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

PUBLIC MEETING MINUTES
July 27, 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 Thursday, July 27, 2023 via Zoom. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act (FACA). Information about BESAC and this meeting can be found at https://science.osti.gov/bes/besac.

BESAC Members Present:

Cynthia Friend, Chair, The Kavli Foundation
Esther Takeuchi, Vice Chair, Stony Brook University, Brookhaven National Laboratory (BNL)
John Allison, University of Michigan
Stacey Bent, Stanford University
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
Tabbetha Dobbins, Rowan College
Helmut Dosch, Deutsches Elektronen-Synchrotron (DESY)
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)
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 Montaño, Northern Arizona University
Abbas Ourmazd, University of Wisconsin, Milwaukee
Jose Rodriguez, BNL
Cathy Tway, Johnson Matthey

BESAC Members Absent:

Lynden Archer, Cornell University
Joseph Berry, National Renewable Energy Laboratory (NREL)
Joan Broderick, Montana State University
Serena DeBeer, Max Planck Institute
Rachel Segalman, University of California, Santa Barbara

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 (CSGB) Division
Andy Schwartz, Director, Materials Sciences and Engineering (MSE) Division

BESAC Committee Manager:
Kerry Hochberger, Management and Program Analyst

Thursday, July 27, 2023

Friend, BESAC Chair, called the meeting to order at 11:00 a.m. Eastern Time (ET) to a virtual audience of approximately 268 people. BESAC members introduced themselves.

Update on BESAC Charges, Cynthia Friend, BESAC Chair

BESAC currently has four charges from the SC. Two are Committee of Visitors (COV)**.** The first charge is to form a COV to evaluate the SC Office of Workforce Development for Teachers and Scientists (WDTS). In addition to the standard charge, this COV is asked to assess the effectiveness of the online technology development and evaluation activities; and diversity, equity, inclusion, and accessibility (DEIA) of participation in WDTS programs, including outreach efforts to enhance DEIA. The COV is currently receiving training and will meet in September. The MSE COV, which includes the DOE Established Program to Stimulate Competitive Research (EPSCoR), follows the 2018 MSE COV and is requested by the end of 2023. Panelist recruitment across demographics and institutions is underway.

Two additional charges stem from the 2021 BESAC International Benchmarking Report. The BES Research Investment Strategies charge 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 Research Strategies for Prioritization Subcommittee is assessing how various organizations in the field have approached this question and how strategies can be applied to BES.

The second charge stemming from the International Benchmarking report requests a subcommittee to assess the impact of the Nanoscale Science Research Centers (NSRCs) and provide strategies for selection of high-impact future directions to better serve the nation and user research. The subcommittee will meet in August, and representatives from each NSRC have been invited to be part of this conversation. The report will review the collective NSRC model and impact, not individual NSRCs.

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

Berhe expressed gratitude to BESAC members for their contributions to and guidance of the SC. Though many exciting opportunities are ahead, the recent Congressional debt limit deal will likely lead to significant budgetary headwinds. The SC appreciates the House and Senate Appropriations Committees for prioritizing SC funding. Although neither the House or Senate Marks reached the FY24 requests, either bill would keep the SC and BES at historically high funding levels. The SC will continue to work aggressively to update its facilities and laboratories and maintain a robust scientific portfolio, despite the challenges to meet ongoing priorities and chart new directions.

BESAC's research prioritization charge is vital. Per the 2021 International Benchmarking Report, learning from other disciplines and building cross-government partnerships are key to making wise investments and forming critical collaborations within the science and technology ecosystem. The SC continues to engage with the global scientific community, with BES making key contributions in these relationships. **Berhe** specifically mentioned meeting with senior leaders in Sweden, highlighting discussions of the Energy Earthshots Initiative and its potential global impact. Attendees are encouraged to be creative in seeking new research collaborations and opportunities in light of science's global nature.

Broadening participation in research continues to be a top SC priority; publicly funded science must serve all of the American public. The new programs and requirements in this area are excellent first steps in enhancing DEIA across SC and include: Reaching a New Energy Sciences Workforce (RENEW); Funding Accelerated, Inclusive Research (FAIR); and Promoting Inclusive and Equitable Research (PIER) Plans. **Berhe** welcomed feedback on these initiatives, urging an introspective look on whether they are lowering barriers and reaching the right communities as intended. Building lasting connections and creating vibrant research communities cannot be done through small, standalone initiatives. Instead, the SC must consider inclusivity as a guiding principle in all its activities. Such efforts will lead to stronger funding proposals and a stronger SC overall.

Discussion

Gagliardi noted that Canada has made work permits easily obtainable for qualified people and wondered if the SC should be acting more aggressively. Making foreigners welcome in the U.S. is important. **Berhe** noted that while work permit issues are not within DOE's purview, retaining and growing the workforce is a high priority.

