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

PUBLIC MEETING MINUTES

July 11-12, 2019

Bethesda North Marriott Hotel & Conference Center
5701 Marinelli Road, Rockville, MD

DEPARTMENT OF ENERGY BASIC ENERGY SCIENCES ADVISORY COMMITTEE
SUMMARY OF MEETING

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) convened on Thursday and Friday, July 11-12, 2019 at Bethesda North Marriott Hotel & Conference Center, 5701 Marinelli Road, Rockville, MD. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act (FACA). Information about BESAC and this meeting can be found at https://science.osti.gov/bes/besac

BESAC Members Present:

Marc Kastner, BESAC Chair, Science Philanthropy Alliance
Cynthia Friend, BESAC Vice-Chair, Harvard University
Kathy Ayers, Proton OnSite
Dawn Bonnell, University of Pennsylvania
Sue Clark, Washington State University, Pacific Northwest National Laboratory
Helmut Dosch, DESY
Thomas Epps, University of Delaware
Yan Gao, General Electric Company
Julia Hsu, University of Texas, Dallas
Despina Louca, University of Virginia
Pietro Musumeci, University of California, Los Angeles
Monica Olvera de la Cruz, Northwestern University
Nai Phuan Ong, Princeton University
Abbas Ourmazd, University of Wisconsin, Milwaukee
Ian Robertson, University of Wisconsin, Madison
Anthony Rollett, Carnegie Mellon University
Maria Santore, University of Massachusetts, Amherst
Andrew Stack, Oak Ridge National Laboratory
Esther Takeuchi, Stony Brook University
Matthew Tirrell, University of Chicago

Designated Federal Officer:
Harriet Kung, Director, Office of Basic Energy Sciences (BES)

Committee Manager:
Katie Runkles, BES Program Analyst

BES Management Participants:
Bruce Garrett, Director, BES Chemical Sciences, Geosciences and Biosciences Division
Linda Horton, Director, BES Materials Sciences and Engineering Division
James Murphy, Director, BES Scientific User Facilities Division

Thursday, July 11, 2019

BESAC Chair, Marc Kastner, called the meeting to order at 9:05 a.m. Eastern Time (ET) to an audience of 155. Kastner requested all BESAC members introduce themselves.

Office of Basic Energy Sciences Update, Harriet Kung, Director, Basic Energy Sciences

Dr. Chris Fall was confirmed May 23, 2019 as the new Director of the Office of Science (SC). Dr. Fall has served as Principal Deputy Director of Advanced Research Projects Agency-Energy (ARPA-E), with the White House Office of Science and Technology (OSTP), and the Office of Naval Research. BES has been approved to post two new positions, Quantum Information Sciences (QIS) and Neutron Facilities Program Manager positions. Daniel Matuszak is the new Separations Program Manager and Emily Smith will join BES in September 2019 as the American Association for the Advancement of Science (AAAS) Science and Technology (S&T) Policy Fellow.

The fiscal year (FY) 2020 President's budget request for BES is $1.858B. Within the budget areas of emphasis and priority include QIS, microelectronics, Energy Frontier Research Centers (EFRCs), Energy Innovation Hubs (Hubs), and data analytics. Two new Major Items of Equipment (MIEs): one will add additional beamlines to the National Synchrotron Light Source-II (NSLS-II), the other will recapitalize equipment and develop new technologies and tools at the Nanoscale Science Research Centers (NSRCs). The FY20 House Energy and Water Development (HEWD) markup provides a $22M increase for facility operations, $42M increase for research in directed priorities, and construction and MIE funding at or above the ideal profile levels.

EFRCs will celebrate their 10-year anniversary this year. The cumulative investment in EFRCs has been $1.3B. A FY20 Funding Opportunity Announcement (FOA) is anticipated for the EFRCs focusing on microelectronics, QIS, science related to the Department's environmental management mission, and other priorities. The EFRC Summit and Forum will be held July 29-30, 2019 in DC; Kung extended a formal invitation to BESAC members. A FOA to recompete the Fuels from Sunlight Hub is expected in FY20.

LCLS is shut down for installations and reconfiguration; LCLS-II early completion is expected 2021-2022. LCLS-II leadership has transitioned from John Galayda to Norbert Holtkamp. Kung formally thanked Galayda for 40+ years of leadership. The Advanced Photon Source Upgrade (APS-U) recently had a successful Office of Project Assessment (OPA) review of critical decision (CD)-3. LCLS-II High Energy (LCLS-II-HE) and the Advanced Light Source Upgrade (ALS-U) have received CD-1. LCLS-II-HE is adding additional cryomodules and extending the energy range to 8 GeV. ALS-U will generate 1,000 times brighter soft x-rays with higher coherence by installing a multi-bend achromat (MBA) lattice, and will develop new advanced instruments.

The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL) is now operating at 1.4MW. The Proton Power Upgrade (PPU) will double the proton beam power to 2.8MW. PPU plans to deliver additional cryomodules, a new target gas injection system, and a redesigned target vessel. The Second Target Station (STS) will move forward as a complementary pulsed source with a narrow proton beam to produce an order of magnitude higher brightness cold neutrons than were previously achievable.

