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

PUBLIC MEETING MINUTES
April 25, 2023

Virtual Meeting

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

The U.S. Department of Energy (DOE) Office of Science (SC) Basic Energy Sciences Advisory Committee (BESAC) convened a virtual meeting on Tuesday, April 25, 2023, via Zoom. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act (FACA). Information about BESAC and this meeting can be found at https://science.osti.gov/bes/besac.

BESAC Members Present:

Cynthia Friend, Chair, Kavli Foundation/ Harvard University (professor emerita)
Esther Takeuchi, Vice Chair, Stony Brook University, Brookhaven National Laboratory (BNL)
John Allison, University of Michigan
Lynden Archer, Cornell University
Joseph Berry, National Renewable Energy Laboratory (NREL)
Donna Chen, University of South Carolina
Lin Chen, Argonne National Laboratory (ANL), Northwestern University
Valentino Cooper, Oak Ridge National Laboratory (ORNL)
Theda Daniels-Race, Louisiana State University
Abhaya Datye, University of New Mexico
Serena DeBeer, Max Planck Institute
Tabbetha Dobbins, Rowan College
Thomas Epps, University of Delaware
Laura Gagliardi, University of Chicago
Jeanette (Jamie) Garcia, International Business Machines (IBM)
Murray Gibson, Florida Agricultural and Mechanical (A&M) University-Florida State University (FAMU-FSU)
Padmaja Guggilla, Alabama A&M University
Javier Guzman, ExxonMobil
Sossina Haile, Northwestern University
Ashfia Huq, Sandia National Laboratories (SNL)
Francis Hellman, University of California, Berkeley
Marc Kastner, Massachusetts Institute of Technology (MIT), retired; Stanford University, adjunct
Lia Krusin-Elbaum, The City College of New York-The City University of New York (CCNY-CUNY)
Marsha Lester, University of Pennsylvania
Surya Mallapragada, Iowa State University, Ames National Laboratory (Ames)
Nadya Mason, University of Illinois Urbana-Champaign (UIUC)
Shirley Meng, University of Chicago, ANL
Gabriel Montano, Northern Arizona University
Abbas Ourmazd, University of Wisconsin, Milwaukee
Jose Rodriguez, BNL
Rachel Segalman, University of California, Santa Barbara
Cathy Tway, Johnson Matthey

BESAC Members Absent:

Joan Broderick, Montana State University
Helmut Dosch, Deutsches Elektronen-Synchrotron (DESY)

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

Tuesday, April 25, 2023

Friend, BESAC Chair, called the meeting to order at 11:00 a.m. Eastern Time (ET) to a virtual audience of approximately 320 people. BESAC members introduced themselves.

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

Berhe thanked committee members for their contributions and highlighted the importance of recent BESAC charges examining the impact and future directions for Nanoscale Science Research Centers (NSRCs) and BES Research Investment Strategies as well as two Committee of Visitors (COVs) to evaluate the BES Material Science and Engineering (MSE) Division and the activities of the Office of Workforce Development for Teachers and Scientists (WDTS). Input received from BESAC and the community informs SC programmatic decision.

BES has a central role to play in achieving DOE core missions and delivering on the Biden Administration's priorities. BES's portfolio spans biothreats, clean energy, new catalysts and chemical conversion for high value and clean chemicals, critical materials and identification of alternative abundant materials, quantum computing, and microelectronics. BES research continues to leverage artificial intelligence and machine learning (AI/ML).

The Bipartisan Creating Helpful Incentives to Produce Semiconductors for America (CHIPS) and Science Act authorizes a historic $50B for SC with $14.7B for BES over five years. If enacted, the fiscal year 2024 (FY24) Presidential Budget Request (PBR) will deliver $8.8B to SC with $2.7B for BES. Funds will support user facility operations, staffing, and maintenance delayed by COVID-19. This budget would double SC's investment in broadening participation programs to support diversity, equity, inclusion and accessibility (DEIA) in the clean energy workforce. Reaching a New Energy Sciences Workforce (RENEW) would receive $56M to continue the recruitment and retention of individuals from underrepresented communities and institutions. Funding for Accelerated, Inclusive Research (FAIR) complements RENEW by building infrastructure and research capabilities at historically marginalized institutions. Additionally, funds would enable the creation of a new graduate fellowship program, continued investment in DOE's Energy Earthshot initiatives towards a net-zero carbon economy in 2050, and allocation of $60M for up to four new microelectronics research centers.

DOE SC is pursing all efforts through the lens of inclusive excellence. Publicly funded scientists have a responsibility to ensure research is accessible to all and that discoveries and innovations support the economic growth and well-being of the entire nation. In FY23, RENEW was expanded across all DOE SC programs. DOE SC also instituted a requirement for Promoting Inclusive and Equitable Research (PIER) plans for all SC-funded research proposals. Science is a team sport that should draw talent from all areas of the nation.