Montaño asked about measuring long-term impacts of SC's DEIA efforts. **Berhe** explained that SC is tracking program performance but needs more than one- or two-years' worth of data. Lessons must be learned in real time to remove barriers, but identifying long-term patterns will require five to ten years of data. Creating change requires long-term support, and the SC is working on multiple data analytics projects to capture as much of the data as possible.

Haile stated DOE's DEIA programs are already making an impact, with effects trickling down in the proposal process. Appreciation was expressed for efforts on reviewer training, as many are unfamiliar with the principles of DEIA. However, there must be a balance between creating new programs and maintaining older programs, as innovative and new directions are not always appropriate. **Berhe** indicated the need to think critically about these programs and reflect on their efficacy. There have been intentional, long-term efforts to exclude certain people and institutions, so it is encouraging to receive feedback that these programs are making a difference.

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

BES's organizational chart was discussed, and recent hires and retirements were highlighted, including director changes at BES-stewarded user facilities.

The Advanced Photon Source (APS) at ANL is being upgraded, and the first accelerator components are currently in the tunnel. The first light at the Linac Coherent Light Source (LCLS-II) at the Stanford Linear Accelerator Center (SLAC) is expected in September 2023. ORNL's Spallation Neutron Source (SNS) is now successfully operating at 1.7 megawatts (MW).

There are two different DOE-wide EPSCoR program funding types available in alternating years: larger implementation awards and smaller state/national laboratory partnerships. Fourteen awards totaling $33M from the implementation cycle were recently announced, covering topics such as grid integration, renewable solar and wind energy, and advanced manufacturing.

BES's peer review process has been completed for the Early Career Research (ECRP), FAIR, and RENEW programs, and awards will be announced soon. BES funding for awards issued under the Small Business Innovation Research and Small Business Technology Transfer (SBIR/ STTR) program is reduced by approximately 50% from the previous year. The FY24 Phase I Release 1 Funding Opportunity Announcement (FOA) for this program will be released in early August. User facility-focused laboratory announcements released in FY23 are supporting the Biopreparedness Research Virtual Environment (BRaVE) and Accelerate Innovations in Emerging Technologies (Accelerate) initiatives, as well as Advanced Scientific Computing Research (ASCR) for DOE User Facilities. Applications are under review for the latter two, while an award announcement is expected shortly for BRaVE.

The Energy Earthshots Research Centers laboratory announcement was initiated jointly by the BES, ASCR, and Biological and Environmental Research (BER) programs. Under this announcement, the three programs will fund Energy Earthshot Research Centers (EERCs)—large, multi-investigator, -institution, and -disciplinary teams focused on advancing foundational knowledge and enabling capabilities in experimental and computational chemical/materials science in support of DOE Energy Earthshots goals. EERC funding will be complemented by smaller, university-led awards in foundational science for Energy Earthshots. Applications are currently under review, and award announcements are expected later in FY23.

Award announcements for the open recompetition of the Batteries and Energy Storage Hub program are expected soon. For the last ten years, the Hub has been the Joint Center for Energy Storage Research (JCESR), which has supported >350 graduate students and postdoctoral researchers among other accomplishments. Science highlights featured research on ultra-low-cost flow batteries made from earth-abundant materials. The results of this work were spun out as a company called Form Energy.

The FY24 BES budget request was ~$2.7B, representing a 6.3% ($159M) increase over the FY23 enacted budget. There was a $56M overall increase in the research program funding request, with a $25M increase to establish Microelectronics Science Research Centers and a $35M increase to expand investment in the SC Energy Earthshots initiative. New start construction funding has been requested for two projects: $13M in support of ORNL's High Flux Isotope Reactor (HFIR) pressure vessel replacement, and $6.6M in support of development and procurement of new beamlines for BNL's National Synchrotron Light Source-II (NSLS-II) (the NSLS-II Experimental Tools (NEXT)-III project). The request for user facilities has only been supported at 90% of the funding required for re-baselined, normal operations. Operations costs are increasing at these facilities due to staffing growth, inflation, and maintenance activities.

The FY24 BES House Mark is ~$2.58B, which is 3.9% below the FY24 request but 2.1% above the FY23 appropriation; the Senate Mark is ~$2.68B, 0.5% below the FY24 request and 5.7% above the FY23 appropriation. SC Energy Earthshots funding is reduced in both marks; support for microelectronics research is supported in the Senate Mark but not explicitly funded. The House Mark has a substantial reduction in funding for BES light sources compared to the request. Funding for construction of the HFIR pressure vessel replacement and NEXT-III was not provided in the Senate Mark. BES looks forward to appropriation committee meetings and reaching a compromise on the budget.

