Stanford University
Joseph Berry, National Renewable Energy Laboratory (NREL)
Joan Broderick, Montana State University
Lin Chen, Argonne National Laboratory (ANL), Northwestern University
Theda Daniels-Race, Louisiana State University
Abhaya Datye, University of New Mexico
Tabbetha Dobbins, Rowan University
Laura Gagliardi, University of Chicago
Jeannette Garcia, International Business Machines (IBM)
Padmaja Guggilla, Alabama A&M University
Javier Guzman, ExxonMobil
Sossina Haile, Northwestern University
Frances Hellman, University of California, Berkeley
Marc Kastner, Massachusetts Institute of Technology (MIT), retired
Lia Krusin-Elbaum, City College of New York
Allan MacDonald, University of Texas, Austin
Nadya Mason, University of Illinois
Shirley Meng, University of Chicago, ANL
Pietro Musumeci, University of California, Los Angeles
Abbas Ourmazd, University of Wisconsin, Milwaukee
Jose Rodriguez, BNL
Rachel Segalman, University of California, Santa Barbara
Andrew Stack, Oak Ridge National Laboratory (ORNL)
Cathy Tway, Johnson Matthey

BESAC Members Absent:

Lynden Archer, Cornell University
Helmut Dosch, Deutsches Elektronen-Synchrotron (DESY)
Thomas Epps, University of Delaware
Murray Gibson, Florida Agricultural and Mechanical University-Florida State University (FAMU-FSU)
Marsha Lester, University of Pennsylvania

Designated Federal Officer:

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

BES Management Participants:

Gail McLean, Acting Director, Chemical Sciences, Geosciences, and Biosciences Division
Andy Schwartz, Director, Materials Sciences and Engineering Division

BESAC Committee Manager:

Kerry Hochberger, Program Analyst

Thursday, July 14, 2022

Friend, BESAC Chair, called the meeting to order at 11:00 a.m. Eastern Time to a virtual audience of approximately 439 people. BESAC members introduced themselves.

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

Sustained support for research and innovation across the DOE SC's broad physical sciences portfolio, including facilities and infrastructure, is key to advancing scientific discoveries and technology development through the lens of inclusive excellence and economic growth. BES's fundamental research mission in understanding and controlling matter and energy is foundational to these efforts. Only through community-driven strategic planning can the nation's and world's scientific priorities be reached.

Achieving the Administration's goals of addressing climate change and developing clean energy technologies will require strengthening relationships between the SC and applied energy offices. The Undersecretary for Science and Innovation is leading joint Science and Energy Technology Teams (SETTs) to build and leverage these relationships through the Hydrogen, Long Duration Storage, and Carbon Negative Energy Earthshots. The DOE SC-supported Energy Earthshot Research Centers (EERCs) are a new research modality to support the initiative's decadal stretch goals through multi-investigator and multicenter collaborations that are closely coordinated with existing cross-office research consortia and demonstration projects. The new Accelerate Innovations in Emerging Technologies (ACCELERATE) initiative, supported in the fiscal year 2023 (FY23) Budget Request, will create highly integrated research teams to accelerate the discovery-to-commercialization path for new technologies. Envisioned novel collaborations will lower barriers to participation for those historically underrepresented in the scientific community. Dr. Berhe is committed to advancing all SC programs as well as emerging technologies such as artificial intelligence (AI), quantum information sciences (QIS), and microelectronics that enable progress in all areas of science.

Beyond internal DOE collaborations, advancing cross-agency collaborations to maximize federal research and development (R&D) investments will benefit the broader U.S. science ecosystem. For example, legislation supports collaborative BES, Department of Defense (DOD), National Institute of Standards and Technology, and National Science Foundation (NSF) semiconductor research through Energy Frontier Research Centers (EFRCs). Expanding international collaborations in a responsible manner will also advance Administration priorities for partnerships that maximize scientific access while maintaining research security.

Healthy stewardship of the DOE national laboratories and user facilities is necessary to expand their roles as regional hubs for economic opportunities and community benefit in partnership with federal, state, and local governments; universities; and the private sector. Partnerships among these facilities through the National Virtual Biotechnology Laboratory have delivered life-saving COVID-19 breakthroughs. Ongoing efforts are developing capabilities for a biopreparedness program across the SC portfolio. As outlined in BESAC's International Benchmarking Report, continued U.S. support of facility operations and construction projects is crucial in the face of intensifying overseas competition. Facilities face unprecedented challenges from supply chain disruption and inflation, and the DOE is undertaking a re-baselining process with community input to understand the resources necessary for future facility operations.

Central to all these efforts is the continuing and vital priority of increasing the accessibility of DOE SC-funded efforts through the principles of belonging, access, justice,

equity, diversity, and inclusion (BAJEDI). The Reaching a New Energy Sciences Workforce (RENEW) initiative will significantly expand training opportunities for undergraduate and graduate students from underrepresented and underserved groups (URGs). Justice40 is ensuring that SC is meeting the needs of communities most at risk, while the Early Career Research Program (ECRP) and Established Program to Stimulate Competitive Research (EPSCoR) are committed to supporting more inclusive generations of scientists from URGs from Minority Serving Institutions (MSIs), including Historically Black Colleges and Universities (HBCUs), and historically underserved states. The FY23 Budget Request also supports the new Funding to Accelerate Inclusive Research (FAIR) initiative to build the research capacity, infrastructure, and expertise at MSIs while developing mutually beneficial relationships with DOE national laboratories and user facilities. Broadening participation to tap into all of America's talent will require invigoration of existing and development of new communication strategies to better share scientific successes within DOE, with Congress, and with the public.

