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

PUBLIC MEETING MINUTES
December 6, 2021

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 Monday, December 6, 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, Massachusetts Institute of Technology (MIT), retired
Lynden Archer, Cornell University
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
Thomas Epps, University of Delaware
Cynthia Friend, BESAC Vice Chair, Kavli Foundation
Laura Gagliardi, University of Chicago
Jeanette Garcia, IBM
Javier Guzman, ExxonMobil
Frances 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

John Allison, University of Michigan
Helmut Dosch, Deutsches Elektronen-Synchrotron (DESY)
Murray Gibson, Florida Agricultural and Mechanical University-Florida State University (FAMU-FSU)
Yan Gao, General Electric Company (GE), retired

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 Division
Andrew Schwartz, Acting Director, BES Materials Sciences and Engineering Division

BESAC Committee Manager:

Kerry Hochberger, Program Analyst, BES

Monday, December 6, 2021

BESAC Chair Marc Kastner called the meeting to order at 11:00 a.m. Eastern Time to a virtual audience of approximately 385 people and requested that BESAC members introduce themselves.

Office of Science Update, Steve Binkley, Acting Director

Binkley reviewed the status of political appointees and DOE Office of Science (SC) staff. Asmeret Berhe, the SC Director nominee, awaits a final confirmation vote before the full Senate. Geri Richmond, a former BESAC Chair, was sworn in last week as the Under Secretary for Science and Energy and is meeting regularly with SC leadership. Adam Kinney is serving as interim SC Chief of Staff. Mailinh McNicholas is a new Special Assistant.

Under the Biden-Harris Administration, the DOE Applied Energy programs were returned to the purview of the Under Secretary for Science and Energy, as organized during the second term of the Obama Administration. This provides opportunities for closer work between the SC and Applied Energy programs.

The 2022 fiscal year (FY22) President's Budget Request (PBR) seeks $7.44B for the SC, which is a ~5.9% (~$414M) increase over the enacted FY21 PBR. The House Energy and Water Development Subcommittee issued a lower markup of $7.32B. The Senate markup is higher at $7.49B. Any increase will be to the overall budget and will not be the same for every SC program.

The Infrastructure Bill allocates $62B to the DOE, primarily for demonstration activities in applied energy areas. SC activities are not targeted. The Reconciliation Bill does provide funds to the SC, but negotiations are still ongoing. The ongoing Continuing Resolution (CR) has been extended from December 3, 2021 through early February 2022. DOE anticipates having a FY22 budget in February 2022.

Discussion

Friend inquired about the FY22 budget. **Binkley** explained that budget increases will not be applied uniformly across programs. For example, proportionally more money will be conferred to safeguards and security activities. There are significant percent increases for each main SC program, including for BES, Advanced Scientific Computing Research (ASCR), Biological and Environmental Research (BER) and others.

Kastner asked how the Applied Energy programs' budget compares to that of the SC programs. **Binkley** has not yet seen detailed funding for the Applied programs. The top-line increase for the DOE is 5.89%. The top-line increase for the Office of Energy Efficiency and Renewable Energy (EERE) is ~20%. The Administration's priorities include clean energy and climate, and these are reflected in the PBR.

Takeuchi asked if new funding opportunity announcements (FOAs) will be postponed until after the CR concludes. **Binkley** said the SC will proceed with FOAs, and several have been issued already. During a CR, the lowest budget number among the PBR, House markup and Senate markup is used to limit funding.

Kastner inquired whether other SC programs are writing international benchmarking or anniversary reports similar to recent reports completed by BESAC. **Binkley** praised BESAC's leadership in paving the way for BER and ASCR to conduct similar studies.

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

Horton shared information about new BES personnel, retirements, and position openings. Several program positions are acting. Noting that Kastner is completing his 2019-2021 term as BESAC Chair, Horton thanked Kastner for his service and recognized BESAC accomplishments under his leadership.

In FY21, new BES grants had a 20% success rate on average, and BES supported ~1,500 core research projects and >200 small business research projects. The 12 BES user facilities supported ~11,300 users of which 64% were remote. BES is paying close attention to this coronavirus (COVID-19)-driven sea change in how user facilities are accessed.

Construction projects for facility upgrades and Major Items of Equipment (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 $1.136B. Critical decision-4 (CD-4) is projected for FY24. COVID-19-related delays have moved dark time for the Advanced Photon Source Upgrade (APS-U) installation to FY23, with CD-4 projected in FY26. APS-U is currently at CD-3 and has a TPC of $815M. The project to double the Spallation Neutron Source (SNS) accelerator beam power to 2.8 MW, the Proton Power Upgrade (PPU), received CD-2/3 in October 2020; CD-4 is projected for FY28, and the TPC is $272M. The Advanced Light Source Upgrade (ALS-U) has a TPC of $590M and attained CD-2 in April 2021 with CD-3 projected for FY23. ALS-U CD-4 is anticipated in FY29. The National Synchrotron Light Source-II (NSLS-II) Experimental Tools (NEXT-II) MIE received CD-2/3 in October 2021 and has a TPC of ~$95M. CD-4 is projected for FY28. New scope was added to the Linac Coherent Light Source-II High Energy (LCLS-II-HE) project, currently at CD-1. The TPC estimate is $660M, with CD-2/3 projected for FY22 (with delay expected to FY23) and CD-4 projected for FY31. The Second Target Station (STS) received CD-1 in November 2020; the TPC range 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), currently at CD-0, continued conceptual design and alternatives analysis. The TPC range is $70M-$98M with CD-1 projected for FY23. The Nanoscale Science Research Centers (NSRCs) Recapitalization MIE is at CD-1/3A and has a TPC of $80M. CD-2/3 is projected for FY22.