Two new MIEs are the National Synchrotron Light Source II (NSLS-II) Experimental Tools (NEXT-II) and the Nanoscale Science Research Center (NSRC) Recapitalization. NEXT-

II will continue the phased build-out of beamlines at NSLS-II. NSRC Recap will upgrade equipment at all five NSRCs.

The FY20 budget request includes funding to support at least one QIS center between Advanced Scientific Computing Research (ASCR), BES, and High Energy Physics (HEP). ASCR, BES, and HEP issued a combined Notice of Intent (NOI) and Request for Information (RFI) to indicate SC is considering an FOA in 2020. The RFI sought community input on elements of a QIS center.

A BES-ASCR Facilities Information Exchange meeting was held at Lawrence Berkeley National Laboratory (LBNL) in June 2019 resulting in a two-year funded BES light source data solution pilot project.

Discussion

Bonnell inquired about a framework to define the intersection of microelectronics and QIS. **Kung** said Horton and her team are considering a framework. A large base of condensed matter physics, material physics, and materials chemistry work exists and might contribute to these areas. The goal is complementarity and delineating new ideas.

National Academies "A Research Agenda for a New Era in Separations Science" Report Presentation, Joan Brennecke, University of Texas

The National Academies of Science, Engineering, and Medicine released a consensus study on separation science in June 2019. Two motivations for the study were time (the last study was in 1987) and remaining fundamental challenges. Compelling reasons to undertake the study included developing a sustainable chemical enterprise, reducing adverse effects of industrial activities, improving human health, addressing new separations challenges, and opportunities for new ways to look at separation science.

The committee focused on a fundamental research agenda considering chemical, analytical, and biological separations. Two research themes, eight research directions, and two crosscuts were identified.

Research theme (RT)-1 is to design systems that can do separations with high selectivity, capacity, and throughput. The research directions for RT-1 include separations in complex systems, thermodynamic and kinetic mechanisms, interface and interfacial forces, and physical changes from external forces.

RT-2 is to understand how separation systems change with time. The four research directions under RT-2 are changes from non-equilibrium states that affect chemical and physical properties, identity of fundamental chemical reactions that change materials and how they are influenced by operating conditions, fate of unwanted products, and alternative strategies to address temporal changes.

Two crosscutting issues were identified and recommendations made. The first crosscut topic was on Standard Systems, Samples and Methods. The recommendation was for NIST and the research community to develop reference standard tests and protocol for each separation material or system. The recommendation for the second crosscut topic, Adapting Theory and Data Science for Separations, was to use data science, modeling, and simulation with experimental measurements to develop a fundamental understanding of separation materials in complex environments and at multiple scales.

Implementing a research agenda will require reinvigoration of a vibrant separation science and engineering community. Challenges to implementation include a decreasing trend in

the number of separation science faculty in the U.S. and minimal conveyance of the excitement of new advances in separation technology in undergraduate courses.

Industry is cautious about adopting new separation technologies or using non-energy sources such as adsorption and membranes. To minimize risk and provide confidence to industry, separation systems must be understood in complex environments.

Discussion

Hsu asked for strategies to excite students about separation science. **Brennecke** explained there is an outreach plan to touch all the stakeholder communities (i.e., a presentation in the undergraduate separation science section at the American Institute of Chemical Engineers (AIChE) meeting this fall). Chemical engineering undergraduates need increased course coverage of adsorption, membranes, and chromatography, not just distillation.

Santore posed a question about the needs, scientific challenges, and impact of technologies where separations are integrated with other operations. **Brennecke** noted the report included such things but there is minimal emphasis on the topic.

Epps was curious if focusing predominantly on chemistry and chemical engineering limited the audience. He suggested including the materials science and environmental science communities. **Brennecke** said there is a section in the report on the intersection of separation sciences with a these disciplines.

Dosch suggested the separation science community meet with other communities to develop a holistic strategy. **Brennecke** explained such discussions have started to take place. For example, there was a special workshop at the APS User Meeting in May 2019.

Kastner called for a break at 10:49 a.m. and reconvened the meeting at 11:05 a.m.

Introduction to the Plastic Issue and the Role of Recycling & Upcycling, Jill Martin, DOW

Martin described the background and challenges for plastics in a circular economy and provided examples of technologies being used for plastics recycling.

The Ellen MacArthur Foundation published the "New Plastics Economy" in 2016. There are now 400 signatories to the directive committing to reduce the use of plastics, to incorporate more postconsumer recycling, and to look at bio-based materials and biodegradable materials. The packaging industry is discussing improvement of their overall environmental footprint, however, some of the challenges are related to infrastructure. McKinsey & Company, in a 2018 publication, "How plastics waste recycling could transform the chemical industry," projected a decline of virgin polyethylene and a balance between mechanical and chemical recycling. From an investment perspective this projection is important.