Berhe recognized the outsized contributions made by the late Dr. George Crabtree, including his nearly 10-year leadership of the Joint Center for Energy Storage Research (JCESR).

Discussion

Gagliardi raised concerns about how a possible change in administration would impact the 2050 net-zero carbon emissions goal. **Berhe** indicated there is no way to predict what will happen but hoped all recognize the gravity of the situation and will let science guide the answers to critical issues that transcend politics.

Meng asked how BESAC can strategically support translation of DOE SC funding authorizations to appropriations. **Berhe** emphasized that all have a role to play in boldly communicating why investment in science is important. The public, policy makers, and other stakeholders may not understand all the scientific details but must understand the inspiration and value proposition behind federally funded science. Further, it must be clear that public investment yields returns to all of society. All are encouraged to engage the public and other stakeholders through their spheres of influence.

Archer appreciated Berhe's holistic recognition of the impact of JCSER — not only in terms of research, but also with regard to society's values in terms of job creation, product development, and national competitiveness. Communicating all facets of the Administration's investments is important.

Dobbins inquired about a federal budget strategy to address the increased cost of living for graduate students. **Berhe** relayed DOE SC increased the annual salary for its graduate fellowships to $45K. DOE SC strongly encourages all principal investigators (PIs) to budget this salary for graduate students supported through other award mechanisms. DOE SC has no direct way of requiring institutions to pay students a specific salary.

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

Presenters shared BES's organizational chart, noting staff openings as well as recent hires. Andy Schwartz is serving as acting director of the new Collaborative Research Division to support efforts related to SC-wide initiatives, including the Energy Frontier Research Centers (EFRCs), Energy Innovation Hubs, and Energy Earthshot Research Centers (EERCs).

The enacted FY23 BES Budget of ~$2.5B represents a 9.8% ($226M) increase over that of FY22. Research program funding increased by ~$104M and included new and expanded investments for Manufacturing, Advanced Computing, AI/ML, FAIR, Accelerate Innovations in Emerging Technologies (Accelerate), SC Energy Earthshots, and RENEW. Within the Research budget, the Established Program to Stimulate Competitive Research (EPSCoR) continued at $25M. A further $119M was allocated for the Computational Materials and Chemical Sciences, Energy Innovation Hubs (Hubs) and the National Quantum Information Science Research Centers (NQISRCs). EFRCs continued with ~$130M, and investments for the SC Energy Earthshots initiative were increased by $25M. The Scientific User Facilities' budget increased by ~$110M, with ~$1.1B for facility operations to continue at 100% of the re-baselined budget levels. Facilities Research included ~$55M for AI/ML, Biopreparedness Research Virtual Environment (BRaVE) and Accelerator Research and Development (R&D). Funding for construction projects and Major Items of Equipment (MIEs) increased by ~$12M, with ~$9M for

the Advanced Photon Source Upgrade (APS-U); $94M for the Linac Coherent Light Source-II (LCLS-II); ~$135M for the Advanced Light Source Upgrade (ALS-U); $17M for the Proton Power Upgrade (PPU); $37M for the Second Target Station (STS); $10M for the Cryomodule Repair and Maintenance Facility (CRMF); $2M for the High Flux Isotope Reactor Pressure Vessel Replacement (HFIR-PVR); $1.5M for the National Synchrotron Light Source (NSLS)-II Experimental Tools (NEXT)-III project ; $25M for NSRC Recapitalization; and $25M for NEXT-II.

All 12 BES user facilities provided re-baselined operations funding requests that include consideration of COVID-19-related impacts to supply chains, as well as inflation, staffing for hybrid and remote operations, required maintenance, and bringing upgrades and new capabilities to remote users. In FY22, BES user facilities supported >15K users, with ~40% of users connecting to facilities remotely.

In December 2022, BES issued a total of ~$11.3M to be delivered over the next three years to five RENEW awards: 1) Controlling Additive Manufacturing Properties of Surfaces (CAMPS); 2) Hydrogen Innovation: Preparing and Obtaining a Workforce in Energy Research (HI POWER); Controlling Reaction Pathways under the Non-ideal Conditions of Seawater Electrolysis; Nanopore Characterization for Geologic Storage of H_2 and CO_2; and Partnership to Increase Representation in Energy Research in Puerto Rico (PIRES-PR).

The Accelerate Request for Information (RFI) issued during the first quarter of FY23 drew >50 responses from national laboratories, businesses of all sizes, universities, non-profits, consortia, individuals, and professional societies. Emergent themes from the responses addressed the need for better data and its reliable management; stakeholder involvement in the initiative from the outset; the need for a holistic systems approach to commercialization; and improved communication of developed technologies to companies of all sizes. Reponses informed the FY23 Accelerate Laboratory Call.