Discussion

Friend asked about areas where BESAC can provide helpful input. **Berhe** advised that BESAC can ensure that SC continues to fund the most competitive and exciting basic sciences. BES and the community have much to contribute to the Administration's priorities of clean energy, climate, microelectronics, workforce development, and others. The climate crisis has not been addressed at the needed level historically. Though BES is focused on curiosity-driven, fundamental science, thinking about how to contribute to ongoing efforts is important.

Dobbins raised impacts of supply chain disruption on user facilities and DOE labs. **Berhe** explained that a roundtable will address this topic next week to generate a clearer picture of current challenges and responses. Infrastructural delays and costs are a major DOE concern.

Takeuchi broached effective strategies for communicating DOE successes. Science communication is personally important to **Berhe.** Public institutions have a responsibility to educate the public about science activities. Even if the public cannot follow nitty-gritty details, sharing awe and excitement has huge impacts as demonstrated by recent images from the James Webb Space Telescope. An engaged public will have an easier time understanding why science needs support, with benefits to advancing science itself as well as providing training and economic growth opportunities. Scientists also have an important role to play in communicating with representatives and other stakeholders. There is no prescription for science communication in an evolving societal landscape. For those interested in participating, ongoing efforts are addressing how to invigorate SC communication strategies and seeking new communication avenues for DOE scientists. There is much to do in this space.

Pointing to SC's greater interest in translational research, inclusion, and community engagement, **Haile** asked about implementation strategies. **Berhe** indicated that engagement from BESAC and the community is welcome in this Administration's efforts. A responsible approach to publicly funded, curiosity-driven science includes thinking about possible applications to benefit society. SC is creating more opportunities for faster and effective translation. All suggestions are welcomed.

Chen appreciated recommendations for communication beyond national labs. Previously, DOE-funded fellowships provided opportunities to expose graduate students to the national labs. Students benefit from these training opportunities, but these programs are contingent on budgets and not well known in academic communities. Important to **Berhe's** own graduate education, such funding opportunities help introduce the next generation to the national labs. At present,

RENEW offers opportunities to broaden participation, and FAIR will do so in FY23 if funded. Future efforts will hopefully create a sustainable path for such funding opportunities to always be part of the SC portfolio. More information is coming this year.

Office of Basic Energy Sciences Update, Linda Horton, Associate Director; Gail McLean, Acting Director, Chemical Sciences, Geosciences, and Biosciences Division; and Andrew Schwartz, Director, Materials Sciences and Engineering Division

Horton presented evolving workplace practices due to COVID-19 and reviewed new personnel, retirements, and vacancies. Gail McLean is serving as Acting Director for the Chemical Sciences, Geosciences, and Biosciences Division.

The Enacted FY22 BES Budget of ~$2.3B represents a 2.8% ($63M) increase over that of FY21. Research program funding increased by ~$117M and includes ~$697M for clean energy, manufacturing, microelectronics, and critical materials as well as funding for RENEW (at $3M), continuation of EPSCoR (at $25M), and the Biopreparedness Research Virtual Environment (BRaVE) effort. Furthermore, ~$119M is allocated for Computational Materials and Chemical Sciences, Energy Innovation Hubs (Hubs) and the National Quantum Information Science Research Centers (NQISRCs). EFRC's budget is $130M. The Scientific User Facilities' budget increases by ~$16M, with $975M designated for facility operations to continue at 97% of the historically optimal level. Facilities Research receives $36M for artificial intelligence and machine learning (AI/ML) as well as Accelerator R&D in addition to $2M for RENEW. Funding for construction projects and major items of equipment (MIEs) decreases by $70M, with $106M for the Advanced Photon Source Upgrade (APS-U); ~$32M for the Linac Coherent Light Source-II (LCLS-II); $53M for LCLS-II High Energy (LCLS-II-HE); ~$75M for the Advanced Light Source Upgrade (ALS-U); $17M for the Proton Power Upgrade (PPU); $32M for the Second Target Station (STS); $3M for the Cryomodule Repair and Maintenance Facility (CRMF); $15M for the Nanoscale Science Research Centers (NSRCs) Recapitalization; and $15M for the National Synchrotron Light Source II (NSLS-II) Experimental Tools (NEXT-II).

In FY22, the ECRP conferred 38 BES awards totaling ~$41M to 31 university faculty, including 8 new BES Early Career institutions and 3 MSIs, and seven national lab scientists. Recipients hail from 20 states, including 8 EPSCoR states. Computational Chemical Sciences issued eight awards totaling ~$6M this first year. Remaining funding of $12M over two additional years is contingent on appropriations. Award teams are led by six universities and two national labs. Proposals are under review for Chemical and Materials Sciences to Advance Clean Energy Technologies and Low-Carbon Manufacturing (CEM, ~50 anticipated awards); EPSCoR, (~25-30 anticipated awards); and EFRCs (~30-35 anticipated awards).