There are numerous challenges to getting plastics into the circular economy, having to do with the value chain, including waste management and geographic location of the plastics plants. Challenges from a scientific perspective include sortation and compatibilization. Investment challenges include funding for fundamental process-level R&D, regulatory support for technologies to be classified as "recycling", process inclusive definitions for recycling and recycled content, and goals and commitments related to the ability to design materials for recyclability. Private and public sector partnerships, as well as new business models, are also necessary. Current activities in the circular economy for plastics are based on strengths in catalysts, technologies, materials science, and characterization capabilities. Creating the circular economy is a long-term commitment that requires significant R&D investment.

Data science in the collection space could help create collection systems where the economics fit the local communities. Material recovery facilities (MRF) are based on entropy and separation into well-characterized streams. Efficiency in a MRF is the ability to detect differences in mono-material as well as multi-material systems.

Challenges in mechanical recycling include odor and color as well as food contact compliant materials; there is not enough food compliant material to satisfy the U.S. market. With chemical recycling the issues have to do with scale, both quantity and quality, of the materials. The end-use markets for current recycled materials are typically lower end markets.

Keeping plastics valuable includes issues of ease and access, using existing infrastructure, and considering end-use markets. DOW developed a recyclable package for Kellogg's using their existing infrastructure which kept the costs lower. Since there is not enough food contact compliant materials available in the U.S. it is necessary to determine which end-use market is appropriate for the materials available.

The Materials Recovery for the Future project focuses on enhanced sortation capability to increase the amount of material that has value for end-use markets. Mechanical recycling is not a trivial matter. The sortation systems see paper and plastic the same way. MRFs are adopting artificial intelligence technologies to teach the equipment to identify what a package is instead of relying on material differentiation.

Existing solvent-based technologies for chemical recycling rely on effective collection and sortation of materials. Collection and sortation improvements are required to achieve any of the recycling solutions at scale. Solvent-based systems, separating polyethylene terephthalate (PET) from polyethylene, can be enormously energy intensive. Feedstock recovery is still challenging at the distributed and consolidated level; both gasification and pyrolysis are particularly energy intensive. Value must be balanced between the feedstock obtained, energy intensity, lifecycle analysis, and carbon footprint.

In gasification, it is permissible to accept municipal solid waste. Because gasification facilities can accept more organic material than a pyrolysis station, the pretreatment cost is lower. However, gasification requires an extremely high monetary investment and energy intensity. While there are different routes back to ethylene, each route has its own efficiency in hydrocarbon production and downstream investments. A pyrolysis facility can be much smaller, roughly the size of a basement, compared to a gasification facility. Pyrolysis primarily produces naphtha and diesel. Naphtha requires additional treatment but there is a good market for diesel.

Discussion

Stack mentioned China's ban on U.S. plastics for recycling and asked if that is related to the current interest in plastics recycling. **Martin** explained China put the ban in place because the U.S. was not sorting the materials well and that caused high contamination levels. Other Southeast Asian countries are now saying the same as China. Such bans, while only one reason for the current interest, are an extremely strong mitigating factor for plastics recycling.

Rollett asked Martin to comment on engagement of the academic community concerning data science for sortation. **Martin** said the original equipment manufacturers, who have adopted some of the sortation technologies, are being consulted now. However, vast opportunities exist to engage the academic community.

Chemical Upcycling of Polymer Roundtable Update, Phil Britt, ORNL

The BES Roundtable was held in April 30-May 1, 2019. Twenty-three people attended and were broken into three panels (chemical mechanisms, integrated processes, and new polymeric materials) with one crosscut panel (experimental, computational, and data science approaches). The four priority research opportunities (PRO) are in reaction pathways, integrated processes, next generation polymers, and novel tools for macromolecular transformations.

PRO-1 centers on converting single polymer waste streams into desirable products. Research opportunities exist for robust catalysts and chemical processes, tandem reactions to selectively polymerize and repolymerize waste plastics, mechanistic understanding of deconstruction and depolymerization reactions, and catalysts and processes that will react with solid polymerics and viscous polymer melts.

PRO-2 focuses on upcycling mixed polymer waste. The research opportunities are in robust catalysts and chemical processes that take advantage of the components in a waste polymer mixture, processes and selective catalysts that react with only one polymer, integrated catalytic transformation and separation for polymer mixtures, molecular interactions between complex mixtures of polymers, and tandem reactions that take advantage of chemocatalytic, biocatalytic, and thermal transformations to create higher value products.

PRO-3 centers on new polymers for chemical circularity. Research opportunities include new depolymerization and repolymerization strategies, reversible polymer chemistries, renewable feedstock integration, and depolymerizing polymers in response to stimulus or embedded catalysts.

PRO-4 focuses on new tools to discover and control chemical mechanisms for macromolecular transformations. This PRO includes experimental tools, predictive computational methods, and integration of experimental and computational data.

A brochure with a high-level summary of the workshop has been drafted and the roundtable report is in preparation.