The FY22 House and Senate marks for BES are similar to the PBR of ~$2.3B (+$55M over the FY21 Enacted Budget). Under the PBR scenario, funding for research programs will increase by ~$109M and will include ~$690M for Research (+$92M over FY21's Enacted Budget) in clean energy, manufacturing, microelectronics, Reaching a New Energy Sciences Workforce (RENEW, at $5M), and continuation of the Established Program to Stimulate Competitive Research (EPSCoR, at $25M). Furthermore, ~$118M is allocated for continuation of Computational Materials and Chemical Sciences, Energy Innovation Hubs, and National Quantum Information Science (QIS) Research Centers; and ~$130M (+$15M over FY21's Enacted Budget) for continuation of the Energy Frontier Research Centers (EFRCs). Funding for scientific user facilities will increase by ~$16M over FY21 levels. Of these funds, ~$975M is designated to support operations at the 12 user facilities at 97% of the optimum level and ~$38M to continue facilities research in artificial intelligence and machine learning (AI/ML) and Accelerator Research and Development. Funding for construction and MIEs will decrease by \$70M with \$106M for APS-U; ~\$32M for LCLS-II; \$53M for LCLS-II-HE; ~\$75M for ALS-U; \$17M for PPU; \$32M for STS; \$3M for CRMF; \$15M for NSRCs Recapitalization; and \$15M for NEXT-II.

BES's FY22 budget reflects Biden-Harris Administration priorities and SC-wide initiatives in clean energy, climate, and diversity, equity and inclusion (DEI). The SC is identifying and developing opportunities to increase research funding applications and success rates from Minority Serving Institutions (MSIs) and to increase recruitment of underrepresented groups (URGs) among students and faculty to SC-sponsored research opportunities, including at the DOE national laboratories. BES FY22 FOAs incorporate new language encouraging applications from MSIs, including Historically Black Colleges and Universities (HBCUs), as well as from individuals from groups historically underrepresented in Science, Technology, Engineering and Math (STEM) fields. BES is also participating in outreach and listening sessions to understand barriers to STEM research faced by MSIs and URGs.

The BESAC International Benchmarking Subcommittee issued a report titled *Can the U.S. Compete in Basic Energy Sciences?* The report examines U.S. competitiveness in BES research areas, facility capabilities, and funding mechanisms. Findings indicate the U.S. has plateaued or fallen behind other global leaders, especially those in China and Europe, in key areas. Recommended U.S. strategies include increased investment in research, facilities, and instrumentation; greater support for early- and mid-career scientists; improved opportunities for facility staff scientists; and better integration of energy sciences research across the basic to applied to industrial spectrum.

In FY21, two BES Roundtables resulted in priority research opportunities (PROs) for 1) Cryogenic Electron Microscopy (cryo-EM) in the Physical Sciences (full report posted); and 2) Advancing Foundational Science for Carbon-Neutral Hydrogen Technologies (brochure posted).

BES is participating in the cross-DOE Energy Earthshots Initiatives, including the Hydrogen Shot, Long Duration Storage Shot, and Carbon Negative Shot.

BES is the leading organization of the planned Foundational Science for CO_2 Removal (CDR) Technologies Roundtable with participation from Fossil Energy and Carbon Management (FECM), EERE, and Advanced Research Project Agency-Energy (ARPA-E). The draft Roundtable scope considers current and new CDR technologies addressing CO_2 capture from dilute sources; durable CO_2 storage in minerals and materials; and geological sequestration. The Roundtable will revisit findings from the earlier National Academies Report, *Negative Emissions Technologies and Reliable Sequestration.*

BES has identified overarching research priorities for the FY22 Solicitation for the Office of Science Financial Assistance ("Open Call") FOA: Fundamental Science to Enable Clean Energy; Critical Materials/Minerals; Fundamental Science to Transform Low-Carbon Manufacturing; AI/ML; and QIS. Invited full applications for the Early Career Research Program (ECRP) are due January 20, 2022. The FY22 EPSCoR FOA focuses on partnerships between institutions and national laboratories; pre-applications are due January 13, 2022. Pre-applications for the BES-issued Computational Chemical Sciences (CCS) FY22 FOA are due January 7, 2022. Per the FY22 PBR, BES plans to issue an EFRC FOA for new and renewal applications. EFRC emphasis may include Science for Clean Energy; Science for Advanced Manufacturing; and Other National Priority Research Areas like QIS or Quantum Materials. BES also plans to issue a FOA for new applications from single PIs and small teams for chemical and materials sciences to advance clean energy technologies and to transform manufacturing. This FOA may include Science for Clean Energy; Science to Advance Low-Carbon Manufacturing; and Critical Materials. Though there are no formal changes in data management plan (DMP) requirements, SC updates to applicant guidance for DMPs will be effective for all solicitations issued after January 1, 2022. Reviewers will be required to read the new Guidance for Reviewers of DMPs.

The forthcoming new charge to BESAC, a COV for the SC Office of Workforce Development for Teachers and Scientists (WDTS), was noted, with report expected in Summer 2022. This was addressed in more detail by WDTS Director Ping Ge later in the meeting.

Discussion

Harriet Kung (DOE SC) thanked Kastner for serving as BESAC Chair and appreciated his skilled leadership. **Friend**, the next BESAC Chair, and **Meng** echoed praise. **Kastner** acknowledged these remarks and recognized contributions from BESAC, DOE, and others.

Friend asked about personnel management at BES user facilities, noting increases in remote users and citing findings from the BES International Benchmarking report. **Horton** said COVID-19 has necessitated innovation and expansion of remote user accommodations at BES facilities. This transition highlighted cyber security and staffing challenges. Funding from the Coronavirus Aid, Relief and Economic Security (CARES) Act supported new remote equipment and user time. However, instrument scientists cannot be replicated; they have reported high stress levels. Moving forward, BES will continue to evaluate remote operations and staffing needs. There is an opportunity to expand facility use to URGs in STEM. The BES International Benchmarking report identified some of these issues, especially for instrument scientists whose workloads and time for personal research were heavily impacted by COVID-19.