In December 2020, SC initiated listening sessions and discussions to gather community input from URGs on barriers to participation in SC-sponsored opportunities. The most frequent comments addressed systemic barriers; lack of awareness of opportunities; implicit bias; access to equipment; solicitation processes; recruitment; promoting diversity, equity, and inclusion (DEI); and mentoring. Responses include new funding opportunity announcement (FOA) Program Policy Factors emphasizing the importance of diversity; expanded outreach including FOA webinars; enhanced user facility actions to engage URGs; issuance of the RENEW FOA; and the proposed FAIR initiative.

BES's RENEW goals are increased participation of URGs in BES's clean energy research portfolio; advancing a diverse, equitable, and inclusive research community; leveraging partnerships with BES's national labs and user facilities; and providing research training

opportunities for students, postdoctoral researchers (postdocs), and faculty from non-Carnegie Research 1 (R1) MSIs, including HBCUs, that are currently underrepresented in the BES portfolio. Non-R1 MSIs will be the primary award recipients and will form partnerships with or conduct internships at DOE labs or user facilities. The RENEW FOA was issued in May 2022 and an outreach webinar held in June 2022. Subject to appropriations, up to $15M in current and future fiscal years will support awards. Letters of Intent (LOIs) are due August 2, 2022, and applications on August 23, 2022. Award selection is anticipated during the first quarter of FY23.

Full reports are expected soon from the DOE Energy Sciences Computer Network (ESnet) Requirements Review for BES and the Foundational Science for Biopreparedness & Response Roundtable cosponsored by BES, Advanced Scientific Computing Research (ASCR), and Biological and Environmental Research (BER). BES's Roundtable on Foundational Science for Carbon Dioxide Removal (CDR) Technologies was held in March 2022, and a virtual Roundtable addressing Fundamental Science to Accelerate Nuclear Energy Innovation is planned for July 20-22, 2022. Finally, a Roundtable for Sustainable Aviation Bio-based Fuels is being planned by BER with Energy Efficiency and Renewable Energy's (EERE's) Bioenergy Technologies Office, ASCR, and BES.

The Carbon Negative Earthshot Summit is scheduled for July 20, 2022.

The BES FY23 Budget Request of ~$2.42B is 4.9% (+$112M) greater than the FY22 Enacted Budget, and the FY23 House Mark of ~$2.49B is 3.1% (+74.6M) greater than the FY23 Request. Under the FY23 Request or House Mark, respectively, funding for Research Programs increases by ~$138M or $84M; Scientific User Facilities decreases by ~$38M or increases by $91M; and Construction and MIEs increases by ~$12M for both. The House Mark reduces the SC Energy Earthshot Initiative from ~$104M to $50M with all other initiatives unchanged from the Request. The FY23 Request allocates ~$785M (increase of ~$88M; House Mark increase of ~$59M) for core research including BRaVE, manufacturing, AI/ML, FAIR, ACCELERATE, the SC Energy Earthshots, RENEW, and EPSCoR, which increases to $35M. Computational Materials and Chemical Sciences, Energy Innovation Hubs, and NQISRCs continue at ~$118M. EFRCs continue at ~$130M. The House Mark reduces the EERCs' FY23 Request from $50M to $25M. BES will complement EERCs with small group awards. Operations at the 12 BES facilities will continue at ~90% of the historic optimal at ~$925M (House Mark of ~$1.046B). Facilities research increases for AI/ML, BraVE, and Accelerator R&D at ~$51M. Funding for construction and MIEs includes ~$14M for APS-U; $94M for LCLS-II-HE; $135M for ALS-U; $17M for PPU; $37M for STS; $10M for CRMF; $2M for the High Flux Isotope Reactor (HFIR) Pressure Vessel Replacement (PVR); $1.5M for a new NSLS-II Experimental Tools project (NEXT-III); $25M for the NSRC Recapitalization project; and $25M for NEXT-II. The FY24 Budget Request is under discussion.

Mandatory LOIs for the FY23 Phase I Release FOA for Small Business Innovation Research and Small Business Technology Transfer (SBIR/STTR) programs are due August 29, 2022. Applications are due October 11, 2022. The FY23 Phase II Release 1 FOA will be issued October 17, 2022.

Upcoming events and items include Clean Energy webinars presenting research opportunities at user facilities; assessment of supply chain, inflation, and other challenges for facility operations and construction; International Benchmarking Reports from other SC offices which build on BESAC's process and report; a refresh of SC webpages; and BES staff travel to other meetings.

Discussion

Stack asked about program policy factors. **Schwartz** responded that every FOA lays out merit review and award selection processes. The latter takes topical diversity, institutional diversity, performance under past rewards, and a policy factor list into account. BES has expanded the policy factor list to support inclusivity and diversity efforts.

Bent wondered whether program policy factors acknowledge applicants' efforts to diversify the workforce. Might factors be expanded to review criteria for all FOAs? **Schwartz** said the RENEW merit review will evaluate applicants' recruitment and inclusion plans. Program policy factors implicitly consider principal investigator (PI) efforts to diversify the workforce. This is a new effort, and future assessments will determine effective practices that can be incorporated more broadly. **Horton** added that program policy factors are evolving; all kinds of team diversity are implicitly considered if not explicitly. This recommendation for broadening review criteria is appreciated.

Haile noted similarities between NSF's Partnerships for Research and Education in Materials Research (PREM) program and RENEW. MSIs may be reluctant to send their best students to premier research institutions because students will no longer produce work at their home institutions. A solution is to create partnerships with flow from the national labs to MSIs. Also, universities may internally downselect proposals due to submission limitations; downselection is not under the DOE's control, and there may be opportunities to expand diversity at this stage. **Schwartz** agreed.