Details about the DOE/BES User Facility Science Webinar series were shared. These webinars are intended to highlight the user facilities' impact on areas of national priority. Future topics include clean energy, bio-preparedness, and advanced manufacturing.

BES research directions come from many sources, including DOE and BES strategic planning. This strategic planning includes input from Basic Research Needs (BRNs) workshops and roundtables, BESAC charges, and engagement between BES leadership and program managers during annual budget planning. Additional input for research direction planning is obtained through BES engagement in National Academy of Science (NAS) assessments and reports and interagency planning. Taken together, this process has been generated an amazing volume of community-driven input over the last 20 years.

Discussion

Ourmazd suggested a process of planning for surprises and allowing some researchers to work on the craziest ideas they could think of without review. **Horton** suggested this is similar to talking with BES program managers about where the leading edges are in their portfolios and working on ways to excite the community to submit proposals based on these types of ideas on a smaller scale.

Dobbins complimented the 20 years of BES strategy reports. These are important resources for two-way communication with the scientific community. **Horton** emphasized the role the community has played in putting together the reports.

Haile asked whether the BES strategy reports have impeded pursuing research directions that were outside of what was covered in the reports. **Horton** stated this concern was what led to the more open-ended Grand Challenge reports. In all reports, the text supporting the priority research directions records broader implications, but a balance between established and new directions is important for avoiding unintended consequences. **Schwartz** agreed and suggested the core BES programs have more flexibility in accepting proposals from broader topical areas.

Gibson wondered whether the ECRP needs to be strengthened to allow for research risk taking instead of only doing research that sells. **Horton** expressed hope that BESAC can help understand what performance metrics should be assessed to enable more risk taking. Applications for the ECRP have historically had a low success rate. In response to concern about the low success rate from a BESAC Committee of Visitors' review, BES has been working to determine the best ways to reduce the number of applications for funding, while still promoting an open call with respect to the science. Currently, many of the core research programs have increased the success rate, and decreased the peer review workload, by including only half of the potential research topics each year, alternating the topics in the calls for proposals from one year to the next.

L. Chen suggested evaluating the impact of previous BRNs to identify future research directions. Research councils could act similarly on a smaller scale. **Horton** stated research councils have historically pulled together small groups to propose workshops with output to be published in the open literature, but for materials science, BES has moved away from this in order to give more of the community an opportunity to provide input.

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

Defining Strategic Directions for Research, George Santangelo, National Institutes of Health (NIH)

Lessons learned were shared from the NIH Office of Portfolio Analysis (OPA), which has been operating since 2011. The goal of the office is to accelerate and optimize research investments within existing and planned portfolios through data-driven decision making. This is achieved through training; consulting and collaborating across the NIH enterprise based on its unique culture, rules, and regulations; developing new analytics, including by leveraging artificial intelligence and machine learning (AI/ ML); building tools; and data cleaning and analysis.

NIH users have four priorities for data management tools: ease of use, which is especially important given that decision makers are very busy; integration of multiple tools, which allows for easy movement from one environment to another; data visualizations, which are essential when working with large portfolios; and an easy-to-use and well-elaborated search process. OPA provides beginner to advanced training so users can fully understand the available resources. Further, scheduled consultations allow the creation of new data analysis methods for specific research questions.

Validation of the data analytics processes confers user confidence in NIH tools. Ongoing work is being done to develop supervised ML utilizing gold standard training data sets having high inter-rater reliability. It's important that you have enough subject matter experts generating gold standards that you measure the degree to which they agree with one another about the data. If they don't agree – if inter-rater reliability is low – you can't trust the data set is a gold standard. When the measured inter-rater reliability is high, everyone can agree that the gold standard data set is a unified representation of what you want to study, and you can leverage ML to identify examples of interest within the data. Similarly, language model-based analysis is being leveraged to analyze scientific content. For example, by using discriminative AI, OPA has agnostically divided different research topics to identify the overlap between the NIH and National Science Foundation (NSF) portfolios to identify support gaps.

OPA is also creating tools to measure productivity, identify emerging topics, and predict which topics will produce transformative breakthroughs. For example, the Relative Citation Ratio (RCR) is a method developed by OPA to measure research productivity and influence. RCR operates at the article-level and is normalized to the scientific field size but does not consider the impact in moving the science forward. With that said, the influence of an article often implies its impact. RCR is publicly available through the iCite 2.0 tool, which in addition to providing a measure of article influence, provides a measure of translational progress (through paper citations by clinical trials) and technological impact (by citations in patents).

OPA has filed a patent for another tool used to predict what topics will produce scientific breakthroughs. Predictions are visualized as heatmaps, and parameters include the relative rate of progress, topic age, funding sources, and number of recent publications. Similarly, OPA has integrated this information to build animated data visualizations, which can be used convey stories about research over time to decision makers.

