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

PUBLIC MEETING MINUTES

March 7-8, 2019

Bethesda North Marriott Hotel & Conference Center
5701 Marinelli Road, Rockville, MD 20852

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, March 7-8, 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. Information about BESAC and this meeting can be found at http://science.energy.gov/bes/besac/

BESAC Members Present:

Marc Kastner, BESAC Chair, Science Philanthropy Alliance
Kathy Ayers, Proton OnSite
Dawn Bonnell, University of Pennsylvania
Joan Broderick, Montana State University
Sue Clark, Washington State University, Pacific Northwest National Laboratory (PNNL)
Beatriz Roldan Cuenya, Fritz-Haber Institute of the Max Planck Society
Thomas Epps, University of Delaware
Cynthia Friend, Harvard University
Yan Gao, General Electric Company
Julia Hsu, University of Texas, Dallas
Stephen Leone, University of California, Berkeley, Lawrence Berkeley National Laboratory (LBNL)
Despina Louca, University of Virginia
Allan McDonald, University of Texas, Austin
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
Maria Santore, University of Massachusetts, Amherst
Andrew Stack, Oak Ridge National Laboratory (ORNL)
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, March 7, 2019

BESAC Chair, Marc Kastner, called the meeting to order at 9:30 a.m. Eastern Time (ET) to an audience of approximately 160 people.

News from Office of Science, Steve Binkley, Deputy Director, DOE Office of Science (SC)

Binkley discussed international interactions and two memoranda concerning sensitive technologies and foreign talent. Representing 16 foreign countries and international organizations are 62 formal (government-to-government) International Agreements (IA), 13 of which involve the BES program. In addition to formal IAs, there are many international collaborations with the national labs, including Memoranda of Agreement (MOA), Cooperative Research and Development Agreements (CRADA), and Strategic Partnership Programs (SPP).

The U.S. is involved in multiple international collaborations at CERN, Large Hadron Collider (LHC) and the High Luminosity (HL)-LHC, in high energy physics at the Long-Baseline Neutrino Facility/Deep Underground Neutrino Experiment (LBNF/DUNE), and ITER. Development of IAs are governed by seven principles: quid pro quo–mutual benefit; Mutual respect; Maintain openness, transparency, respect for individuals; Research for peaceful purposes; Community engagement and buy in; Use of rigorous project management, where appropriate; and Governed by formal, government-to-government agreements, when appropriate.

The Deputy Secretary of Energy issued a memorandum in December 2018 concerning security issues related to sensitive technologies such as Artificial Intelligence (AI) and Quantum Information Sciences (QIS). A second memorandum, issued in January 2019, focused on foreign talent programs. The challenge within DOE is to identify security concerns and put measures in place to protect national interests. SC is working with the national labs' designated Chief Research Officers (CRO) to identify specific touch points within key technology areas of concern, and to develop the types of controls needed. Binkley expects the initial touch points will be identified and measures developed to protect U.S. interests by summer 2019.

Foreign talent programs, largely pioneered by China, task their researchers with bringing information and knowledge about key technologies back to their home country. From DOE's point of view, someone receiving funding from their government while simultaneously receiving money from the U.S. is a direct conflict. The objective of this memorandum is to identify such cases and to ensure this does not happen. There is a two-step process, involving the national labs and universities, to identify such cases and ensure the conflict is avoided. SC is beginning to work directly with universities and professional associations, such as the Association of American Universities and the Association of Public and Land-grant Universities, to gather input and feedback, with substantive information anticipated by summer 2019.

Discussion

Bonnell asked if DOE is being asked to determine what information is an economic threat. **Binkley** said DOE is working with the Department of Commerce to identify national security and economic security threats.

Roldan Cuenya expressed concern on the effect of foreign talent policies on international students, those who bring family to the U.S. and those who work with U.S. user facilities. **Binkley** explained the intent is to target the defined talent programs, non-defined talent programs are not an issue. SC is not making any policy changes in terms of access to user facilities.

Hsu asked if the approaches for these two memoranda are for SC or are DOE wide. **Binkley** indicated they are DOE wide.

Friend asked if the conversations with universities include discussions of sensitive technologies and requested a definition of the talent programs. **Binkley** stated that discussions with universities include both sensitive technologies and foreign talent programs. For example, the Thousand Talent program in China is a defined foreign talent program but the Humboldt Foundation in Germany is not. The differentiating feature is that these programs of concern are essentially state-run and state-managed.

Takeuchi asked how the foreign talent policies might affect students receiving funding from a foreign company. **Binkley** indicated that is not in the purview. He noted that in the last year there have been several instances where a company, who is headquartered in Canada but is Chinese, wants to do work with a lab. DOE's screening process does look for that particular case.

Louca asked if there are guidelines for universities who work with students from sensitive countries. **Binkley** said the purpose of the outreach to universities and other constituencies is to work through the details of the process. Controls will be an outcome of these discussions.

Clark asked about guidance on the threshold between basic research, emerging technologies, and deployed technologies. **Binkley** indicated there would be guidance, and explained some technologies even at Technology Readiness Level (TRL) 0 and TRL 1 can have implications.

Ourmazd inquired about visa designations and limitations on green card holders. **Binkley** explained no particular visa designations were currently identified and green card holders are lawful permanent residents of the U.S.

Kastner asked for specifics on the types of support affected and the ability of students, who are receiving foreign monies, to work on a DOE grant if no funds are coming from DOE. **Binkley** explained the details are being discussed. The ability to work on a DOE grant depends on the source of the student's funding.