Daniels-Race was glad to see RENEW's requirement that non-R1 institutions act as leads and appreciated Haile's remarks. In addition to requiring diverse applications, review processes need to incorporate diverse reviewers who have lived the experiences that the proposals are trying to engage. BES can include reviewers from smaller institutions; avoid using the same people for every review; and reach out to professional societies such as the National Society of Black Physicists, Society of Women Engineers (SWE), and Society of Hispanic Professional Engineers (SHPE) to help broaden the reviewer pool. Has DOE considered future strategies for incorporating diversity in light of possible Supreme Court decisions? For example, an NSF Scholarships in Science, Technology, Engineering, and Math (S-STEM) webinar indicated gender, ethnicity, and race could not be used as DEI criteria. A solution was to consider socioeconomic status. **Horton** commented that this is a difficult question. BES program policy factors are generic and consider all kinds of diversity. RENEW is focused on specific institutions. DOE pays attention to ongoing decisions and will continue to be as agile as possible to meet the goals of a diverse community. BES is engaging with professional societies as part of its outreach activities. **Schwartz** concurred that there is a need to diversify the reviewer pool along many axes. Doing so also expands community awareness of BES.

In reference to comments about Supreme Court decisions, **Hellman** observed that California has long prohibited use of race, ethnicity, and gender in selections. To help eliminate differential outputs from math and physical science programs, a current effort is focusing on recruitment criteria, especially applicants' involvement in activities. The University of Maryland at Baltimore County has succeeded in increasing numbers of African American PhDs by selecting individuals not based on race but on evidence of activity participation.

Meng appreciated BES's emphasis on DEI and the Director's use of BAJEDI. To bring a divided U.S. together, it is important to have a clear definition of justice, including from a socioeconomic perspective. **Schwartz** agreed. Many acronyms are in use; though all are connected, having clear definitions and being thoughtful in each acronym's use is important.

Stack inquired about the role of private industry in EERCs for moving fundamental science towards higher Technical Readiness Levels (TRLs). **Horton** recommended reading budget language. User facilities, but not BES, can support applied research. BES will continue to do basic research, but with a strong partnership with the technology offices. Basic research can be use-inspired to broadly support technology problems. Currently, EFRCs and some of the Hub programs push the boundaries for TRL 2-3.

Pointing to differences between the FY23 House Mark and the Request, **Dobbins** inquired about potentially partnering Earthshot efforts with facilities. Is the Supply Chain Report available? **Horton** replied that BES will accommodate the final appropriation. BES envisions building user facilities and industrial partners into Earthshot activities and will support efforts that bring together dream teams. The Supply Chain Report is available online.

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

EARLY CAREER PANEL: Cynthia Friend, Panel Lead

Friend commented that the BESAC International Benchmarking Report highlighted the need for early career support and continuity, especially in comparison to other international programs. This panel will provide an overview of BES's status on this topic.

BES Early Career Program, Andrew Schwartz, Materials Sciences and Engineering Division

Launched in 2010, the program aims to bolster the nation's scientific workforce by supporting exceptional researchers during their crucial early career years. SC Presidential Early Career Award for Scientists and Engineers (PECASE) candidates are selected from ECRP awardees. Expansion of early career PI engagement and opportunities has been recommended by BES and BESAC reports, Committees of Visitors (COVs), and other advisory groups.

The SC issues a common ECRP FOA with uniform program requirements and award parameters. Each program selects topic areas, conducts a peer review process, and offers selection recommendations. BES offers 25 research topics across its three divisions. To improve award success rate, starting in FY15, some BES program areas began alternating topics every other year. In FY19, program areas with large numbers of preapplications instituted a screening process to improve success rates, reduce reviewer workload, and help proposers maximize their three opportunities for full submissions by limiting full submissions to those with the highest likelihood of success. Eligible individuals from U.S. academic institutions and DOE national laboratories may apply if no more than ten years have elapsed between the year of their Ph.D. and the calendar year in which the FOA is released. Starting in FY20, the SC has considered extending eligibility for qualified life events such as military service or parental leave. Awards provide $150K or $500K per year for five years to recipients at universities or national labs, respectively.

Schwartz reviewed SC ECRP award statistics from 2010-2022, broken down by SC office and by the number of awards granted to recipients at universities or laboratories. BES's award success rate increased from 3% in 2010 to 5.5% in 2016 and was 13% in 2022. Awardees from 2010-2016 have graduated from the ECRP, and BES captured their baseline demographics (gender, minority status, EPSCoR institution, MSI institution), number of application attempts, and years since Ph.D. BES has also tracked award locations. Today, all states except four have received a BES ECRP award. Since awards were issued, approximately 20% of awardees (37 individuals) in the 2010-2016 BES ECRP classes moved. Today, awardees in these classes hold

positions at 11 DOE labs, 74 universities, one industry, and one government agency in 34 states, Washington D.C., and three foreign countries. BES is additionally tracking whether awardees subsequently apply for and receive additional BES funding and act as a senior investigator at a BES center. Finally, analysis of proposal text across topical areas is in progress as well as an ongoing collaboration with the DOE Office of Science and Technical Information (OSTI) to examine publication metrics. Data analytics will offer insights into the impact of ECRP awards on PIs' collaborative networks and the evolution of their scientific ideas.