BES is continuing support for several funding opportunity announcements (FOAs) in FY23, including the annual Open Solicitation; the annual Early Career Research Program (ECRP); the annual Small Business Innovation Research and Small Business Technology Transfer (SBIR/ STTR) program; FAIR; RENEW; and EPSCoR. RENEW funds in FY23 will double the FY22 investment. The BRaVE and Advanced Scientific Computing Research for User Facilities FOAs provide support for research specifically focused on enhancing capabilities at SC user facilities. Preproposals for the latter FOA are due in May 2023.

BES, ASCR, and BER issued an FY23 Lab Announcement for EERCs as part of the SC Energy Earthshots Initiative. EERCs will support large, multi-investigator, -institution, and -disciplinary teams to advance foundational knowledge and enabling capabilities in experimental and computational chemical and materials sciences. Additionally, small group awards are being solicited with the new Science Foundations for Energy Earthshots FOA. These foundational science awards will complement the larger EERCs. Preapplications for both the EERC Lab Call and Science Foundations FOA were due in April 2023;full applications for EERCs are due in May 2023, and for Science Foundations in June 2023.

With coordination across DOE programs that support energy storage research, BES issued an FOA to openly recompete the Batteries and Energy Storage Hub program in January 2023. Full applications are due in May 2023. DOE anticipates awarding $8M-$15M to up to three recipients for five years, subject to future appropriations.

The FY24 PBR for BES of ~$2.7B represents a 6.3% ($159M) increase over that of FY23. If enacted, Research program funding will increase by ~$156M and include new and expanded investments in research for clean energy, microelectronics, manufacturing, critical

materials, BRaVE, and RENEW. Notably, $25M will be used to establish Microelectronics Science Research Centers authorized in the CHIPS and Science Act of 2022. These centers will complement existing SC microelectronics awards in fundamental science, as well asthe CHIPS and Science Act investments to be made by 1) the Department of Commerce (DOC) through the National Semiconductor Technology Center, which will focus on later-stage prototyping and applied research development and demonstration (RD&D); and 2) the Department of Defense (DOD) through the Microelectronics Commons, which will focus on DOD capabilities. A further ~$120M will be allocated for Computational Materials and Chemical Sciences, Hubs, and NQISRCs. EFRCs will continue with $130M and investments for the SC Energy Earthshots initiative will increase by $35M. The Scientific User Facilities' budget will increase by ~$166M to $1.33B, with ~$1.2B supporting facility operations at ~90% of the funding required for re-baselined, normal operations. Facilities Research will offer ~$57M, supporting multiple initiatives: Accelerators and Detectors; AI/ML; BRaVE; and RENEW. Funding for construction projects and MIEs will decrease by ~$63M, with $120M for LCLS-II; ~$57M for ALS-U; $16M for PPU; $52M for STS; $10M for CRMF; $13M for HFIR-PVR; $6.6M for NEXT-III; $5M for NSRC Recapitalization; and $20M for NEXT-II.

BES continues to define research priorities through Basic Research Needs (BRN) strategic planning workshops and roundtables.

The BES User Facility Science Webinar series was successfully launched in January 2023. Future topics include World Quantum Information Science (QIS) day (held April 14), microelectronics, clean energy, biopreparedness, and advanced manufacturing.

With operations beginning between 2006 and2008, the five NSRCs have shown impressive growth in their user communities —including remote users — over their 15 years of service to the nation. The NSRCs mission to support materials synthesis/fabrication and microscopy is differentiated from that of BES's scattering user facilities. The future of the NSRC's highly collaborative research environments will be further explored in a panel discussion during the meeting.

Discussion

Daniels-Race has been thrilled to see a more diverse range of institutions supported by DOE and urged BES to fulfill today's DEIA ideologies in filling BES staff positions. In years past, the DOE organizational chart has lacked gender, race, and ethnic diversity. Recruiting from underrepresented populations takes concerted and aggressive effort. Future DOE searches will hopefully represent all faces of the public. **Horton** commented BES is working towards these important goals. Gender balance has improved with recent hires, but recruitment of minorities continues to be challenging. All are encouraged to share open positions with interested parties. **Montano** added recruitment is not the only consideration for improving workforce diversity. Hiring committees must also consider how candidates are evaluated and take systemic issues related to achievement gaps into account. Evaluation metrics and how they impact representation at all levels are broadly a higher education and science, technology, engineering, and mathematics (STEM) problem. Current criteria in hiring tend to overvalue end points and undervalue the journey. **McLean** requested attendees share a currently open position [- the CSGB Division Director -] with colleagues.

Guzman inquired if the user facilities re-baseline activity considered how to leverage remote capabilities more efficiently. **Horton** said an SC facilities review conducted one year into the pandemic found remote access opened user facilities to broader audiences. Allowing remote

operations to continue is a priority, and SC is considering staffing and cybersecurity needs to enhance remote engagement. Some of BRaVE's funding is designated for automated equipment.