Archer asked about the EFRC FOA and BES engagement in the Earthshots. **Horton** cannot say when the FOA will be released. However, since the EFRC is a longstanding program, its release is not contingent on an appropriation. All discussed Earthshots will require discovery science to enable stretch goals. BES, BER, and ASCR facilities and capabilities are critical assets, and BES will help ensure a strong science foundation that intersects with technology research. The Infrastructure Bill allocates investments to the Applied Energy programs for demonstration projects or applied research. BES's FY22 Request asks for additional funds for more research in this area.

Meng hoped the planned CDR Roundtable will directly address the challenges with direct air capture of CO_2 raised by a 2011 American Physical Society report and will use breakthroughs during the intervening years to justify the re-visitation of this topic. Many in nanoengineering are excited to see this topic return. **Garrett** replied that individuals from the community have pointed to substantial thermodynamic challenges with CO_2 capture from dilute sources, but the topic is considered worth pursuing.

Gagliardi requested long-term perspectives on the engagement of MSIs and minority students in BES proposals and activities. **Horton** said new text encouraging applications from MSIs has been added to FOAs. The implicit need for diversity of all kinds has always been present, but words guiding activities have been strengthened, including program policy factors and review criteria related to diversity of PIs and teams; these parameters will be considered when selecting awards and examining the diversity of the BES portfolio. The RENEW program will require an appropriation to be launched. This activity will support internships for faculty and students from MSIs at national laboratories to grow DOE partnerships with and the scientific portfolios at these institutions.

Kastner dismissed the meeting at 12:25 pm for a break and reconvened the meeting at 12:45 pm.

Office of Science Distinguished Scientist Fellow Presentation
New Tools for Mechanistic Transient Studies in Catalysis, José Rodriguez, Senior Chemist, Brookhaven National Laboratory

DOE guidelines include developing technologies to reduce emissions and generate novel, marketable products using CO_2 or coal as a feedstock. The Catalysis Group at BNL is working on converting CO_2 into multiple products, including alcohols, methane, and syngas, by using well-defined interfaces of metals with oxides, carbides, sulfides, and phosphides. The BNL Group has pioneered numerous synchrotron-based techniques, enabling a multi-modal approach to *in situ* characterization of catalysts using both steady-state and transient methods to understand mechanisms behind materials' catalysis properties. Innovation in NSLS-II instrumentation has been key to studies and new methods under development, which include infrared/X-ray absorption fine structure (IR/XAFS), IR/X-ray diffraction (IR/XRD), IR/pair-distribution function (IR/PDF) analysis, and ambient-pressure X-ray photoelectron spectroscopy (AP-XPS). A portable, automatized transient/time-resolved setup optimized for one-carbon (C1) chemistry will be transported to NSLS-II in 2022 and used in *operando* studies with XRD, PDF, and XAFS.

Scientists have been working on the conversion of CO_2 to methanol through hydrogenation for more than a century. Cu/ZnO is a typical industrial catalyst used for this process. However, more efficient catalysts are needed along with system characterization under high pressures and temperatures. Studies in the 1980s found that the dissociative sticking probability of CO_2 on pure copper using Cu(111) or Cu(100) is extremely low while addition of Cs to Cu(100) helps to bind and dissociate CO_2. Recent research has determined that Cu nanoparticles are more active than Cu(111) for methanol synthesis via CO_2 hydrogenation. Furthermore, the oxide used as a support for the Cu nanoparticles affects catalytic activity by conferring special structural or electronic properties. Promising catalysis results have been obtained with CeO_x/Cu(111). Ongoing, systematic transient studies are exploring the behavior of CeO_2/CuO powders to identify active sites and reaction mechanisms and to optimize catalytic performance.

Discussion

Garcia asked about Cs and Ce catalysts. **Rodriguez** said Cu alone is a poor catalyst, but an interface between the Cu metal and a cesium oxide or cerium oxide binds CO_2. The cerium-oxide and Cu interface is so effective for methanol production that cesium use is not necessary. Future studies will use cesium oxide and Cu to generate higher alcohols like isopropanol.

Chen inquired about surface-specific phenomena. **Rodriguez** remarked that cerium oxide is a robust chemical and displays no signs of synchrotron beam damage. To make the system surface-specific, small amounts of cerium oxide are used, and nearly all the oxide resides at the surface. XRD is not surface-specific, but AP-XPS is. Also, XRD coupled with IR spectroscopy can provide surface-specific information. Multiple techniques are need to tackle this problem.

Gagliardi called attention to theory. **Rodriguez** remarked that 25%-50% of the BNL Catalysis Group works in theory and 40%-50% of the Group's publications involve theory. All study rationalization, and conceptual frameworks arise from theory. Today's presentation focused on instrumentation.

SC Quantum Information Science Centers, Irfan Siddiqi, Director, Quantum Systems Accelerator, Lawrence Berkeley National Laboratory

The National Quantum Information Science Research Centers effort is the first large-scale QIS endeavor to cross the SC's technical breadth. Five Centers were launched in 2020: Co-design Center for Quantum Advantage (C^2QA) led by BNL; Next Generation Quantum Science and Engineering (Q-NEXT) led by ANL; Quantum Systems Accelerator (QSA) led by LBNL; Quantum Science Center (QSC) led by ORNL; and Superconducting Quantum Materials and Systems Center (SQMS) led by Fermi National Accelerator Laboratory. Each Center represents a partnership of labs, universities, and industry. The Centers take distinct yet complementary approaches to tackle major cross-cutting challenges, integrating fundamental science, devices, systems, prototypes, and applications across the QIS innovation chain. The Centers' portfolio addresses advanced materials for quantum technologies, entanglement distribution networks, high-performance instruments and sensors, and full-stack quantum computation, the latter including programmable quantum systems, integrated quantum engineering, and algorithms and applications. An Executive Council maintains cross-Center coordination.