The beta version of a new public-facing tool called iSearch Analytics will be available in September 2023. While the data is sourced mostly from biomedical research, the tool will also include other types of science. OPA is also looking to expand the tool to include all sources of research funding worldwide. iSearch Analytics' major features include literature expansion by delivering preprints and progressing towards comprehensive coverage of publications; person disambiguation through highly cleaned person-level data and metrics; and reimagined visualizations through language model organized information.

Discussion

Bent sought elaboration on the decision to build tools instead of buying them. **Santangelo** alluded to the IBM Watson tool and how its capability was oversold. A tool like that cannot capture the complex administrative structure of NIH investments. Tools must be built internally and customized to understand institution-specific structures to be effective. Similarly, tools must be validated to ensure a unified approach, which is difficult to do for off-the-shelf tools.

Mallapragada asked how NIH decision makers use these tools to shape their funding portfolios. **Santangelo** emphasized how new this technology is but suggested its use in finding research topics with inadequate funding, as well as helping remove hurdles for investigators on slowly progressing topics.

Allison asked about the input for determining the relative rates of fields' progress, especially if fields have been around for a long time. **Santangelo** explained the calculation as the fraction of literature that has been recently generated, with entropy (in terms of the areas of study within the field) as another component. Older topics can still show high levels of relative rate of progress similar to emerging areas, but findings rely heavily on granular discrimination between topics.

PROGRESS TOWARDS LIQUID SOLAR FUELS: Panel Moderator Gail McLean, Acting Director, CSGB

The process of producing liquid solar fuels is sometimes referred to as artificial photosynthesis and involves a direct conversion of solar energy into chemical energy. The Fuels from Sunlight Hub program currently targets the chemical transformation of carbon dioxide (CO_2) and potentially other small molecules into liquid fuel using sunlight as the energy source. Work is ongoing at the two BES Fuels from Sunlight Hub awards: the Liquid Sunlight Alliance (LiSA) at the California Institute of Technology (Caltech) and the Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE) at the University of North Carolina – Chapel Hill.

The Liquid Sunlight Alliance, Harry Atwater, LiSA Director, Caltech

LiSA aims to create tools and capabilities to develop a circular economy for carbon, collecting and capturing CO_2 from hard-to-decarbonize emission sources like industrial processes and power plants. Through electrochemical, biochemical, thermochemical, and photochemical methods, the goal is to create liquid fuels, chemicals, and materials and to close the carbon cycle. The need for solar fuels is based on the alternative processes for generating liquid fuels; gridpowered electrocatalytic and thermocatalytic approaches are carbon positive until approximately 2050, when the grid is expected to be decarbonized.

Artificial photosynthesis is a direct pathway from solar energy to liquid solar fuels, as opposed to a number of indirect routes DOE is also studying. Contrasting with previous artificial photosynthesis approaches, which focused on photocatalysis at individual reaction centers, LiSA seeks to generate solar fuels through co-designed coupled microenvironments and associated cascading reaction centers, mirroring those observed in natural systems. LiSA's three goals are to: 1) understand and integrate multi-component systems of coupled microenvironments, tailoring molecules and materials for achieving targeted functionality in transport and activity around an active site; 2) discover photon, electron, and molecular processes, from light excitation to the catalytic center, to realize ensembles of molecules and material that achieve efficiency and selectivity beyond those available with conventional electrochemical processes; and 3) develop and validate predictive models for component and interface durability, and understand the implications for solar to fuel efficiency and selectivity under real world conditions.

The first phase of LiSA began in 2021 to understand the science of the building blocks of molecular design in microenvironments, especially the photodynamics and stability of components. The second and current phase is focused on exploring coupled microenvironments and their integration, which includes understanding how to use light-driven processes to control reactions and assess degradation mechanisms.

Key knowledge advances from LiSA research in 2023 addressed: 1) foundations of coupled microenvironment cascades; 2) how to control selectivity with copper as a performative heterogenous catalyst using molecular additives and ionomer coatings to tailor the productivity and product distribution; 3) ultrafast soft X-ray characterization of carrier dynamics as a mechanism for probing relaxation and photoelectrodes; 4) characterizing surface instabilities of CO_2 reduction catalysts and relating catalyst morphology to corrosion mechanisms; and 5) discovering new photoelectrode and amorphous photoanode materials like zinc titanium nitride ($ZnTiN_2$) and nickel antimonate (Ni-Sb), respectively. The use of Earth abundant materials offer alternatives to rare materials like iridium oxide (IrO_2).