Discussion

Dosch voiced concern that 30+ years of intensive polymer research has not answered the upcycling questions. **Britt** explained that polymers are non-equilibrium structures. The goal is predictive understanding and insight, and a huge number of science questions are still unanswered. **Dosch** asked about the use of existing knowledge and expressed worry about the risk of reinventing previous technologies. **Britt** said it is still impossible to make a polymer with a specific property, a specific glass transition temperature, and a specific strength. He reasoned if this knowledge was available over the past 30 years, it should be possible to predictably design new polymers.

Epps inquired if there is a mismatch between upcycling and scale. For example, volume versus the capacity of commodity materials that are being produced. **Britt** held that one challenge to making the possibilities available is determining the fundamental science questions. Illustrating possibilities, he said even with economies of scale, it is expensive to truck plastics over long distances to upcycle. One possible alternative is to upcycle in a community or region, allowing the region to define the percentages of materials they possess. Having the fundamental knowledge allows the region to mix the materials and create products. At the moment there is a problem of scale. There are huge amounts of polyolefins but very little of anything else.

Hsu was curious if other countries are engaged in more advanced upcycling. **Britt** said Europe is far ahead of the U.S. in some areas but polyethylenes are still a challenge. **Dosch**

confirmed there is substantial activity in Europe and asked if microplastics in the environment were discussed in the roundtable. **Britt** explained that microplastics were out of scope.

National Academies "Sexual Harassment of Women" Study Presentation, Irene Ngun, National Academies

Sexual harassment is a form of discrimination consisting of three types of behavior: sexual coercion, unwanted sexual attention, and gender harassment. There were five key findings from the National Academies' consensus study: extensive sexual harassment exists in science, engineering, and medicine; gender harassment is most common; sexual harassment undermines research integrity, reduces the talent pool, and harms targets and bystanders; legal compliance is necessary but not sufficient; and changing the organizational climate and culture can prevent and effectively address sexual harassment.

Severe, pervasive gender harassment can do the same professional and psychological damage as an isolated instance of sexual coercion. Sexual harassment has adverse effects on bystanders, co-workers, workgroups, and the entire organization. Research shows that those who simply witness sexual harassment will report negative outcomes that parallel those of direct victims; these effects emerge for both male and female employees.

In research environments, sexual harassment violates the standards and values of research integrity. The committee concluded that the cumulative effect of sexual harassment is significant damage to research integrity and a costly loss of talent.

The least common response to sexual harassment is formal reporting. Targets of sexual harassment are unlikely to report the harassment and often face retaliation. The committee recommended moving away from a culture of compliance and toward a culture of respect.

Organizational climate was found to be the greatest predictor of sexual harassment. Four recommendations from the report included creating diverse, inclusive, and respectful environments; diffusing hierarchical and dependent relationships between trainees and faculty; providing support for targets; and improving transparency and accountability. The committee also made four recommendations to federal agencies focusing on evaluating the effectiveness of policies; providing attention and resources; instituting rewards and incentives; and requiring violations be reported.

Discussion

Olvera de la Cruz mentioned scenarios where scientists hire their partners or spouses for post-doc positions and asked if that should be considered unethical. **Ngun** said the topic came up in conversation. There is a section in the report about consensual relationships, but more research is needed in this area.

Gao asked why sexual harassment in medicine is higher than other areas. **Ngun** explained the committee was not able to determine why it was high in medicine, but concluded it may be because medicine has a unique environment. Medicine is very hierarchical, has huge power differentials, and certain fields are extremely male dominated. All of those factors create the potential for sexual harassment to thrive.

Rollett highlighted the student portability idea, allowing students more portability in who they work for. **Ngun** added that one of the outcomes of this study was the creation of an Action Collaborative that includes 60 member institutions. The hope is to consider the portability question and find best practices that help diffuse power differentials or help students be independent of a single principal investigator (PI) or faculty member.

Kastner adjourned the meeting for lunch at 12:20 p.m. and reconvened BESAC at 1:33p.m.

Exascale Computing Project (ECP) Update, Lori Diachin, Lawrence Livermore National Laboratory

The ECP mission is to deliver exascale-ready applications and a vertically-integrated software stack to address the competitiveness of the high performance computing (HPC) industry. ECP, a part of the Exascale Computing Initiative (ECI), is a 7-year, $1.7B R&D effort involving 6 core labs and 81 R&D teams.

Exascale means running 10^{18} flops per second. ECP is measuring application capability improvement relative to the applications performance in 2016. ECP expects a 50x increase in the work rate. HPCs massively parallel, distributed memory, MPI-based systems have been stable, allowing PIs to conduct productive science for decades. ECP is tackling a shift in the architectures, which are much more specialized and designed to get performance gains. The new architectures represent a significant departure from many applications and software codes. Exascale computing will require novel or augmented programming models, more parallelism, new concurrency, and new algorithms. Data movement is increasing in cost; computation is considered free but communication is very expensive.