The Centers play a central role in stewardship of the QIS ecosystem, including support for the development of a diverse and inclusive workforce through programs targeting fellowships for underrepresented minorities, including those from HBCUs, to those targeting training for Kindergarten through 12th-grade (K-12) teachers. The Centers also broadly engage with industry partners to accelerate deployment of quantum-enabled technologies. To forge connectivity across the QIS ecosystem, the Centers create new synergies between DOE programs by leveraging user facilities. Cross-center workshops and other activities introduce QIS-relevant facility capabilities to the research community. The Centers also share anticipated community needs with user facility experts to guide development of new capabilities.

During their first year of operation, the Centers jointly conducted activities in technical coordination, instrumentation and facilities, workforce development, cross-center management, and communications/outreach. Future joint plans include developing a database of quantum materials characteristics; a cross-Center workshop on algorithms and co-design approaches; workshops for existing researchers on the application of user facilities to QIS; identification and promotion of additional instrumentation and facilities resources; a second annual career fair; a second meeting of Centers' Chief Diversity Officers for continued exchange of best practices for QIS DEI; and a coordinated QIS summer school.

Center science highlights include the development of a quantum network simulator by Q-NEXT; investigation of a spin system's quantum phases using a programmable quantum simulator by QSA; discovery of room-temperature, single-photon emitters in SiN by QSC; development of an efficient, fully-coherent Hamiltonian simulation by C^2QA; and discovery of niobium nanohydride precipitates in superconducting transmon qubits by SQMS.

Discussion

Archer asked about QIS ecosystem gaps and leveraging laboratory successes to advance industry. **Siddiqi** said gaps are currently being identified. A working group is examining actions DOE can take to promote efforts in this area, and there are ongoing interagency discussions, including with the National Science Foundation, to identify roles and fill gaps. There has been strong industry participation from IBM at the BNL Center. SQMS is also working with companies for advanced materials characterization. LBNL's Center established an Industry Council to elicit company input on technical areas that would benefit industry.

Garcia inquired about benchmarking to compare technologies across Centers. **Siddiqi** remarked that circuit and application benchmarking are being deployed along with identification of characteristic problems for benchmarking technologies. There are also efforts to develop more-fundamental benchmarks based on quantum mechanics and inequality methods, such as those assessing Hilbert space size. In the absence of a universal system, it is likely that variegated benchmarks will be used.

Meng appreciated Siddiqi's well-structured presentation, inquired about SQMS's use of cryo-EM, and advised greater outreach to middle- and high-school children on quantum topics. **Siddiqi** explained that cryo-EM studies were conducted at 106 kelvin. Study of some phenomena, such as condensation of parametric oxygen, may require colder temperatures. Examining effects across temperature fields is exciting. Advancing educational outreach now is a good idea; doing so later presents a greater opportunity cost.

BES Roundtable on Foundational Science for Carbon-Neutral Hydrogen Technologies, Karren More, Director, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

The Virtual Roundtable on Foundational Science for Carbon-Neutral Hydrogen Technologies was charged with discussing scientific and technical barriers associated with carbon-neutral hydrogen production, storage, and utilization. The Roundtable recognized the importance to two prior reports issued by BES and DOE titled *Basic Research Needs for the Hydrogen Economy* (2003) and *DOE Hydrogen Program Plan* (2020), respectively. The DOE's H2@Scale initiative and Hydrogen Earthshot have placed additional emphasis on this area, reflecting the current Administration's priority of clean energy.

Held in August 2021, the Roundtable was led by SC-BES with participation from EERE's Hydrogen and Fuel Cells Technology Office (HFTO), FECM, and Nuclear Energy (NE). Participants were initially organized into four topical panels: Hydrogen Production; Hydrogen Storage; Hydrogen Utilization; and Cross-cutting Topics. Following discussion, four PROs were identified: 1) Discover and control materials and chemical processes to revolutionize electrolysis systems; 2) Manipulate hydrogen interactions to harness the full potential of hydrogen as a fuel; 3) Elucidate the structure, evolution, and chemistry of complex interfaces for energy- and atom-efficiency; and 4) Understand and limit degradation processes to enhance the durability of hydrogen systems. For PRO1, the development of *in situ* and/or *operando* characterization techniques and computational and/or data science tools is needed to capture the evolving complexity of systems under working conditions. For PRO2, the ability to characterize hydrogen interactions and dynamics for storage and utilization processes at surfaces and interfaces, in molecular species and confined environments, and in integrating these data into predictive models is key. PRO3 requires development of integrated, predictive approaches that involve the coupling and parallel application of diverse techniques. Understanding garnered through PRO4 will lead to new design principles and result in more robust, stable materials with significantly enhanced lifetimes, especially when synthesis and performance are coupled with predictive modeling.

The Roundtable Brochure and Technology Status Document were issued in October 2021. A final report will be released in early 2022.

Discussion

Roldan Cuenya inquired about ammonia as a hydrogen carrier and evaluating U.S. hydrogen research activities in an international context. **More** explained that the Roundtable did not specifically address ammonia as a carrier. Rather, discussion of this research area more broadly identified the need for studies elucidating underlying mechanisms in this topical field. Other DOE reports have addressed the international context for hydrogen. The Roundtable's final report will also contain an international assessment.

Kastner dismissed the meeting at 2:10 pm for a break and reconvened the meeting at 2:30 pm.

Presentations and Panel Discussion: Science and Energy Technology Teams (SETTs)

John Vetrano (BES), session moderator, introduced the SETT panel and remarked that the Office of the Under Secretary for Science and Energy now encompasses both the science and technology offices to facilitate better linkages between them and to help achieve the Administration's clean energy goals. The Energy Earthshots represent a portion of the broader topics being coordinated across the DOE.