Discussion

Garcia observed that many awardees are at universities, and few move to industry. Is there an opportunity to collect data about award impact on educators and their students? **Schwartz** agreed that this information would be interesting. It is challenging to track ECRP PIs and even more so to track students and postdocs. This was done temporarily for the EFRC program, but it is difficult to track individuals once funding ends.

Daniels-Race inquired whether the PIs that left academia did so before or after receiving tenure and about different award sizes to recipients at universities versus national labs. Award requirements could include an exit interview to aid in data collection. Is vertical position in the cloud chart of proposal text meaningful? **Schwartz** does not know if questions are asked about tenure and ECRP PI departure from academia. In the cloud chart, density, not position, is meaningful. Robin **Hayes**, BES Program Manager, added that density indicates correlation among items, and the color blue corresponds to proposal frequency in a given area.

Pointing to the low percentage of MSIs among award institutions, **Chen** inquired what percentage of universities are MSIs out of all U.S. universities. **Horton** appreciated this question. [Subsequent investigation indicates about 14%.]

Bent asked about the distributions of applicants and awardees as a function of years post-Ph.D. **Schwartz** clarified that BES has this data, and a comparison would be interesting (and could be included in future discussions).

Berry asked about the larger trend of PI movement from labs to universities; more information could inform community building. OSTI records offer a way to track awardees' effects on their fields, including translational impact in the context of other awards and publications. **Schwartz** agreed that publication records can reveal awardee career trajectories. Data currently do not offer insight into awardee movement from labs to universities. Subsequent to 2016, there are examples of individuals moving from universities to labs and joint appointments. However, this is a smaller trend.

Allison appreciated data illustrating awardee success in acquiring subsequent BES grants. Outreach to MSIs and EPSCoR institutions may encourage faculty to bring their best ideas to BES for ECRP awards not only because of renewal rates for DOE core programs but also because of the BES community.

MacDonald asked how ECRP interacts with early career awards from other agencies. **Schwartz** commented that ECRP takes awards from NSF, DOD, and other agencies into account. Selection can be challenging because the best applicants may be receiving awards from multiple agencies. There is no significant direct interaction among agencies, but early career awards are part of the overall dialogue. **Horton** added that DOE program managers have presented information to NSF awardees about broader opportunities.

Musumeci encouraged using data to compare how effective the BES ECRP is relative to other U.S. early career award programs and international programs. Data may also offer

preliminary guidance on differences between university and laboratory awards and whether the difference in award size is justified. **Schwartz** agreed that benchmarking across other national and international programs is important as well as comparing awardees with those who apply but do not receive an award. Adjustment of award size can be considered.

Dobbins suggested creating data teams to track the longitudinal impact of FAIR and RENEW. **Schwartz** concurred; BES is currently discussing data collection.

To assess selection effectiveness, **Kastner** relayed that the Sloan Foundation tracks the recipients of its early career awards and those applicants who just missed receiving an award. In the absence of a complete publication analysis, awardee publication citations offer a measure of how well the program is selecting awardees.

BES Early Career Network, Robin Hayes, BES Program Manager

The BES Early Career Network (ECN) was launched in 2015 to share best practices between centers, provide workforce development opportunities, and create a network of early career scientists. At present, the ECN's >1.6K members include graduate students, postdocs, and early career scientists from universities, national laboratories, industry, and current EFRCs, BES Energy Innovation Hubs, Computational Materials Sciences (CMS) awards, and Computational Chemical Sciences (CCS) awards. Centers may appoint one representative to the ECN's planning group. There have been 247 BES ECN representatives from 78 institutions in 30 states and Washington, D.C.

Planned events organized by BES ECN representatives include panels and workshops, with examples addressing career pathways; diversity; the budget process; communication; industry; science policy; and elevator pitches. Representatives also organize social events.

The ECN hosts two to four webinars per year that are now open to the public. Grant writing is a favorite webinar topic; this year's writing webinar was attended by ~2K individuals.

Representatives also select five topics each year for internal discussions. Past topics include careers, DEI, early career engagement, mental health/work-life balance, mentoring, networking, outreach, science communication, and team science. Representatives share discussed information with their communities.

The BES ECN website (https://www.energyfrontier.us/ecn-events) provides an overview of the network, representatives' information, and event information. Event information is cross-posted with other organizations. Additional communication channels include the BES ECN GovDelivery list, which is open to the public, and the DOE BES ECN LinkedIn Group. Representatives have access to an internal Microsoft Teams channel.

To gain experience writing for the general public, ECN members are encouraged to write EFRC Newsletter articles. To date, 154 ECN authors have contributed 316 articles.

Discussion

Segalman asked about retaining ECN members in the DOE envelope. **Hayes** presents information about BES and the graduate fellowship to new representatives each year. Career and grant writing webinars are popular; grant writing webinars discuss how to submit a BES grant, and career webinars showcase national laboratory speakers.

Mason inquired about tracking ECN impact on member success. **Hayes** explained that there has been no long-term, systematic study. Some individuals share where they wind up. Participants are asked to provide feedback at the end of each event and to conduct an annual self-reflection exercise.

Hellman expressed interest in industry participants. **Hayes** said that this contingent is a small pool, mostly funded by BES. Typically, individuals are already involved in a research center and have permission to engage in ECN activities. Relatively few are directly from industry.