There are 24 applications for Applications Development across six areas (national security, energy security, economic security, science, earth systems science, health care); three are funded by National Nuclear Security Administration and 21 by SC or the National Institutes of Health. Application teams were required to define an exascale challenge problem, one that could not be performed on the systems available in 2016 and could not even be performed on the systems available today (200 petascale systems). Teams developed the criteria for completing these challenge problems. All challenge problems were reviewed by external subject matter experts and program offices helped define the most impactful applications.

The six co-design centers are important bridges between the 24 applications and the hardware itself. Co-design centers address computational motifs common to multiple applications. Six common challenges were identified across the 24 application projects. These include porting to accelerator-based architectures, exposing additional parallelism, coupling codes to create new multiphysics capability, adopting new mathematical approaches, achieving algorithmic or model improvements, and leveraging optimized libraries. Teams have discovered that to meet project goals, on the more challenging architectures, broader expertise is needed.

Eight applications of interest to BES were described QMCPACK, EXAALT, GAMESS, ExaFEL, NWChemEx, PELE, Subsurface, and ExaAM. Two applications, ExaFEL and EXAALT, were explored more deeply.

Discussion

Ourmazd asked how the community was engaged to identify codes to develop and how ECP is ensuring the goals remain current. **Diachin** explained there was a call for exascale application teams in 2016. The proposals were reviewed by a committee of experts and viable candidates were brought to the program offices for discussion. Two primary mechanisms to ensure continued impact are briefings to the program staff and annual subject matter expert reviews for each project team.

Advanced Scientific Computing Advisory Committee Exascale Computing Project Subcommittee Update, Roscoe Giles, Boston University

Giles focused on the transition from ECP to the next round of ASCR activities. The subcommittee charge was to examine ECP lessons learned for managing large collaborations, ASCR's fundamental research investments, and new R&D priorities. The subcommittee was charged to provide recommendations for capturing the lessons learned from ECP, supporting the software and hardware developments, and informing ASCR's future investment strategy.

Key issues considered by the subcommittee include ASCR support for medium and long-term research, sustained benefits of ECP, workforce impact, and management lessons for large projects. The subcommittee has been interviewing stakeholders about forthcoming critical issues related to the ECP, aspects of ECP to be sustained, and the impact of ECP to their community. Questions concerning the near future for ECP focused on the best model to bring the benefits of advanced computing to communities, new science enabled by exascale, and interactions with national and international computing efforts. Longer-term future questions include hopes for the impact of post-exascale, engaging ASCR on post-exascale computing paradigms, and transcending algorithmic/computing barriers. Organization and workforce questions include resources to take advantage of emerging and future computing, developing and growing crosscutting themes and interactions between the SC offices, and developing computational skills by young scientists. The subcommittee will conduct more small-group interviews and hold two workshops, likely co-located at ASCR town halls.

Discussion

Rollett asked about the change in performance measurement, from Linpack-based to algorithms. **Diachin** explained it is difficult to get 50x performance on real applications. The class of applications that were petascale ready in 2016 are the ones required to get to 50x. Algorithmic improvements cannot reduce accuracy of the results and have to be shown to be equivalent to their baseline calculation.

Stack said as a user what he would like from ECP is access to the codes. **Giles** mentioned on the software technology side there is a significant effort to package, organize, and holistically validate the libraries. Giles was less sure if sets of applications, developed using the common software framework, are equally visible to other developers. **Diachin** noted that some applications are widely available. The intent is to make the software available to the community, but certain codes may have export control issues to resolve.

Dosch said exascale operations in the U.S. need to integrate industry. **Diachin** noted that ECP has an Industry Council that meets every six months, but agreed that European efforts have a stronger connection with industry.

Spallation Neutron Source/ Proton Power Upgrade (PPU)/ Second Target Station Update, Paul Langan, ORNL

Today the SNS is operating at its maximum design level of 1.4MW and the user program is producing tremendously impactful science. The First Target Station (FTS) is optimized for thermal neutrons while the STS is optimized for cold neutrons. PPU increases the brightness of beams and doubles the power of the existing accelerator structure. The STS project will include an initial suite of beam lines optimized for cold neutrons. Peak brightness allows much improved time resolution and real-time, time-resolved experiments on connected processes, as well as the use of radically smaller samples.

PPU has achieved CD-0, CD-1, and CD-3a. Partner labs (Fermilab, LBNL, and Thomas Jefferson) have been selected. The project successfully completed a CD-3b review in June and is preparing for CD-2 review at end of 2019; early project completion is expected in 2024.

STS has received CD-0. The implementation plan is finalized and conceptual design packages are completed. STS is developing a bottom-up cost-estimate; the first draft will be ready by August 2019. STS is preparing for a CD-1 readiness review; early project completion is expected in 2028. Construction has minimal impact on First Target Station (FTS) operations.

Japan recently demonstrated neutron production at 1MW and the European Spallation Source will deliver a 2MW capable source in 2025 with an upgrade to 5MW by end of the 2020s. The landscape of neutron sources is getting more competitive; SNS upgrades will provide world-leading neutron capabilities to U.S. researchers.