One of the key mandates of the Fuels from Sunlight Hub program is to develop photochemical architectures that incorporate light absorbers and a multi-catalyst cascade to achieve CO_2 reduction to methanol. The first of LiSA's approaches uses a tandem photoelectrode with two catalytic centers that operate in a cascade format, which enables independent control of potential and current density at the two electrodes. Substantial progress has been made in showing cascaded solar to fuel conversion from CO_2 with a faradaic efficiency (FE) of approximately 5%. A second architecture focuses on coupling a photoelectrochemical system for generating ethylene to a solar-driven thermochemical system to selectively make hexene from CO_2. First indications of liquid fuels have been seen from this process.

The Center for Hybrid Approaches in Solar Energy to Liquid Fuels, Jerry Meyer, CHASE Director, University of North Carolina – Chapel Hill

The five-year goal of CHASE is to develop a fundamental molecular level understanding of how hybrid photoelectrodes can couple single photon absorptions to the chemical transformations necessary to generate liquid solar fuels. These hybrid photoelectrodes are comprised of molecular catalysts with tailored microenvironments integrated with silicon semiconducting light absorbers. The electric fields in these semiconductors can be tailored to transfer electrons towards the catalyst for the CO_2 reduction reaction. One of the challenges is the transition metal complexes used as molecular catalysts. While they are very good at converting CO_2 to C1 products, CHASE is interested in higher energy density liquid fuels like butanol. To reach that goal, multiple catalysts will be used, and the initial products generated by one catalyst will be transferred to another, utilizing the cooperative interactions of catalyst cascades.

Further, a vision has been set forth for CHASE: liquid fuels can be generated using the small molecules found in air as the only chemical feedstocks and sunlight as the only energy source. This challenge of practical liquid solar fuel production can only be met through the cooperative interactions of molecules and materials.

CHASE is currently working on two proposed architectures to achieve this. The first is referred to as the wired architecture, as the cascading catalysts are directly integrated into the semiconductor surface and accept electrons directly from them. The second is the decoupled architecture, where all the cascade catalysis is done in the dark, using hydrides that can transport to a catalyst cascade to drive the reduction reactions. Once these hydrides deliver their payload and become oxidized, they are regenerated at an illuminated architecture.

The decoupled architecture is defined by the catalysis occurring remote to the light absorbing semiconducting hybrid photoelectrode. Organic hydrides like nicotinamide adenine dinucleotide + hydrogen (NADH) and benzimidazole, along with transition metal hydrides, can regenerate at a photoelectrode surface, so they are not simply sacrificial reagents. CHASE has not yet been able to link the catalysts to secondary supports in this architecture. One of the key challenges is finding conditions where all these catalysts can work in concert, but good progress is being made. This architecture forms the basis for a catalytic cycle to reduce carbon monoxide (CO) to a formyl, which is then converted to the hydroxymethyl complex and, upon illumination, releases methanol. Following this conversion, CO can rebind to the catalyst, completing the catalytic cycle.

The key difference between the wired architecture and the decoupled architecture is the direct electron transfer from the hybrid photoelectrode to the catalyst, which drives the reactions in the cascade to generate liquid fuels. The wired architecture is defined by each catalyst in the cascade being integrated into a single hybrid photoelectrode as the illuminated semiconductor transfers electrons directly to the molecular catalysts. CHASE's success in this architecture has been integrating the catalyst cobalt phthalocynine (CoPc) with p-type silicon. This is used as a hybrid photoelectrode to generate methanol, CO, and hydrogen, with the FE of methanol production currently at 8%. Incorporating carbon nanotubes coated with CoPc into standard photoelectric cells forms the same products but increases the FE of methanol production to 20% while increasing the current density.

Discussion

Friend sought comments on the durability and the challenges of molecular-based catalysts. **Meyer** agreed any molecular approach to energy conversion raises concerns about durability. CHASE's current durability is approximately 2 hours under air mass 1.5 conditions, which is not sufficient. However, there are a number of strategies to improve durability, such as atomic layer deposition (ALD) to put a thin layer of an oxide on top of the molecular catalyst. Similarly, rigorously excluding oxygen from the system is vital for practical applications. **Atwater** explained LiSA's multipart strategy to durability. First, some chalcogenide materials (e.g., zinc telluride), in the absence of a co-catalyst, are performative for the CO_2 reduction to CO, which might contribute to durability. Second, co-catalysts like copper may appear to be durable, but research shows that copper does remodel itself, leading to durability issues through the loss of activity by changing the morphology of the actual heterogeneous catalyst site. However, LiSA has shown molecular additive coatings and ionomer films are very effective in increasing durability and selectivity in the systems examined.