In Memory of George Crabtree, Marc Kastner, Massachusetts Institute of Technology (retired), Stanford University (adjunct)

Dr. George Crabtree will be greatly missed. He was an outstanding scientist and leader who made vital contributions to BES research priorities and strategic planning. Workshops and subsequent reports led by Dr. Crabtree advocated for the assembly of research dream teams and the creation of the early career program. Among many illustrious accomplishments led by Dr. Crabtree with lasting community impact, JCESR will conclude its 10th and final year in 2023.

Friend dismissed the meeting at 12:47 p.m. for a break and reconvened the meeting at 1:17 p.m.

MSE COV, Andrew Schwartz, Director, Materials Sciences and Engineering Division

BESAC has been charged with forming a committee to conduct the seventh MSE COV. The COV will consider a) the efficacy of MSE solicitations, awards, and performance monitoring of projects and programs, and b) the breadth, depth, and scientific and technical quality of portfolio elements from FY18-FY22. A COV chair has been selected, and leads are being identified for four panels: 1) Scattering and Instrumentation Sciences; 2) Materials Discovery, Design, and Synthesis; 3) Condensed Matter and Materials Physics, and 4) EPSCoR. A virtual format is being considered.

BES has taken steps to address recommendations from the 2018 MSE COV, including conferring the flexibility to hold COVs less frequently than every three years; ways to reduce the number of ECRP proposals; longer award terms; expansion of communication pathways; increased travel funds for program mangers; and filling vacancies and adding staff.

Discussion

None.

FUNDAMENTAL RESEARCH AND FACILITIES FOR MICROELECTRONICS PANEL, Andrew Schwartz, Director, Materials Sciences and Engineering Division, and Panel Lead

Most SC programs, including BES and its associated user facilities, have supported semiconductor and microelectronics research for several years. BES user facilities have made important contributions to advancing U.S. innovation and competitiveness in this space. In 2018, BES and other SC programs held a Basic Research Needs Workshop for Microelectronics to define priority research directions for SC. Following release of the workshop report, SC has made several investments, including through the EFRC program in 2020 and 2022, and with 10 DOE National Laboratory-led co-design research projects in 2021. With passage of the CHIPS and Science Act, it is important to consider the role of BES user facilities in future microelectronics research.

Microelectronics: Anticipating the 2050 Alligators, Nancy Haegel, NREL

Five decades of semiconductor science following trends laid out by Moore's law and Swanson's law have driven a computing revolution and positioned the world for an energy revolution. Microelectronics will be even more ubiquitous but will also operate with fewer atoms

under more extreme environments. Framing basic science questions and priorities will be vital to enabling innovation for sustainability and equitable access to energy and innovation.

Microelectronics operate at the intersection of information/computing, energy, and sensing control with quantum materials. Important basic science questions include understanding structure and properties at incommensurate interfaces; spin-based room temperature information processing; replacing or reducing critical or expensive materials (i.e., circularity); and fundamental conditions/mechanisms that integrate degradation. Anticipated challenges (i.e., "alligators") include the inability to exploit the highest degree of functionality due to integration limitations; macroscale system degradation to due to nanoscale interface instability; infrastructure limitations (i.e., power electronics) for the new economy; material abundance/supply chain limitations; energy consumption as a limitation to computing and information storage; and balancing microelectronics' connection to work, heat, and information.

NREL science highlights addressed Topological Semimetals for New Energy Frontiers; Nitrides for Microelectronics; 2-D Perovskite Spin-LEDs; Perovskite Photonic Synapses; and Low-Power Optical Synapses.

Microelectronics, Supratik Guha, ANL and University of Chicago

Future pathways to advanced microelectronics must consider computing energy efficiency, increased connectivity between memory and logic functions, and system fragmentation into chiplets with assembly on a common substrate (i.e., heterogenous integration). Those in the community that are aware of these challenges often lack the skills necessary to solve them; new materials knowledge in physics and chemistry is needed.

Materials research imperatives for microelectronics encompass studies in 1) physics, chemistry, and computational science; 2) atom-scale, deterministic nanofabrication in 3D; 3) carrier and thermal transport physics and materials for 3D, multiscale, and imperfect heterogenous environments; 4) new physics-based computational models and architecture; and 5) characterization of 3D structures.

Science highlights from ANL featured research in ultra-dense, near-perfect atomic and synaptic memory; AI approaches to extracting/processing data from high-rate detectors; and new microelectronics synthesis approaches.

Current and potential future BES contributions to Chips and Science Act, Susan Trolier-McKinstry, Penn State University

BES has been a leader in identifying and addressing numerous microelectronics challenges. Research from the Center for Ferroelectric Microelectronics — a DOE EFRC — has addressed issues such as computational energy consumption/microelectronics functionality; developing new materials and understanding the fundamental underpinnings of behaviors, including those of ferroelectronic materials; engineering challenges associated with joining materials; development of automated microscopy; and materials co-design for data-intensive applications.