Discussion

Gao stated users will need a detailed explanation of the benefits of PPU. **Langan** explained the BESAC presentation provides a bigger picture view. Users have noticed, and are excited about, the improved performance. The benefits are seen in different ways, through more experiments or accelerated access, as well as the use of smaller samples or more complex measurements that take the same amount of time. **Gao** mentioned the possible impact on users during the beamline construction. **Langan** said SNS has worked extensively with DOE to ensure the impact to the user program is minimal. Once the STS is built, both FTS and STS can operate at the same time or individually while the other is being worked on.

Louca asked if measures are in place to reduce and avoid redundancy in the three neutron scattering sources. **Langan** said there is a long-term strategy. STS will do different types of experiments than FTS, and each source is best matched for a different type of experimental technique using a different neutron energy range.

Kastner called a break 3:18 p.m. and reconvened the meeting at 3:48 p.m.

Neutron Subcommittee Update and Discussion, Marc Kastner

The High Flux Isotope Reactor (HFIR), built in 1965, uses highly enriched uranium (HEU). A National Academies 2016 report on HEU use in research reactors encouraged conversion to low enriched uranium (LEU). The American Physical Society Panel on Public Affairs 2018 report stated HEU use is a problem and needs to be addressed.

The neutron subcommittee charge is to provide the science case for a high flux reactor, its merit and significance, global facilities that could address the science case, important applications, performance that is not available at the spallation sources, feasible upgrade paths to keep HFIR as a forefront facility, and the possibilities of using LEU for steady state neutron sources. The scope of the study is to comprehensively cover a wide range of topics across a large number of communities beyond BESAC and BES.

A kick-off meeting will be held at LBNL in August 2019, a workshop in Washington, DC in November 2019, and site visits to ORNL, other DOE labs, National Institute of Standards and Technology (NIST), and possibly to international facilities (Institut Laue-Langevin (ILL), Forschungsreaktor München II (FRM-II), and Belgian Reactor 2 (BR2)).

Discussion

Dosch mentioned the compact neutron sources work in Japan and asked if that is out of scope. **Kastner** said the committee is supposed to look at alternatives and requested Dosch send an email with contact recommendations.

Subcommittee Rules of Engagement Overview, BESAC Members

Setting the backdrop, Kastner said there is sometimes a tendency for subcommittee members to become overly enthusiastic about pursuing the charge. Kastner introduced the Subcommittee Rules of Engagement document and asked BESAC to discuss the contents. BESAC was reminded that any information to one member of a subcommittee should go to all members of the subcommittee. The chairperson should ask all questions intended for DOE employees.

Hsu asked if the rules of engagement are guidelines for all subcommittee members or just BESAC members serving on subcommittees. **Kastner** said it is for all subcommittee members; the same thing should hold true for BESAC members as well. Issues that arise in BESAC should come to Kastner and he will speak to Kung. **Rollett** suggested inserting "committee and any sub-committees" in the text.

Tirrell clarified that when Kastner mentioned "the Chair" he was referring to the Chair of the subcommittee.

Rollett moved to accept the document allowing minor edits. **Tirrell** seconded the motion. BESAC unanimously accepted the document.

Public Comment Session

Leland Cogliani, Lewis–Burke, invited BESAC members and attendees to National Lab Day on the Hill (July 24). One of the exhibits will be on LCLS-II. There will be a cavity exhibit for members of Congress and their staff. It will show the construction of a world-class leading user facility. The theme of the exhibit is the national labs as a network, highlighting how various labs contributed S&T to make LCLS-II possible. The target audience is primarily the 100+ new members of Congress, most of whom do not have national labs in their states. There will be a showcase with examples of how each national lab is contributing, from basic science to physical and cyber protection of the grid. Paul Dabbar will host a panel discussion with all the former Undersecretaries of Science.

Kastner adjourned BESAC at 4:08 p.m.

Friday, July 12, 2019

Kastner, BESAC Chair, called the meeting to order at 9:00 a.m.

Basic Research Needs (BRN) for Manufacturing Workshop Update, Linda Horton, Director, Materials Sciences & Engineering Division

The first BES BRN on manufacturing is planned for December 2019 in Rockville, MD. Manufacturing is an emphasis area for DOE. The charge is to identify fundamental research to overcome scientific and technical barriers for innovations that would transform manufacturing in the future. Manufacturing roadblocks include poor device performance, defects introduced on scaling, non-linear scaling relationships, processing effects, and poor quality products. Science

solutions include control of atomic-level interactions, precision synthesis, understanding non-equilibrium chemistry, synthesis simulation methods, and robust catalysts. The BRN will consider enabling science that could support some of the Energy Efficiency and Renewable Energy's (EERE) Advanced Manufacturing Office focus areas. Panel topics include precision synthesis, processing and scale-up science, system integration science, and sustainable and digital manufacturing, as well as crosscutting subjects.

Discussion

Friend asked if instrumentation would be discussed. **Horton** stated the topic had not come up. She agreed it was a valid point; DOE develops many instruments that might allow innovation in some of the areas.