Hydrogen and Fuel Cell Perspectives, Sunita Satyapal, Director, Hydrogen and Fuel Cell Technologies Office, and Coordinator, DOE Hydrogen Program

The *DOE Hydrogen Program Plan* highlights DOE-wide coordination to meet the Hydrogen Program's priorities: 1) Low-cost, clean hydrogen; 2) Low-cost, efficient, safe hydrogen storage; and 3) Enabling end-use applications at scale for impact. The H2@Scale initiative depicts the versatility of hydrogen for multiple domestic applications presenting decarbonization opportunities. The Hydrogen Energy Earthshot seeks to reduce the cost of clean hydrogen to $1 per kilogram in one decade ("1 1 1"). This initiative was launched in June 2021, and a Hydrogen Summit was conducted in the late summer of 2021. All pathways that could lead to "1 1 1" are under consideration, including electrolysis, waste conversion with carbon capture and storage (CCS), and advanced pathways.

There is strong coordination among DOE basic science and applied programs to reach near- and long-term goals related to hydrogen production, delivery, storage, conversion, and applications. Several mechanisms foster within-DOE and external collaborations including through consortia such as H2NEW that engage the national laboratories, universities, non-profits, and industry. Consortia have clear, well-defined stack metrics and goals. Integrated efforts between SC user facilities and hydrogen-related consortia have resulted in >70 joint publications. DOE also supports >25 Cooperative Research and Development Agreement (CRADA) projects with the private sector that are aligned with the H2@Scale's vision. Other mechanisms enabling collaboration include cross-office and interagency participation in annual merit reviews of DOE hydrogen programs, job rotations, joint planning activities, and the SETTs. Cross-sector and cross-disciplinary efforts have yielded successes, such as the development of advanced durable fuel cell electrocatalysts and commercial collaboration towards their deployment.

Storage Connections across DOE, Eric Hsieh, Director, Grid Components and Systems, Office of Electricity

The DOE's Energy Storage Grand Challenge (ESGC) released a Roadmap in December 2020. The Roadmap works backwards from Storage Objectives, including decarbonization, reliability, resilience, and equity, to identify Use Cases. In turn, Use Cases map to Technology/Product Development that is grounded in Foundational R&D spanning electrochemical, mechanical, thermal, and chemical fields. Of note, the Facilitating Grid Decarbonization and Serving Remote Communities Use Cases were incorporated into the Long Duration Storage Shot. This Earthshot establishes a target to reduce the cost of grid-scale energy storage by 90% for systems that deliver 10+ hours of duration within one decade. The path forward indicates that storage will be used in many different ways. Thus, no one technology is likely to dominate all uses. While lithium-ion technologies currently represent 99% of storage on the grid today, DOE is investing in a much broader array of chemical technologies, with lithium-ion technologies receiving <50% of funding.

In addition to a broad research portfolio, meeting the ESGC's goals will require the capacity to manufacture and commercialize technologies. Furthermore, policies must ensure a market for such technologies and support the workforce that will be needed to install and maintain energy storage systems. Multiple funding opportunities are available across DOE programs, with several efforts supported through joint program solicitations to leverage funding. The 2021 fall Storage Summit led to the launch of a Storage Lab Partnering Portal that highlights storage capabilities across the national laboratory complex and facilitates DOE-industry connections. Major energy storage highlights in 2021 reflect DOE investments sustaining research, policy, and communication initiatives within diverse sectors, including industry.

Carbon Management and the Carbon Negative Energy Earthshot, Emily Grubert, Deputy Assistant Secretary, Office of Carbon Management

Carbon management approaches, including carbon dioxide capture, utilization, and removal, are key to the U.S.'s goals of a fully decarbonized electricity system by 2035 and a net zero greenhouse gas emissions economy by 2050. Meeting these goals will require performance-based standards and will likely generate new industries. Additionally, DOE activities in these areas must be informed by and enable climate justice and DEI.

Announced in November 2021, the Carbon Negative Shot calls for innovative and scalable technologies to remove atmospheric CO_2 and durably store it for <$100 per net metric ton of CO_2-equivalent (CO_2e) within a decade. Success entails a robust accounting of full lifecycle emissions, long-term storage of at least 100 years, and affordable gigaton-scale removal. CDR is not only necessary for the U.S. to meet its 2035 net zero target, but also for addressing legacy emissions. Though DOE does not believe CDR will replace mitigation, a long-term industry is anticipated in this area, and the U.S. can take a lead role in developing and enabling large-scale approaches.

Discussion

Takeuchi inquired about the intersection between the Federal Consortium for Advanced Batteries (FCAB) Blueprint, ESGC, and Long Duration Storage Shot. **Hsieh** explained that the

ESGC was created in response to a Congressional request for a strategic DOE approach to organize major cross-cutting activities. The ESGC is the structure in which DOE will implement the Long Duration Storage Shot's cost-performance goals by 2030. The FCAB Blueprint is a strategy document addressing manufacturing and supply chains for a specific set of technologies with mobility applications. Information will be shared across efforts. For example, FCAB findings that reduce costs could support ESGC goals. Likewise, an ESGC discovery of materials that enable a more diverse supply chain would support FCAB.

Stack asked about efficient approaches to fund the transition from fundamental science to applied solutions. **Satyapal** observed that there are different funding models. For hydrogen, the Energy Materials Network Consortia use a two-pronged approach. Funding on the basic/foundational end of the spectrum requires a low technology readiness level (TRL), and work may have a higher risk. On the applied end, concrete targets and metrics are set. Consortia principal investigators (PIs) often receive basic and applied funding. Work is linked to the EFRCs, national laboratories, and user facilities. Success requires innovation along a continuum; issuing one big mandate across the spectrum with stringent targets would reduce flexibility. This approach allows for a basic-to-applied ecosystem. Models that foster cross-spectrum connections are helpful, such as accelerated stress-testing of electrodes. **Hsieh** echoed Satyapal's final remarks; researchers are seeking material property validation, supply chain availability, and end-user requirements at the earliest possible R&D stage using bench-top devices, modeling, or other approaches. On the CDR front, **Grubert** commented that many appropriations mandate spending funds on the deployment of more mature technologies. Finding ways to address the requisite basic work is important. Supporting the overarching ecosystem is a big priority.