Guzman asked about the processes' overall efficiency and whether the final liquid fuel should be made in the device or an intermediary fuel should be taken out to be intensified elsewhere. **Atwater** acknowledged diminishing returns with respect to moving towards large, multi-carbon products. LiSA is focusing on a coupled microenvironment architecture that cascades products from a gas diffusion electrode to produce C2 products like ethylene, which then allows the use of a solar-driven thermocatalytic reaction center. The eventual technological goal is to build systems operating under ambient conditions with no other external chemical plant to perform this coupling of photoelectrochemical catalysis to thermocatalysis, in order to produce more complex and higher molecular weight distribution products. **Meyer** recognized the challenge of making carbon-carbon bonds with a molecular approach. CHASE views ethanol as a key intermediary from primary photoelectrodes. Ethanol should then be able to be upgraded to butanol, which is much more miscible with gasoline.

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

Basic Research Needs Update, Gail McLean, Acting Director, CSGB; and Andy Schwartz, Director, MSE

BES workshops and roundtables are important tools to provide strategic input for BES-supported research. They are highly structured to engage the community and ensure that participants meet the stated goals. Roundtables are oriented around focused topics, while workshops look at broader research fields. The output of these are reports that guide BES research strategies and serve as resources in high-priority topical areas. The first BRN workshop, held in 2002 in response to a BESAC charge, surveyed science needs across the energy technology landscape and established the model for future BRN workshops. This set of workshop helped provide the foundation for the BESAC Grand Challenge report in 2007. These workshops and roundtables cover the breadth of the BES portfolio and have often engaged with other SC programs and DOE technology offices.

Examples of the initiatives that have directly resulted from these strategic planning efforts include the Energy Frontier Research Centers in 2009; the ECRP and Energy Innovation Hubs in 2010; the National QIS Research Centers in 2020; and the upcoming EERCs.

The next BRN workshop is on accelerator-based beam instrumentation in Fall 2023. Possible topics for future workshops and roundtables include science foundations for critical materials sustainability; next-generation fabrication for microelectronics and QIS; basic research needs for the subsurface; future BES computation sciences, including theory, data and AI/ ML for exascale and beyond; bioinspired chemical and material sciences for sustainable energy and products; and materials and chemistry in extreme environments, focusing on renewable energy, manufacturing, and end use. BESAC's input on future workshops and roundtables, including on topics not mentioned, is invited.

Discussion

Kastner suggested van der Waals heterostructures as a future topic. **Schwartz** appreciated this suggestion and wondered whether it could fit under the next-generation fabrication topic.

Haile proposed the topic of co-designed materials and architectures, on scales from nanoscale to civil engineering architectures. **Schwartz** acknowledged this idea and supposed it might fit into some of the topics already mentioned.

Takeuchi emphasized the usefulness of BRNs and commented on the upcoming accelerator-based beam instrumentation workshop, asking how these tools' software can better interface with their hardware to maximize scientific output? **Schwartz** stated that facilities are considering this topic. **Horton** mentioned a previous workshop on data at user facilities, but discussions may not have sufficiently covered this concept.

Huq asked how interagency hubs operate with multiple interests involved. **Schwartz** clarified that the National QIS Research Centers are not multiagency, but involve multiple programs across the SC, with the intent for interdisciplinary activities crossing over the priorities of the multiple programs. BES began the BRN process, but other SC programs have since adopted this model to look at the scientific directions relevant to their program missions in a given area like QIS. The hub model for QIS Research Centers was intended to cover that broad landscape.

Gagliardi proposed a workshop on best practices for data acquisition, storage, and use across experimentation, computation, and AI. **Schwartz** recognized this suggestion and saw it as particularly crosscutting.

Ourmazd brought up the topic of applying AI/ML to data as both an interpolation and extrapolation technique. In light of this, how can predictions be made on the evolution of complex systems? Industry does not seem to be interested in this aspect of AI/ML. **Schwartz** potentially saw this as part of the previously mentioned future BES computational sciences topic. Moving in the direction of predictive capabilities is extremely important. **McLean** noted the relevancy of this idea to modeling the complexities of enhanced geothermal systems. The topic is not only pertinent to computational science, but also many other topics.

L. Chen commented on the accelerator-based beam instrumentation workshop and the importance of considering feedback from facility users on their future needs. As a follow up, would the idea for the next-generation microelectronics and QIS workshop focus on the science of fabrication or the dynamic phenomena related to it? **Schwartz** stated the workshop has not been scoped yet, but the discussions have been around fabrication, as previous workshops have not focused on this area.

Guzman asked whether enough workshops and roundtables have been done on the basic science behind the Energy Earthshots. **Schwartz** said some topics have received more focus than others. The suggestion of basic research needs for the subsurface was included specifically for this reason. **McLean** added that the bioinspired chemical and material sciences for sustainable energy and products topic was added in response to the Energy Earthshots Initiative. **Horton** (via chat) mentioned that the Floating Offshore Wind Shot was a driver behind the materials and chemistry in extreme environments workshop idea.