Hsu asked Horton why roll-to-roll processing was not being discussed, noting it is an alternative to traditional heating, and rapid in-situ characterization is promoted by roll-to-roll manufacturing because of the high throughput. **Horton** explained a lot of modeling that is associated with roll-to-roll manufacturing is well known, it is well established, and is specific to particular manufacturing. However, improved efficiencies of roll-to-roll may be uncovered in the BRN.

Olvera de la Cruz mentioned the non-equilibrium grand challenge and self-healing chemical reactions. **Horton** said biomimetics includes some of those elements.

Roundtable on Liquid Solar Fuels, Bruce Garrett, Director, Chemical Sciences, Geosciences, & Biosciences Division

A BRN workshop on liquid solar fuels will be held in August 2019 and focus on artificial photosynthesis. Challenges span length and time scales, require appreciating and controlling individual steps in the process, as well as understanding processes that degrade components and mechanisms that increase durability. The Hubs are efforts that cross fundamental research with applied research and proof-of-concept prototypes.

The changing landscape since the 2005 Solar Energy BRN is driving the need for the 2019 BRN; upcoming opportunities, such as the recompetition for the Fuels from Sunlight Energy Innovation Hub, is driving the timing. A 25-person group will identify PROs for the next 5-10 years. Chairs and participants have been confirmed, the date and location have been selected, the factual document is moving forward, and the panel topics have been identified. The panels will focus on the science of selectivity and efficiency, science of integration, science of durability, and crosscutting issues.

Discussion

Friend asked to what extent building on the JCAP infrastructure would be considered. **Garrett** said the roundtable will focus on the science and the PROs, not on JCAP.

Kastner asked BESAC to consider extending the period between COV meetings.

Scientific User Facilities Committee of Visitors (COV) Report, Tony Rollett, Carnegie Mellon University

In April 2019, 17 individuals convened to review the management processes of the light sources, neutron sources, NSRCs, and construction projects, and to consider proposal actions,

monitoring activities, portfolio breadth and depth, and preparedness to meet future challenges in the Scientific User Facilities Division (SUFD).

The COV stated staffing in SUFD is lean thus planning and leadership succession is important. SUFD is encouraged to work with labs and facilities to improve workforce diversity and address cultural issues at the facilities. The Accelerator and Detector Research program is highly effective; all white papers should be entered into the Portfolio Analysis and Management System (PAMS). The COV encouraged considering the use and development of software analytical tools, high throughput hardware, and better support at existing instruments. In addition, SUFD should find new ways to inform potential industrial users of the ways user facilities can solve problems that standard tools cannot address.

The COV found the 2016 recommendations had been acted upon and commended SUFD for its effective leadership. SUFD has an effective set of systems and practices in place, and the Triennial facility review process was highly effective in all sectors. Several facilities have overcome significant technical challenges. The diversity of the user body appears to be similar to that in the physical sciences and engineering, however the user facility staff and management are noticeably less diverse. Recapitalization is an ever-present need and expanded beamline internship opportunities for students and postdocs could increase the pipeline of new facility staff. The COV commends the work of the light sources staff in planning for the data explosion.

Louca added that interagency collaboration was recommended in the report and discussed by the COV. Louca, responding to Kastner's question about the frequency of COVs, shared that the amount of material a COV reviews is immense. Extending the timeline to five years between COVs may double the volume of material.

Gao expanded on the beamline staff development recommendation. The beamline staff have a difficult job; they support users but also have to innovate. As light source instruments become increasingly complex the role of beamline scientists in innovation becomes more important. It is vital to have a culture that encourages and supports those who want to innovate.

Discussion

Kastner thanked the COV on behalf of BESAC. He asked if issues raised in the 2016 report were much the same now or were there new issues. **Louca** said the management change is something to be followed. Looking ahead, five years is a long time to see if SUFD implemented the recommendations. **Rollett** added that the data issue is much larger now than three years ago.

Hsu asked if there is a mandate to differentiate the five NSRCs, or if they must be geographically distributed for user's access. **Kung** said the NSRCs serve some geographical purpose; it is absolutely necessary to have complementarities without undue duplication. **Friend** added that the COV recommendation was not that all the centers had to be completely different but that there might be existing points of emphasis where the investment could occur. **Rollett** explained one could think of the recommendation as pragmatic. Funds from recapitalization are limited; it makes sense to encourage the NSRCs to think about their future direction.

Friend extended thanks to Rollett for his great leadership on the COV.

Musumeci stated, in light of long-term sustainability and growing international competition for the BES facilities, one should recognize it is not only the research contribution but also the formation of the workforce, beamline and accelerator scientists, which add greatly to the facilities. He asked if the COV found a balance between national labs and academia for early career. **Rollett** said the COV did look at that and the balance seemed reasonable.

Bonnell moved to accept the report, **Robertson** seconded the motion. BESAC unanimously accepted the COV report.

News from Office of Science, Chris Fall, Director, Office of Science

Fall thanked BESAC for their work for DOE and the scientific community. Fall understands the value of BESAC's advice in shaping SC's programs, the value of the trust that open and transparent dialog engenders, and BESAC's concern about potential changes to the way SC gets advice from the scientific community.