Roldan Cuenya asked how the "1 1 1" estimation was made. Though electricity is cheaper in the U.S., reducing hydrogen costs to \$1 per kilogram is very ambitious. Germany's current goal is to reduce hydrogen costs to 2.5 euros per kilogram. **Satyapal** noted that DOE is coordinating hydrogen efforts through several international collaborations and partnerships like Mission Innovation whose most recent clean hydrogen target was \$2 per kilogram from production to end use. DOE had conducted analyses to justify the \$1 target and identify tipping points for different applications. U.S. natural gas costs are so low that hydrogen must almost be less than \$1 to be competitive. Aside from funding hundreds of projects, DOE has also held confidential discussions with companies to estimate their lowest prices; some companies thought they could price hydrogen at \$1.50 per kilogram. Chile is seeking an aggressive target of \$1.15. DOE has set an ambitious target to catalyze innovation.

Bent drew attention to technology information flow from companies to national laboratories and universities. **Satyapal** referenced several examples of two-way information transfer between industry and labs in the hydrogen arena. DOE hosts workshops and invites industry, with the Roundtable on Foundational Science for Carbon-Neutral Hydrogen Technologies being the most recent. DOE also has formal industry partnerships through H2@Scale, the 21st Century Truck Partnership, and U.S. Driving Research and Innovation for Vehicle efficiency and Energy sustainability (U.S. DRIVE). The annual merit review issues feedback to projects. Regarding intellectual property (IP), the HFTO tracks patents and their commercialization. Currently there are ~1,100 hydrogen patents, 30 are commercialized, and an additional ~65 could be commercialized in the next few years. Other mechanisms include the

Small Business Innovation Research (SBIR) program along with the Technology Commercialization Fund (TCF). HFTO sets aside ~1% of its funding to support lab and industry collaborations, especially when a company is licensing lab technology. Echoing Satyapal's comments, **Hsieh** highlighted examples from electricity storage. Releasing a public draft roadmap with a request for information (RFI) elicited industry input. More formally, Congress requires DOE's Electricity Advisory Committee to conduct a formal review of energy storage technology activities every two years. Finally, CRADAs and other requests where companies invest money to use lab capabilities indicate that the DOE is on the right track. Somewhat unique to FECM, **Grubert** noted that carbon capture and CDR activities are essentially pollution control technologies, and FECM tends to be aware of this commercialization space. This offers scope for close interactions with industries. Recently, FECM has been identifying the information needed from projects to reach deployment targets. Many performance targets depend on dynamics outside of DOE's control, such as electricity costs. FECM is considering modeling approaches to evaluate different scenarios.

Pointing to recent large-scale explosions in Asia and Europe, **Robertson** inquired about the safety of hydrogen production and distribution in the context of the $1 target and the national gas pipeline. **Satyapal** remarked there are almost 2,000 miles of dedicated industrial hydrogen pipeline with 90M metric tons of hydrogen used already. Like all other fuels, hydrogen is flammable and must be handled appropriately. DOE launched a global Center for Hydrogen Safety. Modeled after the American Institute for Chemical Engineers guidelines for industrial processes and safety, the Center offers trainings, lessons learned and best practices. Anyone can join the Center, which has >60 partners including major companies like Shell. Though the Hydrogen Shot is focused on production, DOE has many concurrent efforts examining storage, delivery, and dispensation. DOE recognizes that costs can vary widely across applications; support from the bipartisan Infrastructure Deal will help address this.

Guzman asked if the aggressive Earthshot cost targets are based on the free market or assume policy to incentivize technology use. **Grubert** said achieving the CDR target of $100 per metric CO_2e ton in concert with policy would facilitate at-scale deployment. CDR generally does not have a product, and adding CDR to processes with a product tends to make products more expensive. Earthshot conversations focused on how much CDR is needed to meet climate targets, and the conclusions could serve as a leading indicator for policy. When determining cost targets, the Earthshot considered what it believed the market could bear. DOE is unlikely to reach deployment at $100 per CO_2e metric ton and anticipates participation by an emerging industry. Discussion also considered international carbon markets and proposals for Q credits. From a storage perspective **Hsieh** added that the five cents per kilowatt hour goal assumes no policy changes and that the marginal fuel in 2030 will be natural gas for the grid. A policy to internalize carbon prices would make the Storage Shot goals considerably easier to attain.

Chen asked about derivation of Earthshot cost analyses from the basic to applied ends of the spectrum, and how basic sciences can support Earthshot goals. **Satyapal** stated the 2020 hydrogen baseline is $5 per kilogram assuming capital costs at a low volume of $1,500 per kilowatt. Efficiency, durability, and electricity costs can be broken into component targets, like the cost of bipolar plates. These can be collectively translated into high-level targets for basic R&D. From a CDR vantage, **Grubert** remarked that much is still unknown, and basic science can engage with this challenge on many fronts, such as materials science for direct air capture. Basic science is also needed for sensor development and verification technologies for biologically based approaches.

Archer commented that the original Moonshot cost $280B in today's dollars to put someone on the moon. While the Earthshot moniker creates a sense of excitement, are the designated resources enough, and is industry expected to contribute in ways it did not or could not for the original Moonshot? Also, lithium-ion technologies are unlikely to reach five cents per kilowatt hour amortized. Is there a plan to shift to more earth-abundant and inexpensive chemistries and will there be a related request for proposals (RFP) focused on reaching the five-cent target? While more resources would certainly help achieve targets sooner, **Hsieh** observed that the Infrastructure Bill supports demonstration of technologies at scale in a way that could not be done before. Regarding industry participation, DOE is thinking more holistically about open data to facilitate commercialization and avoid barriers like nondisclosure agreements. With funding, there are opportunities to share lessons learned with industry more quickly. While future RFPs cannot be discussed, the ESGC Roadmap explicitly notes the need to diversify away from lithium, with opportunities in stationary applications for use of cheaper materials like salt, iron, or sand.