Early Career Programs at Lawrence Berkeley National Laboratory (LBNL), Horst Simon, Lawrence Berkeley National Laboratory

LBNL's Early Career Lab-Directed Research and Development (LDRD) Program was created in FY17 to develop more diverse PIs with early career project leadership experience and to prepare participants for successful ECRP proposals. The program provides awardees with $225K/year for two to three years and operates on ~10% of LBNL's annual LDRD costs. Since FY19, six individuals have been selected each year based on the strength of their science proposals, and three individuals from the FY18 and FY19 classes have received ECRP awards. Others have moved onto strong national laboratory careers with programmatic funding. The LDRD program has succeeded in engaging ~30% female PIs, a noteworthy figure when compared to LBNL's ~14% female staff scientists and senior scientists.

The Cyclotron Road (CR) program is DOE's first fellowship program for technology entrepreneurs focusing on national energy challenges. CR has fostered participants from 56 companies that have raised >$400M in follow-on funding.

LBNL's Career Pathways Office (CPO) was created in FY18 by consolidating several lab-funded career development programs. The Berkeley Bridge Graduate Summer Fellowship, started in 2018, is a graduate student summer program designed to engage top University of California, Berkeley graduate students from URGs in active research roles at LBNL. The Early Career Enrichment Program (ECEP), launched in 2018, expands the lab's early career researchers' awareness of the diversity of LBNL science, engineering, and operations, and helps them develop meaningful connections with lab leadership, staff, and each other. The CPO also addressed a gap in postdoctoral career development support and serves as a central resource. In 2019, >200 postdocs attended the first annual Postdoc Career Fair. In February 2020, the lab's K-12 STEM program with CPO launched the Teaching Scholars Program for postdocs interested in education. Other postdoc resources include workshops and a Postdoc Training Grant opportunity. The CPO also organizes an annual LBNL Research SLAM that challenges early career researchers to present short, compelling research presentations for broad audiences.

The Berkeley Lab Postdoc Association was formed in 2016 and engages ~1K LBNL postdocs. Its three committees address Outreach, Lab-Industry Networking Connections, and Social & Outdoor events.

The LBNL Postdoc Alumni Project tracks the broad career paths pursued by postdocs. Statistics from 2015-2020 alumni indicate ~1/3 pursued careers in a) industry, b) academic, and c) government or nonprofit sectors each. Due to LBNL's international pool of postdocs, it is not surprising that postdocs pursue work in many different countries. Of the ~1K alumni, ~15% transition to LBNL scientific roles and relatively few transition to other national labs.

A relatively small investment in early career development can have a large impact on future lab staff development. Such support is particularly important for increasing diversity and engaging millennials. There are opportunities to further integrate DOE SC early career programs and create multi-lab postdoc programs that will help early career scientists develop careers spanning multiple national labs.

Discussion

None.

Science and Energy Crosscuts and Energy Earthshots Overview, Kelly Visconti, Crosscut Team Lead, Office of the Under Secretary for Science and Innovation

The Administration's climate and energy goals of halving carbon dioxide (CO_2) emissions by 2030, achieving power sector net-zero emissions by 2035, and deploying economy-wide net-zero emissions by 2050 requires an all-hands-on-deck approach. The Office of the Under Secretary for Science and Innovation (S4) Science and Energy Crosscut Team is spurring progress towards these goals through a fully integrated science and applied energy research, development, demonstration, and development (RDD&D) paradigm within and across key DOE technology domains and is leading the DOE Energy Earthshots Initiative.

Science and energy crosscuts prioritized in FY21-22 include but are not limited to hydrogen; energy storage; carbon management; grid modernization; critical minerals and materials; industrial decarbonization; STEM; subsurface clean energy applications; clean energy technology manufacturing; net-zero buildings; sustainable fuels; and the energy-water nexus.

The Energy Earthshots Initiative targets a subset of the hardest remaining RDD&D challenges to solve within a decade to reach the 2050 net-zero goal. Three Earthshots have been launched thus far: the Hydrogen, Long Duration Energy Storage, and Carbon Negative Earthshots. Formation of each initiative is advised by the Energy Earthshots Working Group, consisting of DOE Senior Leaders from the Office of Energy Efficiency and Renewable Energy (EERE), Fossil Energy and Carbon Management (FECM), Office of Nuclear Energy (NE), SC, Office of Electricity, Office of Technology Transitions, Office of the Secretary of Energy, Office of Policy, Advanced Research Projects Agency-Energy (ARPA-E), Office of Economic Impact and Diversity, and the SunShot Initiative. Earthshot facilitation is supported by the Hydrogen, Energy Storage Grand Challenge, and Carbon Management SETTs. Each Earthshot was developed through an ideation, scoping, and development process before being launched through a summit. Implementation includes processes around stakeholder engagement, planning and execution, and progress tracking and reporting.

Discussion

Friend asked how the Earthshot process integrates feasibility considerations and mechanisms for course corrections. Successes en route are important. **Visconti** stated that while each Earthshot is in a different technology area, a deep dive is initially taken to create a baseline assessment of technology cost performance and to understand where there are foundational barriers that need to be addressed through funding opportunities. BES roundtables provide useful information about foundational barriers. As advised by the SunShot Initiative, understanding the baseline, ensuring progress, and realizing that roadblocks may require a course adjustment are baked into the Earthshot initiatives.