BES can further support microelectronics by catching up to Asian and European investments in foundry capabilities; considering other parts of electronics infrastructure such as ceramic capacitors; and facilitating lab-to-fab as well was fab-to-lab transitions.

Light sources for microelectronics, John Hill, BNL

Light sources, including the NSLS-II, and nanoscience centers offer unique capabilities to understand and improve all steps in the microelectronics life cycle — from materials synthesis and processing to device characterization. Existing work has had and continues to have an impact on microelectronics development. Moving forward, capabilities should be expanded to include *operando* imaging and characterization. Success requires dedicated instrumentation and expertise at the interface between synchrotron science and the microelectronics industry.

Highlighted science from light sources included: lensless 3D imaging of integrated circuits with hard X-rays; strain mapping at the 10-nanometer scale; spatial resolution of diffraction patterns; characterization of the process dependence during formation of the ferroelectric phase of Hafnium Zirconium Oxide during rapid thermal processing; synthesis of next-generation materials via novel tools (i.e, the Quantum Material Press); and extreme ultraviolet capabilities for materials processing.

Discussion

Archer asked to what extent industry challenges are informing basic research questions and if there is room for improved research-industry interactions. **Haegel** commented there is always room to improve interactions. Crosstalk among the national labs, academia, and industry is common, and industry is often integrated into research efforts as part of the team or advisory committee. How industry is engaged varies by topic. Forums for engagement are critical.

L. Chen wondered about translating research results to American semiconductor industries**. Haegel** believes in acceleration, though sometimes going faster does not always yield the best results. NREL has 400 industry partners, and other labs have similar partnership levels.

Garcia sought input on how quantum computing may assist in the microelectronics space. **Guha** envisions quantum computers acting as a processor embedded in a larger classical computing ecosystem. Much research is needed to determine how quantum capabilities will be incorporated into, and how information will be exchanged with, classical computing systems. Quantum computers will be important going forward.

Allison observed that databases are needed for AI-guided discovery of materials; these databases largely do not exist outside of atomistic databases. This is an issue in most physical science fields. **Guha** suggested a separate program is needed, and that there must be a united, concerted effort within communities. For example, journals must request specific information formats from researchers. At present, different teams are thinking about this topic, but each team has its own curation and storage methods. The medical research community is ahead in this domain.

Ourmazd raised the issue of navigation of industry confidentiality requirements. **Trolier-McKinstry** stated negotiations with industry are easiest when funding agencies impose boundary conditions. For example, the National Science Foundation (NSF) Industry-University Cooperative Research Centers (IUCRC) program confers non-exclusive, royalty-free licenses to any industry partners that are active research participants. Negotiating conditions in advance is critical and has become more complex when working with a number of leading-edge companies.

Rodriquez inquired how NSLS-II divides appropriations among various facilities' capabilities and research programs. **Schwartz** remarked that this question can be generalized across BES. Allocating funds is an ongoing balancing act. Conversations with the community, BESAC, and others help guide decisions. BES generally dedicates ~40% of its budget for research. The FY24 budget request allocates approximately 42% of BES funds for research. Facilities are expensive and must be maintained in order to enable research. **Horton** shared that

the general SC budget guidance suggests 40% for research, 40% for facilities operations, and 20% for construction. This ratio may fluctuate from year to year. For example, sometimes construction requires a larger budget. A current BESAC charge is seeking strategies for BES research investments. BES aims to balance research funds across recipients (e.g., academia, national labs), institutional partners, and research modalities. Community input on strategies to balance investments is welcomed.

Takeuchi observed that connections between research and industry were a repeat theme in presentations. Such interactions are something BESAC may need to think more about; connections can be a thorny issue as many industries and manufacturers are no longer onshore. **Trolier-McKinstry** concurred that interactions are critical. Putting a new material in the process line requires understanding the entire infrastructure for depositing and patterning materials, as well as needs for cleanliness.

Archer wondered to what extent industry needs push or pull facility capabilities. **Hill** said IBM has pulled on BNL capabilities with industry seeking facility tools to help solve problems. From NSLS-II's side, a full understanding of industry challenges is lacking; NSLS-II does not have employees that were previously embedded in industry. Discussing challenges helps bridge this gap.

Huq asked about interagency coordination for microelectronics. **Schwartz** explained that the Subcommittee on Microelectronics Leadership, authorized by the National Defense Authorization Act of 2021, is led by the Office of Science Technology and Policy (OSTP) with involvement of the DOE, DOD, DOC, and other agencies. There is an active dialogue about different agency roles. DOC, and to some extent DOD, is focused on later-stage prototyping and the transition to commercialization. DOE is focused on early-stage innovation, which feeds into later prototyping.

Krusin-Elbaum cited light source capabilities at facilities in Switzerland and Germany that would enable research opportunities in low dissipation chiral logic and topological spintronics. Do U.S. user facilities have these capabilities? If not, why not? **Hill** was not aware of such capabilities. At present, experiments could be conducted at U.S. user facilities in demonstration form. There is no reason in principle that a dedicated end station could not be constructed at a U.S. facility. To do so, a proposal and funding will be needed. **L. Chen** resonated with the importance of new light source capabilities.