Tway brought up the idea of a workshop to map out potential unmet needs and gaps in basic science resulting from the net zero transition. **Schwartz** appreciated this suggestion.

Allison seconded Gagliardi's suggestion for a data best practices workshop and Takeuchi's idea to examine the software component of accelerator-based beam instrumentation. Revisiting the topic of Computational Materials Science and Chemistry was also put forth.

Schwartz acknowledged these comments. **Garcia** (via chat) added AI and QIS as potential topics as part of a data best practices workshop.

Gibson suggested a workshop around the sustainability of making polymers. A roundtable on understanding nucleation and its control of determining structures was also raised. **Schwartz** noted these ideas.

Mason advocated for repeating topics that have been covered recently if they are important. A best practices workshop for DEIA in energy research was also suggested. **Schwartz** remarked that the latter workshop idea could be SC-wide.

Friend mentioned using data analysis tools to look at the impact of the last BRNs and emerging fields in the energy sciences space.

UPDATE ON COMPUTATIONAL CHEMICAL AND MATERIAL SCIENCES: Panel Moderator Andy Schwartz, Director, MSE

The first Computational Materials Sciences (CMS) projects were initiated in 2015, and the companion Computational Chemical Sciences (CCS) program was launched shortly after in 2017. These programs support basic research to develop validated and robust open-source codes and accessible databases that allow for the modeling and simulation of a wide array of materials and chemical systems. Thanks to ASCR, DOE has one exascale computer online and another one coming soon. This increase in computing power is driving an increased focus on data science in the research portfolio. In interest of this, updates from two current CCS/CMS projects were given.

The Computation Chemical Sciences Program at BES and PNNL, Sotiris Xantheas, Pacific Northwest National Laboratory (PNNL)

A 2016 BESAC meeting recognized the importance of creating a new electronic structure calculation capability that was U.S.-developed, open source, and scalable. Needed software capabilities included efficiently scaling to about a million processors, handling relativistic effects, properly treating d- and f- electrons, and improving on density-functional theory (DFT). Increased performance and scaling would need to come from parallelization as advances in processor speed were nearly exhausted. To this end, BES funded the CCS program, of which there are 16 projects currently ongoing. Projects include the Scalable Predictive Methods for Excitations and Correlated Phenomena (SPEC) project at PNNL. The software libraries for previous and current CCS projects are being hosted on a website administered by the University of Minnesota.

SPEC brings together people from domain science, computer science, and applied mathematics to realize CCS goals. Specifically, SPEC looks to implement state-of-the-art, many-body electronic structure methodologies; deliver scalable, open-source electronic structure software libraries; address challenges in excited-states of complex chemical systems; and interpret signals from data collected at DOE's light source facilities.

Within the DOE complex, investments in scientific user facilities and computation facilities should be linked by software development in order to enable new scientific discoveries. PNNL has developed a number of scalable software programs. SPEC's performance is in the range of 50-60 petaflops, which is optimal for research like studying light-harvesting antennas in dye-sensitive photocells or developing descriptors of chemical transformations. PNNL manages its software collections through the Computational and Theoretical Chemistry Institute (CTCI), which serves as an umbrella for the ecosystem of methods used.

In two scientific highlights, Tensor Algebra for Many-body Methods (TAMM) was shown being used to determine the excited state spectral function of DNA base pairs and to determine the low-lying excited states of dynamic correlation of the FeMo-cofactor in the enzyme nitrogenase.

Going forward, SPEC is looking to address a number of challenges, including: moving from a model system to real systems resembling those measured in DOE's light sources; realizing the full potential of upgrades at DOE computational facilities; involving the scientific community in a concerted effort to realize the full potential of developed software; and training young scientists to fully realize the advantages of heterogenous hardware architectures. First steps have been made on these challenges through a workshop and paper to chart a path forward.

Computational Materials Science Centers: Midwest Integrated Center for Computational Materials (MICCoM), Giulia Galli, ANL/University of Chicago

The major CMS projects are located at national laboratories and have the same broad mission as the CCS projects, but each focuses on different properties or materials. Smaller projects at universities were started in 2019.

MICCoM is located at ANL and develops and disseminates interoperable computational tools, including open-source software, data, simulation templates, and validation procedures, to enable simulations and predictions of properties of materials for low-power electronics and quantum technologies. Distinctive features of the center are the development of interoperable codes for simulation of materials at multiple length and time scales; the focus on heterogenous materials, including defects, interfaces, and building blocks; and the emphasis on spectroscopic and coherence properties. MICCoM's guiding principles center on scientific innovation, sustained methods for algorithmic development, and improvement of existing algorithms; the coupling of methods and of codes across centers to target multiple properties of heterogenous materials; the importance of hybrid computational strategies and running on multiple architectures, including quantum computers; integration with experiments; and making computational data robust and available, especially in the age of AI/ML.