Berry drew attention to an asymmetry between energy generation and longer-term storage in the current Earthshot array and invited perspectives on a gap analysis in this context as well as takeaways from the SunShot Initiative. **Visconti** relayed that the current Earthshots are crosscutting in nature. Hydrogen is a broad technology with applications in almost every sector. Long-duration storage efforts can be connected to the grid. CO_2 removal is an extensive clean-up effort. Future Shots may consider the economy-wide footprint of major sectors like production,

industry, buildings, and transportation and may determine if an Earthshot initiative is the right model. Regarding the SunShot Initiative, this effort alone is not responsible for all advances in solar energy, but there is tremendous power when the government elevates conversation to the national level around a priority. International competitors also pay attention to where the U.S. spends money. The Earthshots are also considering domestic manufacturing supply chain issues in the context of energy justice, equity, and workforce.

MacDonald sought additional Energy Storage Earthshot details. **Visconti** explained that batteries served as the Shot's baseline. For grid-scale systems, however, batteries are only one approach, and the goal of long-term storage is technology-agnostic. Beyond daily storage cycles, other technologies rise to the top, as detailed in NREL's Storage Futures Study.

Allison posed a question about industry involvement. **Visconti** reflected that this initiative, launched a year ago, is a work in progress. Industry involvement mechanisms are still being determined. DOE's applied offices do engage with industry, and the SETTs are ensuring that industry connections are being built. BES roundtables also offer connection opportunities. All suggestions are welcome. **Horton** added that communication is a hallmark of the interactions involving the technology offices and the S4 Crosscut Team. BESAC's comments underscore the importance of appropriately connecting basic and applied efforts, which include the national labs and technology offices, and their contacts with industry.

Meng stressed the importance of communication; those from the fundamental and applied sciences can say things differently, inadvertently creating barriers. Bringing expertise from international allies is important. Japan has had consistent hydrogen technology policies for 20-30 years. **Visconti** agreed.

Friend dismissed the meeting at 3:02 pm for a break and reconvened the meeting at 3:32 pm.

***OPERANDO* SCIENCE AND INSTRUMENTATION PANEL**: Esther Takeuchi, Panel Lead

Takeuchi defined *ex situ* methods as removing parts for analysis outside the functional environment; *in situ* methods as measuring a property or material in a working environment, but the system may not be operating at the time of measurement; and *operando* methods as probing the system while operational to gain information on kinetics and transient species in a functioning environment. There has been a huge growth of *in situ* studies over the last ten years. Use of *operando* studies is still nascent. Due to the many time and length scales impinging on a system, multiple techniques are often needed for full interpretation.

Synchrotron X-ray Characterization of Lithium-Ion Batteries, Johanna Nelson Weker, SLAC National Accelerator Laboratory and Stanford University

Batteries offer an excellent system for *in situ* and *operando* studies using different techniques across length scales from angstroms to millimeters. Research efforts have developed a robust *operando* pouch cell design for multiple techniques (scattering, spectroscopy, microscopy); long-term cycling (e.g., months); and fast data collection (e.g., one-minute charge/discharge cycles). The setup enables simultaneous characterization of multiple cells.

Presented science highlights addressed stabilizing alloying anodes and interfacial engineering with hard x-rays as well as probing fast-cycling anode materials with x-ray diffraction (XRD) and x-ray absorption spectroscopy (XAS).

Beyond energy storage systems, ongoing work is utilizing synthesis and small-angle x-ray scattering (SAXS) to optimize atomically precise catalysts; SAXS and polymer deconstruction for upcycling; synthesis with XRD for examination of metal-organic frameworks, and XRD and extended x-ray absorption fine structure (EXAFS) and annealing techniques to study perovskite photovoltaics (PV).

***In situ/Operando* Studies of Energy Storage Materials using Neutrons,** Ashfia Huq, Sandia National Laboratories

Neutron spectroscopy complements x-ray scattering by detecting light atoms, even in the presence of heavy atoms, and can track movement of lighter elements such as lithium and hydrogen through a system. Neutrons additionally distinguish between isotopes. Being electrically neutral, neutrons can penetrate bulk material. Other pertinent techniques include reflectometry, small-angle neutron scattering, vibrational spectroscopy, and quasielastic neutron scattering. *In situ* and *operando* studies open the window for non-equilibrium characterization and leverage fast spectroscopy techniques along with large-volume data analysis complemented by modeling. Basic exploratory research to understand fundamental working principles and mechanisms driving operations, performance improvement, process development, and failure analysis is vital for industry applications.

Science highlights addressed oxygen flow in solid oxide fuel cells; lithium dendrite growth to understand mechanisms of short-circuiting in an all-solid-state battery; methods of solid-state synthesis of the lithium lanthanum zirconium oxide (LLZO) electrolyte that reduce energy usage and lithium loss; and real-time battery cycling using Australia's Wombat High-Intensity Power Diffractometer.

***Operando* Electron Microscopy for Energy Generation, Use, and Storage**, Katherine Jungjohann, National Renewable Energy Laboratory

Multiple BES reports have highlighted the importance of characterizing atomic-scale energy phenomena, including interfaces, impurities, transient states, reaction mechanisms, and degradation pathways. *In situ* and *operando* transmission electron microscopy techniques probe systems at the nanoscale under various environmental conditions using *in situ* holders or micro-electromechanical system (MEMS) devices. MEMS devices additionally enable transitioning among multimodal techniques. However, beam effects on samples may limit atomic-scale *operando* EM approaches. Comparing *operando* results with those of other imaging and analytical techniques is essential for an accurate understanding of observed phenomena.