Facility Updates

Linac Coherent Light Source Scientific Leadership Strategy, Mike Dunne, Director, Linac Coherent Light Source, SLAC National Accelerator Laboratory

LCLS enables the ability to tailor and measure X-ray beams from linear to controlled polarization; from durations of 200 femtoseconds down to 200 attoseconds; from statistically fluctuating to controlled pulse widths and spectra; and from single-pulse to tunable multi-pulse and two-color X-rays. These beam characteristics empower precision studies across a wide range of disciplines in biological and chemical dynamics, catalysis, materials physics, and quantum materials.

First operated in 2009, LCLS's parameters were groundbreaking and made LCLS the world's first hard X-ray free-electron laser (XFEL). However, XFEL capabilities are now available around the world, with the Pohang Accelerator Laboratory (PAL)-FEL in Korea, Swiss-FEL in Switzerland and the Spring-8 Angstrom Compact free-electron LAser (SACLA) in Japan all exhibiting capabilities similar to LCLS-I. The European XFEL (EuXFEL) in Germany and the Shanghai HIgh repetitioN rate XFEL and Extreme light facility (SHINE) under construction in China are high-repetition rate facilities. The performance of these facilities is impressive and setting new operating standards.

The LCLS has a broad community of users, with ~1,300 individuals from around the world registering for the 2021 Annual Users Meeting. At present, LCLS's productivity compares very favorably with other international facilities, especially in the area of publications produced relative to user beam time. This is because LCLS is full-service facility with support from beamline scientists. However, international competition could increasingly challenge U.S. leadership. In 2017, LCLS and EuXFEL had similar materials budgets and employed comparable numbers of beamline operations and development staff. In 2020, EuXFEL's materials budget and staff numbers outstripped those of LCLS by ~60% and ~70%, respectively. BESAC's recent International Benchmarking report highlighted upgrades to EuXFEL and planned capabilities at

SHINE indicating that instrumentation and source capabilities at these facilities could create a significant imbalance in the XFEL landscape within ten years.

Currently, construction projects at the LCLS facility are being rolled out in three phases. Phase 1 installed two LCLS-II variable gap undulators in 2020. Phase 2 is scheduled for 2022 and will result in an LCLS-II 4-GeV superconducting accelerator. LCLS-II-HE is scheduled for around 2027 and will increase beam energy to 8 GeV. Collectively, these projects will increase laser pulses from 120 Hz to 1 MHz and transform the breadth and scale of LCLS's impact.

The LCLS has developed a four-point strategy to extend and retain leadership in the international arena: 1) Establish a defining set of scientific priorities, with decadal-scale ambition; 2) Drive step-changes in source and facility performance; 3) Foster a vibrant research ecosystem, taking advantage of DOE's unified structure, including considerations of career development; and 4) Full build-out and exploitation of the LCLS platform with more dedicated and specialized instrumentation and a suitable breadth of instrumentation. This plan is manifesting through LCLS Scientific Campaigns that allow community-wide teams to tackle strategic grand challenges; teams are granted access to LCLS for coordinated research activities. Each of the concurrent Campaigns represents a major cross-cutting effort of theory, synthesis, experiments, and analysis with a beamtime allocation of three or more years. The scientific goals drive strategic R&D to transform LCLS's capabilities and inspire new approaches to X-ray science, including innovative X-ray sources; improvements to beam quality; ultra-stable X-ray optics; new sample environments; kHz to MHz X-ray detectors; and real-time data analytics. Improvements are captured in the LCLS instrument development plan, which will fully leverage the large-scale investments over the period of 2005-2027.

Update on Neutron Facilities, Ken Andersen, Associate Laboratory Director, Neutron Sciences, Oak Ridge National Laboratory

The High Flux Isotope Reactor (HFIR) and SNS are co-located at ORNL and offer the world's highest continuous neutron brightness and the world's highest peak neutron brightness sources, respectively. HFIR and SNS, respectively, house 12 and 18 neutron scattering instruments. ORNL's neutron science program envisions a three-source strategy, including HFIR, the SNS First Target Station (FTS), and eventually the SNS STS, with each designed to have complementary capabilities and instruments. Research at SNS and HFIR supports critical areas outlined in BESAC's International Benchmarking report, including those related to energy applications, matter for energy and information, and industrially-relevant science for sustainability.

Though COVID-19 has disrupted onsite user visits, SNS and HFIR have been able to operate a similar number of experiments to pre-pandemic times due to remote direction, a mail-in program and onsite activities by facility staff. SNS and HFIR have the third- and sixth-highest publication output of world-wide neutron facilities, respectively. Together, SNS and HFIR boast the highest publication output per instrument at worldwide facilities, though output from the ISIS Neutron and Muon Source and the Institut Laue-Langevin (ILL) is similar. HFIR and SNS subscription rates are similar to those of ILL, with SNS leading slightly. Though world leading, HFIR's steady-state performance is similar to that of Forschungsreaktor München II (FRM-II) and ILL, and the pulse brightness of SNS will be challenged by that of the European Spallation Source (ESS) when it is running.

Ensuring that SNS and HFIR instruments are upgraded to provide high source brightness is challenging, and upgrades must balance new capabilities with higher throughput. Currently, several instruments at HFIR are outperformed by more modern instruments at other facilities. Many projects are ongoing, and several additional projects are prioritized but not funded.