Fall assured BESAC that his perspective in life is as a scientist. Fall shares the values of science, the rigor, the evidence, and the scientific method. He cares about the traditions of science and the history of science.

Fall stated he is not trying to upset the momentum SC has generated going forward. The priorities include exascale computing, artificial intelligence, QIS, biosecurity, microelectronics, and accelerator S&T, and new ideas such as polymer upcycling and separation sciences. Fall is interested in convergence opportunities (next generation biology, physics, math, and computational science).

Fall wants to understand SC's business model better, explore the EFRCs and Hubs and their value proposition. While SC may be optimally structured for QIS and accelerator S&T, he wants to examine if there is a better configuration.

SC is famous, across the federal government, for project management, and Fall has high expectations for continued exceptional project management. Fall is paying attention to the reasons for the problems with HFIR and SNS.

DOE has labs that date from the Cold War and needs to clean up some sites. Fall is intent on ensuring the labs are in good shape for the next generation of scientists and science. He plans to attend to the infrastructure needs and balancing research and facilities, noting there is no reason to run facilities at less than optimal levels.

Fall wants SC to communicate what it does better. It is important to tell Congress and the American people what SC is doing with the money they allocate. SC must continue to generate support from Congress, but also thank the American people for their trust and make them feel part of the activities and accomplishments. Most importantly, the message must motivate the future generation of scientists as well as the citizens who know science is important.

Fall is interested in new business models for accomplishing new science ideas. It is okay to experiment with other business models for SC. He thanked Paul Dabbar for putting a roadmap in place and setting priorities that allow him to concentrate on these issues. Fall closed by saying he knows he can trust remarkable public servants, like Kung and her colleagues across the leadership of SC, to nurture the details of the science mission.

Discussion

Katsner expressed gratitude, on behalf of BESAC, for Fall taking on the Director responsibilities and for his careful consideration of so many of the issues.

Rollett suggested community support will be needed for the change of exascale performance metrics. He said Congress needs to hear why things are done a certain way and why the HPC machines are effective for solving scientific and engineering problems.

Friend thanked Fall for taking on the role of Director of SC and for his thoughtful remarks. She asked Fall to elaborate on the process for evaluating the SC business model and his criteria. **Fall** said the process and criteria are not yet formed. Concerning measuring, it is a

matter of resources and SC allocation preferences. Other agencies are studying where money is spent and the effect on science using sophisticated data mining and data analytics. He is willing to take risks and chances. The DOE leadership is not risk averse in terms of trying new things. SC is looking for a bottom-up approach on the quantum centers and potentially microelectronics. A bottom-up approach works best for innovation and exploration of new collaboration and cooperation models. **Friend** suggested consulting the BESAC and COVs reports on the value proposition. **Fall** explained that Congress has communicated the urgency to start spending money. SC has limited time to study the problems and begin moving forward. Flexibility will allow SC to try new things; if they do not work, it is possible to move in new directions.

Bonnell asked Fall for his thoughts on international collaborations, national security, and how the community can help. **Fall** explained DOE wants meaningful cooperation on science for the public good and S&T for economic impact and for national security. DOE has taken steps at national labs but the problem is much more difficult with external partners. DOE is in the middle of the conversations. While there may never be agreement on a shared set of values, it is imperative to get to a mutually agreeable working point. DOE is trying to understand where intellectual property is going and why it is leaving. The situation is clearly not right; the solution is less clear.

National Academies "Gaseous Carbon Waste Streams Utilization" Report Presentation, Nilay Hazari, Yale University

The National Academies' study was motivated by an interest in carbon waste gas utilization, a part of a capture, utilization, and sequestration system. The report addressed seven tasks: global status and progress, emerging technologies, commercial viability, assessment criteria, major technical challenges, current research efforts, and a comprehensive research agenda. The most relevant of these tasks to BES are the current research efforts and the comprehensive research agenda.

The committee gathered data from public sources, committee member knowledge, meetings and webinars, literature, and community input. They considered research needs for CO_2 and methane waste gas utilization. The report only looks at utilization pathways that result in chemical transformation of CO_2 into a valuable product

The report is organized around key features of the carbon utilization system. These key features include enabling technology and resources, life-cycle assessment and techno-economic analysis, and three technical pathways (mineralization, chemical, and biological utilization).

The committee identified economic, commercial, and environmental factors and criteria that may be used to assess commercial viability of carbon utilization technologies (economic, commercial, and environmental factors). The committee identified six chemical utilization research areas (chemical catalysis, stoichiometric additives, integrating catalyst and reactor design, non-traditional targets, coupled oxidation and reduction, and reactor technologies). The committee's recommendation is to implement the research agenda and coordinate with existing efforts in carbon utilization.

Discussion

None.

Public Comment Session

None.

Kastner adjourned BESAC at 11:39 a.m.

Respectfully submitted,
Tiffani R. Conner, PhD, PMP, AHIP
Science Writer
ORISE/ ORAU
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