Presented science highlights characterized lithium grain formation to elucidate battery degradation pathways using *in situ* and *operando* electron microscopy (EM) and cryogenic EM.

This research relies on DOE SC's five NSRCs to provide state-of-the-art capabilities and generate new techniques. Workforce development in this area is critical; time is needed to develop expertise in these methods.

***Operando* Science Enabled by the Linac Coherent Light Source (LCLS),** Leora Dresselhaus-Marais, SLAC National Accelerator Laboratory and Stanford University

Advanced microscopes, rare-event cameras, and AI for analysis, reactor modeling, and control facilitate metals processing science across time and length scales to enable sustainable technology.

Science highlights showcased advanced x-ray imaging techniques to characterize phonon interactions with material defects; failure mechanisms of new ultra-hard materials; and alloy selection using shock waves to test failure. Additional research investigated materials performance and chemistry in hydrogen environments using ultrafast electron diffraction.

The LCLS-II-HE will augment x-ray free electron laser (XFEL) capabilities to provide ultrafast, coherent, hard x-rays; an ~3K-fold increase in average spectral brightness; and an ~8K-fold increase in repetition rate. This technology will enable advances in *operando* studies for mapping reaction landscapes in real environments, materials characterization, and advancing understanding of biological function and structural dynamics. Ongoing efforts are designing detectors and AI for data capture of ultrafast and stochastic processes.

Discussion

Jose Rodriguez inquired about the relationship between spatial and time resolutions across techniques. **Dresselhaus-Marais** replied that XFEL techniques are broad, offering access to time scales from 200 attoseconds to minutes. Length scales will depend on time scales, and coherent diffraction imaging offers access to lengths from 5-30 nanometers up to a millimeter. **Weker** noted that time and length scales also vary with synchrotron x-ray techniques. It is possible to achieve angstrom-level resolutions in milli- to nanoseconds. Nanometer imaging resolution is possible in half-seconds as well as micron resolution at 20 kilohertz. **Jungjohann** commented that femtosecond reversible processes are observable at the atomic-scale resolution. Irreversible processes may require sacrificing spatial resolution. Increasing beam power will show what is happening but may cause too much damage. Some researchers image over months.

Garcia inquired about methods to address the lithium dendrite problem in shorting batteries and whether the dead lithium is produced during battery operation or is initially present as lithium metal impurities. **Jungjohann** advised that coatings may protect the lithium from interacting with the battery electrolyte; this is a challenging problem as this interface evolves over battery cycles. Lithium stripping does not remove the entire grain, leaving small deposits bound to the solid electrolyte interphase and creating electronic bridges.

Datye praised development of new capabilities and inquired about facility funding in the context of the university user community. **Horton** offered that funding is a work in progress. The FY23 mark increases operations funding for the user facilities in recognition of challenges. Additionally, SC is reviewing operations funding models because inflation and staffing situations have changed. *Operando* experiments are challenging and require more time, better computer interfaces, and greater staffing. DOE supports graduate research programs that enable three-month stays at national laboratories. The RENEW program targets specific institutions, and funding will ensure that laboratory staff will have time for mentoring and training activities. **Weker** added that *in situ* and other techniques are often developed with EFRC or Hub funding and subsequently rolled out to broader community use. Efficient use of funding and crosstalk has also led to transfer of preexisting software to battery applications.

Berry observed that measures are not completely independent from the measurement techniques used. Are there opportunities to use probes to manipulate systems more directly? **Huq** remarked that synthesis reduces phase space and can create a feedback loop. Obtained measurements can inform materials synthesis strategies that save months of trial-and-error work. **Dresselhaus-Marais** replied that XFEL inevitably causes damage, but pulse duration is so quick that diffraction occurs before material destruction. More recent studies have examined using XFEL as a gentle heater to access different pieces of the phase space with each pulse so that the entire temperature curve of a phase diagram can be obtained in a millisecond. There are interesting opportunities for thermal engineering projects.

Public Comment

Jacquilyn Weeks (Sandia National Laboratories, via chat) asked if *operando* techniques are likely to be priorities for future funding opportunities such as the ECRP. **Horton** indicated that technological advances are supporting the vision of probing systems in real time. There are opportunities for proposing *operando* techniques across multiple BES programs, including those focused on techniques for electron microscopy, x-rays, or neutrons, as well as the ECRP and the regular annual FOA that is open year-round to researchers at all career stages. *Operando* techniques touch on many priorities, including energy research, advancing world-leading techniques, and data and AI/ML. **Friend** added that BES's unique and cutting-edge user facilities add tremendous value in this research area, as highlighted in the BESAC International Benchmarking Report.

Julia Hsu (University of Texas, Dallas, chat) questioned the distinction between *in situ* and *operando* techniques. **Takeuchi** explained that *in situ* refers to a sample in its native environment, but with no intentional, dynamic processes. For example, *operando* studies would examine a functioning battery or changes to reagents during an active chemical synthesis.

Kathryn Perrine (Michigan Technical University, chat) asked if R2 institutions are eligible for FOAs other than RENEW. **Horton** explained that RENEW is the only BES FOA with institutional restrictions. R2 institutions are eligible for all BES FOAs.

Horton mentioned that additional charges may be presented at the next BESAC meeting.

Friend adjourned the meeting at 5:05 p.m.

Respectfully submitted on July 25, 2022
Holly Holt, PhD
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