Facility upgrades at SNS include the PPU, which will double the power of the existing accelerator structure by 2024, and building STS with the initial suite of beam lines by 2034. Based on the recommendations from a committee of national and international experts, eight STS project-constructed instruments were selected to address key science themes from the 2020 SNS STS *First Experiments* report. Several other instruments are in the pipeline for the SNS FTS or HFIR, including the Versatile Neutron Imaging Instrument (VENUS), Diffractometer for Materials Discovery (DISCOVER), Multi-Analyzer Triple Axis (MANTA) Spectrometer, and High-Resolution Neutron Spin-Echo Spectrometer.

The HFIR Beryllium Reflector Replacement (HBRR) and upgrades are scheduled for 2025. Ongoing evaluations are determining whether HBRR can be combined with the HFIR Sustaining and Enhancing Neutron Science (SENSe) replacement of the HFIR pressure vessel, which received CD-0 in November 2020. Together, these projects will position HFIR for an additional 80 years of operation.

In addition to hardware, ORNL's neutron facilities are making significant investments in data analysis and experimental software with the goal of real-time data analysis and semi-autonomous experiments guided by AI/ML approaches.

Accelerating Climate and Clean Energy Innovation: Role of the DOE Nanoscale Science Research Centers, Jeff Nelson, Director, Center for Integrated Nanotechnologies, Sandia National Laboratories

The five NSRCs operate within six of the DOE's national laboratories: 1) the Molecular Foundry (TMF) at LBNL; 2) the Center for Integrated Nanotechnologies (CINT) co-located at the Los Alamos National Laboratory and Sandia National Laboratories; 3) the Center for Nanoscale Materials (CNM) at ANL; 4) the Center for Functional Nanomaterials (CFN) at BNL; and 5) the Center for Nanophase Materials Sciences (CNMS) at ORNL. These BES user facilities offer unique expertise and research equipment in nanoscale synthesis, characterization, modeling, and fabrication; a merit-review process for brief research proposals; and free access to staff support and equipment for science that will be published in open journals. Since inception, the NSRCs have supported ~33,000 users on ~16,400 projects leading to ~19,300 publications. The NSRCs' total FY21 operating budget was $134M.

The NSRCs can play a critical role in accelerating clean energy technology needed to reach climate goals. Shared collaboration highlights emphasized research in 1) improving performance in energy storage, including high energy density, high-nickel-content cathodes, and use of a drug discovery toolbox for designing selective battery membranes; 2) understanding degradation in energy storage, featuring a short-circuit mechanism in lithium-metal batteries revealed by cryogenic laser ablation, and structural changes in conversion-type electrodes examined via X-rays and transmission-electron microscopy; 3) novel catalysts for carbon-neutral hydrogen, such as a platinum group metal (PGM)-free catalyst for polymer electrolyte fuel cells and a branched ruthenium nanoparticle catalyst for water splitting; 4) CO_2 conversion catalysts for sustainable fuels, as demonstrated by a semi-artificial photosynthetic biohybrid and di-tungsten carbide-driven catalysis of CO_2 reduction; 5) stabilizing Perovskites for solar energy and solid-state lighting, including metal halide Perovskite nanocrystals stabilized in a metal-organic framework and use of chemical robotics for discovery of metal halide Perovskites and their stability; and 6) enhancing membrane selectivity for water purification, showcasing removal of trace organic compounds from the water supply via ultrathin nanoparticle membranes, and fresh water provision from a bio-inspired electrodialysis membrane.

The NSRCs have also supported basic to applied research to combat the COVID-19 pandemic, including studies to 1) understand the virus and develop novel detection methods such as fast, nanotechnology-based portable diagnostics sensors; 2) synthesize custom nanoparticles for vaccine encapsulation and delivery; 3) improve effectiveness of personal protective equipment including masks and of nanoparticle-based antiviral coatings; and 4) develop epidemiological models to predict virus spread.

Discussion

None.

Pre-Committee of Visitors (COV) Overview: SC Workforce Development for Teachers and Scientists (WDTS), Ping Ge, Director, Workforce Development for Teachers and Scientists

The SC has charged BESAC to establish a subcommittee to serve as a COV to examine the activities of WDTS over FY17-FY21 and to deliver a report in the summer of 2022.

WDTS's mission is to ensure a sustained STEM workforce pipeline to support the DOE. In an average fiscal year, WDTS is appropriated ~$28M. The majority of funds (~75%) support undergraduate or faculty internships or graduate student thesis research at DOE national laboratories through four programs: Science Undergraduate Laboratory Internships (SULI); Community College Internships (CCI); Visiting Faculty Program (VFP); and Office of Science Graduate Student Research Program (SCGSR). These programs collectively involve ~1,400 participants annually and serve as a touchpoint for engaging URGs. About 25%, 50%, and 15%, of CCI applicants, VFP participants, and SCGSR participants, respectively, are from MSIs, and ~1/3 of SCGSR participants are rising female scientists. SULI, CCI, and VFP support science across DOE's mission scope. SCGSR supports graduate student theses in SC priority areas. Participants apply to programs through the WDTS Online Application and Review System (WARS).

A portion of WDTS funds (~14%) are distributed to pre-college programs, including the National Science Bowl (NSB) and the Albert Einstein Distinguished Educator Fellowship, respectively geared towards K-12 students and teachers. The NSB engages ~5,500 high-school and ~2,500 middle-school students annually. Remaining funds support cross-program activities, including online technology development, evaluation of program effectiveness, and strategic outreach.

This will be the third WDTS COV, with all reviews conducted by BESAC. Prior COVs in 2010 and 2016 led to major restructuring of the WDTS programs, centering focus on lab-based training programs as well as an improved online system for applications reviews and participant selection, leading to WARS. In addition to the standard charge, the COV is requested to comment on the effectiveness of the online technology development and evaluation activities in support of WDTS programs and outreach efforts to enhance diverse and inclusive program participation.

Discussion

None.

Public Comments

None.

Kastner adjourned the meeting at 5:01 p.m.

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Oak Ridge Institute for Science and Education and Oak Ridge Associated Universities