To address the electronic and dynamics properties of heterogenous systems, research is done on the structure of the materials at an atomistic scale. Once complete, more advanced properties are examined, such as the electronic properties of strongly correlated regions, optical properties, and spin coherence and dynamics. Such research requires multiple methods, algorithms, and codes and has led to methodological advances and new computational protocols during the investigation of the synthesis of atomistic level point-defects.

In terms of data, MICCoM has focused on "bringing published papers to life" by providing all data and procedures presented in these papers in a decentralized and distributed manner. To that end, data is available through the open-source software Qresp - Curation and Exploration of Reproducible Scientific Papers – which was developed by MICCoM and is available at the website qresp.org. It was shared that getting participation in this project has been a struggle, as it is a significant change from the status quo.

In summary, MICCoM aspires to be a sustained innovation factory for new methods and new strategies while providing exemplary open-source software to the community; a proponent of coupled simulation strategy on hybrid architecture; a champion for the stewardship of first-principles molecular dynamics and many-body perturbation theory reference data and open papers; and an advocate for workforce development and community engagement.

Discussion

Garcia asked how the chemical and materials science fields are perceiving the movement towards quantum computing. **Galli** explained no one is putting all of their efforts into quantum computing. Instead, researchers are trying to figure out how to link their studies to these efforts. There is an awareness that some questions in materials sciences can only be answered with quantum computers but accessing machines remains an issue. **Xantheas** agreed there is a level of excitement around quantum computing and explained the classical computing approach will benefit from the increase in computing power quantum computing enables.

Rodriguez sought information on data validation efforts in these programs. **Galli** stated that for each advanced property of the materials that is calculated, there are specific validation methods, which include photoluminescence, optical spectra, and coherence times. **Xantheas** said the spectral functions of DNA base pairs are reproducible. SPEC is working closely with experimentalists at lights sources to reproduce the data for core excitations.

Mallapragada asked if mechanisms are in place to ensure codes are being maintained for quality assurance and continued community use. **Xantheas** reminded attendees of the software libraries hosted by the University of Minnesota; whether those libraries are interoperable is being evaluated. Software sustainability requires consensus on common programming practices and that must come from the community. **Galli** voiced the challenges of sustainability and the lack of a career path in universities for those with a special expertise dedicated to these codes. There might be opportunities in national laboratories, but they do not exist yet. **Xantheas** heartily agreed and remarked on the issue of the lack of career path for consultants that can assist the software users as well.

Allison wanted to hear more about the pros and cons of using centralized or decentralized software databases. **Galli** said MICCoM is using the web as a centralized database. If data is publicly available, not just in a portable document format (PDF) file, having searchable metadata is more important than the nature of the database. Funding agencies and publishers should be doing more to encourage this type of data sharing. **Haile** (via chat) shared that crystallographers have published Crystallographic Information File (CIF) data for a long time. **Gagliardi** (via chat) stressed the importance of sharing data in a standardized format.

Public Comment

James Kubicki (The University of Texas at El Paso, via chat) suggested a BRN workshop on the integration of DOE science with social science research. **Horton** and **Schwartz** acknowledged this comment.

Venkat Bommisetty (Princeton Plasma Research Laboratory, via chat) asked about the role of BES regarding microelectronics and next-generation lithography. **Schwartz** said these topics span both MSE and CSGB divisions. There are materials science challenges along with associated chemistry and processing challenges that the scientific community did not face during the complementary metal-oxide semiconductor (CMOS) scaling of the past. This is on the list of potential BRNs to help BES optimize its investments in this area of research. **Horton** remarked on the potential role of BES user facilities in exploratory research for next generation microelectronics, noting that the NSRCs have clean room capabilities that commercial nanofabrication facilities do not.

An attendee (via chat) wondered whether an increase in funding is anticipated for non-SC DOE laboratories. **Horton** responded that funding proposals are assessed based on merit and not source. Non-SC laboratories are always considered for funding, and there is no inherent bias against any of the national laboratories.

An attendee (via chat) commented on ensuring data is stored permanently as opposed to temporarily. There should be dedicated funding from BES for data portals.

An attendee (via chat) mentioned the fourth BES research division being formed and voiced concerns around the optimization of funding distribution, especially in relation to single PIs and centers. **Horton** stated BES budget distribution is determined by the budget and not by the research division. This organizational change is a way to manage existing funding, not move funding from one organization to another.

Friend adjourned the meeting at 5:03 p.m.

Respectfully submitted on August 10, 2023,
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