Meng asked about the future roadmap for microelectronics. Industry prefers nondestructive, high-throughput characterization while BES pushes for precision and sensitivity at the molecular and atomic levels. The future will require going beyond Moore's Law. How can BES facilities give the U.S. an edge like Europe's special capabilities in optics? Thinking about next-generation manufacturing devices with high-end x-rays and AI is critical for facilitating industry acceleration. BES can have an impact in helping to identify the descriptors that qualify materials for the microelectronics industry. **Hill** agreed that the U.S. needs to think about translating capabilities from characterization at a synchrotron to high-throughput industry fabrication lines. BNL has some thoughts on this. **Haegel** stressed letting the questions inform what tools are needed. Future fabrication tools may be very expensive — perhaps $500M. New technologies may also change paradigms. The field must remain open to possibilities and continue collaborating and learning. **Guha** commented that setting the descriptors for microelectronics materials is a complex discussion.

Mallapragada revisited whether there are opportunities to develop nondestructive, high-throughput characterization tools and requested more information about supply chain challenges

for critical materials. **Guha** highlighted procurement of bulk crystals and supply chains for rare earth and isotopically pure materials as major challenges. Bulk crystal research has declined in the U.S., and China is currently a leader in producing nonlinear crystals. **Schwartz** added that the DOE Isotope Program (IP) is part of the previously mentioned interagency subcommittee, and that the interagency dialogue is also addressing supply chains for certain critical materials.

Allison raised coordination among BES and other federal agencies to integrate materials with processing fundamentals and computational architecture. **Schwartz** said BES is working closely with the SC Office of Advanced Scientific Computing Research (ASCR), which is focused on development of architectures and algorithms. The BRN for Microelectronics workshop held five years ago addressed closing the loop between materials development and integration with architecture, but this continues to be a challenge. **Trolier-McKinstry** stressed architecture-informed materials development is a critical need and is challenging to do in BES programs. Materials discovery/characterization must inform architecture and vice versa.

L. Chen asked about the role of basic research in understanding coupling in microelectronics. **Hill** confirmed research can support scientific understanding of dynamics and phase change memory. Being able to watch devices operate under real-world conditions will be important, and this is something synchrotron-based light sources can do.

Segalman wondered how CHIPS and Science Act language about research security will affect the BES program. **Schwartz** commented that most security language is targeted towards commerce and manufacturing and not earlier research stages. This is an ongoing discussion.

Update on BESAC Charges for 2023, Cynthia Friend, BESAC Chair

Two of BESAC's four current charges are COVs. Along with the MSE COV, BESAC has been charged with forming a COV to evaluate the SC Office of Workforce Development for Teachers and Scientists (WDTS) for FY17-22. This charge was initially delayed due to COVID-19. Previous BESAC COVs evaluated WDTS in 2010 and 2016. In addition to the standard charge, this COV is asked to assess 1) the effectiveness of the online technology development and evaluation activities; and 2) DEI of participation in WDTS programs, including outreach efforts to enhance DEI.

The remaining two charges stem from the 2021 BESAC International Benchmarking Report, which characterized the standing of BES research in six critical areas against international competitors. The report found China is surging in research and funding in many critical areas, Europe leads in QIS, and the U.S. is flattening or falling behind. The report additionally suggested strategies to enhance the U.S.'s position in the global arena for these critical areas. Accordingly, one of the current charges seeks area-agnostic strategies to direct investments in BES-supported domains in the medium to long term. Specifically, the charge seeks input on strategies to identify topical priorities and balance research investments across recipient types, infrastructure, and modalities as well as discovery versus use-driven science. The charge also requests guidance on how BES should take international competition and collaboration into account across research domains and how frequently evaluations should be revisited in the future. The second charge stemming from the International Benchmarking report requests the subcommittee to assess the impact of the Nanoscale Science Research Centers (NSRCs) to date and provide strategies for selection of high-impact, future directions to better serve the nation and user research. Both subcommittees are currently being formed.

Discussion

Horton reiterated the BES Research Investment Strategies charge seeks input to BES on how to make assessments, not to deliver final assessments. **Friend** added the importance of fields can change, so strategies to determine where to emphasize efforts are important.

Archer reasoned that in order to define a strategy, the committee will need past data to form and test hypotheses. Strategies become actionable when one has a clear-eyed understanding of the past. **Kastner** clarified the committee will formulate strategies and identify the types of data BES will need in order to make decisions. BES will be responsible for gathering data. **Takeuchi** commented that the International Benchmarking Report offers different types of metrics for success, such as publication impact, conferences, etc. These metrics can serve as a jumping off point, but the committee will need to determine whether other metrics should be added to the mix. **Friend** emphasized the committee should focus on identification of strategies to inform decisions and the types of data needed to support such strategies; the committee should avoid getting overly involved in data collection.

Berry stated having a strategy is predicated on having a goal. Presumably, the goal of the Research Investments Strategy charge is to fulfill the DOE mission. Metrics of success may extend beyond publications. **Friend** agreed and clarified that the goal is specifically to evaluate strategies to bolster BES research. The Benchmarking subcommittee used BRN goals to identify critical BES areas. **Takeuchi** agreed.

Friend deferred additional charge-related discussion to the end of the meeting.

Friend dismissed the meeting at 3:10 p.m. for a break and reconvened the meeting at 3:40 p.m.

NANOSCALE SCIENCE RESEARCH CENTERS PANEL: Murray Gibson, FAMU-FSU, Panel Moderator

Center for Nanophase Materials Sciences (CNMS), Karren More, Director

CNMS is co-located with BES user facilities in Oak Ridge, Tennessee. CNMS excels in imagining and spectroscopy, soft matter science, and autonomous experiments, with unique capabilities, instrumentation, and/or expertise in these domains. Future science for this facility will target multiscale dynamics; harnessing complex macromolecular conformations; and heterogeneities in quantum materials.

CNMS supported ~800 users and contributed to 360 peer-reviewed publications in FY22, with ~40% of publications demonstrating collaborations with other NSRCs, BES User Facilities, and DOE programs. Although >60% of users originate from outside of Tennessee and 13% are international, many users are from eastern/southeastern portions of the U.S. CNMS is working to increase the number of users from industry and other underrepresented groups, including Historically Black Colleges and Universities (HBCUs). Remote access has improved the diversity of the user population. Coordinating with other NRSCs, CNMS also contributes to SC Data Workshops and Reviews.

Center for Integrated Nanotechnologies (CINT), Jeff Nelson, Co-Director

CINT is one program carried out at two facilities: CINT-Core in Albuquerque and CINT-Gateway in Los Alamos. CINT's scientific thrusts address *in situ* characterization and nanomechanics; nanophotonics and optical nanomaterials; quantum materials science; and soft, biological, and composite nanomaterials. Science highlights were presented across these focal

drives. CINT's NSRC recapitalization investments will continue to position the user community to advance microelectronics, quantum, and clean energy science and technology.

Following passage of the CHIPS and Science Act, CINT is leading an NSRC Working Group on Microelectronics to identify collective resources that can accelerate provision of expertise, instrumentation, and facilities to meet industry and university research needs.

The user community shows strong regional support, with a balance of user projects across academia, government, and industry, including regional small businesses. CINT is working on a number of programmatic and outreach initiatives to continue to grow the community in numbers and all aspects of DEI.

The Molecular Foundry (TMF), Kristin Perrson, Director

TMF at Lawrence Berkeley National Laboratory (LBNL) is collocated with several other national user facilities, Energy Innovation Hubs, and EFRCs. Scientists may have joint appointments across facilities, and collaborations drive synergistic activities in synthesis, characterization, fabrication, and theory. Likewise, shared data and software across the complex advance discovery and innovation. TMF itself is guided by five cross-cutting research themes: 1) architecting information-dense control of energy and information flow; 2) atomically precise control of energy and information flow; 3) nanoscience towards a sustainable future; 4) accelerated materials discovery and prediction; and 5) physical and digital infrastructure as drivers for innovation. Science highlights include sequence-defined hierarchical peptoids; fully recyclable peptoids; and pioneering techniques and instrumentation in advanced electron microscopy. The facility's future vision includes a focus on accelerated discovery through AI synthesis and robotic workflows, as well as QIS and characterization of quantum materials and behavior with an all-superconducting electron microscope (1K-TEM).

TMF User Program served >950 users from 36 countries in FY22 alone and plays an important role in workforce development through training post-doctoral researchers. Proximity to Silicon Valley contributes to the large industry user pool. Active outreach to MSIs and other underserved institutions and groups will continue to increase user diversity in an equitable and inclusive manner.

Center for Nanoscale Materials (CNM), Ilke Arslan, Director

The CNM at ANL has its own beamline at the APS but leverages many ANL resources, including the Argonne Leadership Computing Facility (ALCF). CNM also collaborates with other user facilities. For example, the Digital Twin for Spatiotemporal Experiments is a collaboration across the NSRCs, APS, ALS, and SLAC National Accelerator Laboratory. Science highlights of CNM's impact include discovery of borophene and borophane; selective photocatalytic reduction of CO_2 into methanol fuel; and a new qubit platform allowing manipulation of a single electron by a superconducting quantum circuit. Future scientific opportunities lie in quantum coherence by design; interfaces, assembly, and fabrication for emergent properties; ultrafast dynamics and non-equilibrium processes; AI/ML accelerated analytics and automation; and nanoscale discovery for a sustainable energy future.

By pivoting to remote access during the pandemic, the CNM was able to continue growing its user pool. In FY22, the number of CNM users exceeded 700. CNM leverages ANL's

educational and outreach programs to broaden its user base and is engaged in targeted initiatives to increase users from industry and underrepresented groups and institutions.

Center for Functional Nanomaterials (CFM), Chuck Black, Director

The CFN, co-located at BNL and the NSLS-II, strategically focuses on nanomaterial synthesis by assembly; *in situ*/*operando* science; and accelerated nanomaterials discovery using AI capabilities. Science highlights showcased capabilities related to DNA-mediated nanomaterial assembly; electron and X-ray probes for *in-situ* and *operando* characterization; and 2D materials synthesis, characterization, and assembly. Partnerships with NSLS-II and the NSRCs are important for advancing discoveries. CFN leads the NSRC-Recapitalization Project team and participates in several other cross-NSRC efforts. Future research and advanced capabilities are aligned with national initiatives and will support QIS, clean energy, and microelectronics. There is also the opportunity to link individual NRSC efforts through a common platform spanning all Centers for users to combine systems in their research.

The CFN primarily supports users from the northeastern U.S., including leading research institutions, EFRCs, and the Co-design Center for Quantum Advantage (C^2QA), one of DOE's 5 National QIS Research Centers. The CFN has strong ties with MSIs, and remote operations have broadened the geographic diversity of the user pool. The CFN is continuing initiatives to expand the user pool to industry and national labs aside from BNL.

Discussion

Gibson thanked the NSRCs directors for their presentations.

Daniels-Race asked about proposal acceptance rate. **More** said the acceptance rate is typically between 60%-70%, but the rate varies by year. Some proposals are accepted with limited access to specific capabilities.

Datye wondered whether processes for industry participation are too onerous and what TMF is doing differently to have so many industry participants. Industry participation is not an issue in Europe. **Persson** commented that travel and outreach can be bottlenecks. TMF users stay three months on average. However, TMF is located near Silicon Valley and the Bay area. Many industries are aware of TMF because they hire graduate students. The proposal is only two pages, and access is free. **More** clarified access is only free to industries if they agree to publish. Publishing can be a barrier and paying an hourly fee can be problematic for applicants unwilling to publish. **Nelson** commented that working with startups is easy, because their resources are limited. Engaging large companies takes much more work. Setting up a recent project with Intel took six to nine months. It will be crucial for the NSRCs to leverage resources and personnel through the microelectronics interagency working group to offer a better value proposition to industry.

Montano appreciated statements about increasing participation of underrepresented groups. Facility collaborations can have a tremendous impact on MSIs and non-Carnegie Research I (R1) institutions. Funds to support travel can be an access barrier. Also, if users are seeking high-impact publications because this is an evaluation metric, users may be less likely to collaborate with MSIs or non-R1 institutions. **Horton** commented that Congress does not allow BES to pay users. **Persson** said TMF uses company donations for travel grants to support users

from institutions in EPSCoR states and MSIs. **More** revisited remote access as a way to successfully engage users for whom travel is a barrier. CNMS publications are highly collaborative, and the staff work with users to make publications that are high quality. It is in all parties' best interests to collaborate. **Nelson** cited use of host lab funds, for example Laboratory Directed Research and Development (LDRD) grants, as a way to support travel. CINT has used these funds to bring high school students to the facility for summer experiences. There are efforts to connect with professors as well. **Black** echoed comments that remote access broadens user communities. BNL's Office of Educational Programs helps identify internship programs that can offset travel costs.

Archer asked about special accommodations for new faculty access. While it is great to have high scientific review standards, perhaps accommodations could factor in through a separate process. **More** explained special considerations are not given to early career individuals. However, CNMS's website encourages applicants to contact staff for help in writing a successful proposal. **Persson** said proposals are selected by an external review board. TMF checks after selection to see if all are obtaining access. **Arslan** added industry typically does not write the same kind of proposals as academics, and industry proposals frequently are not rated as highly. CNM does offer help.

Daniels-Race asked about remote access and reiterated earlier comments that review panels should consider how barriers for some populations may impact performance on selection metrics. The review process is a bottleneck, and reviewers are not always in sync with expanding the user base. **Nelson** cited rapid access proposals as a useful tool for engaging industry and new users. Proposals provide more limited access to facilities; the review process is rapid and more internal.

Guzman appreciated ongoing collaboration among the NSRCs and asked about factors limited further collaboration. **Black** observed that instances where NSRCs have worked together have been resourced. If a charge were delivered requiring greater collaboration, the NSRCs would be capable of this. **Arslan** agreed funding is a limiting factor. Data calls for AI/ML and the Recapitalization project demonstrate how all the centers can work together.

Public Comment

None.

Friend adjourned the meeting at 4:53 p.m.

Respectfully submitted on May 5, 2023,
Holly Holt, PhD
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