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

Kung stated that over the past decade BES has been guided by BESAC and followed one central tenant, to understand, predict, and control matter and energy flow at the levels of electrons, atoms, and molecules. The 2020 budget was not released to the public as of the BESAC meeting; Kung focused on the 2018 and 2019 budgets.

The Fiscal Year (FY)18 BES budget exceeded $2B, receiving an 11.7% ($218M) increase over FY17. BES was directed to devote $130M to construction and monitor and evaluate (M&E) projects. Within the funding BES was given flexibility to operate facilities at greater than 95% optimal level allowing over $60M for research increases. The extra funding enabled BES to pull forward high priority research directions, to maintain the Energy Frontier Research Centers (EFRC) funding recompetition, launch a renewal of the Batteries and Energy Storage Hub, and renew the Joint Center for Energy Storage Research (JCESR) for another five years. BES has also been able to support 40 Early Career Awards (ECA), and provide 82 supplemental awards to DOE national lab programs. In FY18 BES reached a record number of users supported at the BES facilities.

In FY19, BES received an additional 3.6% increase from the 2018 level. Congressional direction is towards construction and M&E projects. Four FY19 Funding Opportunity

Announcements (FOA) were released to expand research in the areas of next-generation quantum systems and quantum computation, and the Established Program to Stimulate Competitive Research (EPSCoR) Implementation Grants.

In December 2018 Congress passed the National Quantum Initiative (NQI) Act. The NQI directs the President to enact a 10-year program and specifies quantum information theory, quantum physics, quantum computational science, quantum sensing, and materials science and engineering for DOE. The NQI is very specific about DOE's role, and authorizes up to five QIS centers.

BES user facilities reached a record number of users, 16k+ users and 300k companies, in FY18. The High Flux Isotope Reactor (HFIR) has been shut down since November 2018. ORNL is developing a restart plan for the reactor to be online by the end of FY19. Based on the 2016 BESAC facility upgrade prioritization study there is strong support for all of the upgrade projects.

Two new charges have been issued to BESAC focused on funding mechanisms and international competition, and assessing the scientific justification for a U.S. domestic high-performance reactor-based research facility.

Kung thanked BESAC for their past guidance, stating the work BESAC has done matters, has shaped the BES program, and has set the trajectory across a broad disciplinary field.

Discussion

Olvera de la Cruz inquired about continued support for research areas outside of the QIS Initiative. **Kung** explained that BES takes a very close look at the balance between core research and newer initiatives.

Roldan Cuenya asked about the 3-4 year funding barrier to grants and for information on the Stanford Synchrotron Radiation Light Source (SSRL). **Kung** shared that the average time duration of grants exceeds three years, but they must be reviewed on a 3-year cycle. BES takes a long-term view towards stewarding the disciplines. In terms of SSRL, BES is working with each lab to discuss the future of their facilities and ensuring that capabilities will be maintained through incremental upgrades.

Kastner called for a break at 10:48 a.m. and reconvened the meeting at 11:05 a.m.

BES40 One Page Summaries Panel, Marc Kastner, Leland Cogliani (Lewis Burke), Philip Lippel (MIT Washington Office), Al Hammond (Science Writer)

Kastner explained the generation of one-page summaries is the next step of the BES40 report. The BES40 report was generated from community ideas woven into stories about BES research that lead to new science and new technologies important for industry and other DOE missions. Working with the stories, Hammond interviewed expert scientists and translated the science for a wider audience. While the report was well received, the feedback indicated a need for shorter stories to support the case for continued funding for BES.

Hammond stated that in the BES40 report the science was explained at least in passing. Since the one-page summaries have restricted space, the science was reduced to a bullet called breakthrough. Breakthrough is followed by several bullets about impacts, and a final bullet restating the breakthrough. There is also a two-page summary of the entire report; that document is only about 23 "innovations that matter" which are grouped by industry category.

Cogliani, speaking as the co-chair of the Energy Sciences Coalition (ESC), expressed there are more than 80 new members in Congress who have never heard of DOE SC and it is the perfect time to use the one-page summaries to introduce SC. He characterized the one-page summaries as a menu of options that appeal to a Congressperson's background, committees, and their legislative interests. The summaries are currently integrated into the FY20 funding statement from the ESC.

Lippel explained that budgets involve both authorization and appropriations stages. When he and Cogliani meet with key budget committee staffers and Congresspersons, the one-page summaries help tell the stories of BES and SC. Lippel and Cogliani's colleagues requested shorter messages with relevance to particular meetings. Lippel suggested that university or lab personnel utilize the one-page summaries that resonate with the meeting attendees' interests. Lippel said that although the stories are historical, the impact and take away points are designed to be forward looking.

Discussion

Ourmazd commented that the American Physical Society (APS) publication, "Industrial Physics, The Impact of Industrial Physics on the U.S. Economy" illustrated that 12% of the U.S. gross domestic product (GDP) comes directly from physics-based industries.

Friend asked how the stories will be kept fresh. **Hammond** stated these stories were designed to be a 40-year backward perspective but the same process could be used to create forward looking claims. Where the context is clear, such as international competitiveness or critical sectors, it would be useful to have a one-page summary that showcased program funding in an area and why it is important. Further, there are many reports already completed that need to be reduced to one-page summaries. **Kastner** expressed these could be created for each Basic Research Needs (BRN) workshop. **Lippel** explained not all BRN reports have to be at the same level of production and use. The one-page summaries are starting points for discussions. The BRN summaries may not use the same format but would definitely use the same level of description of the work.

Roldan Cuenya suggested some of the national labs' annual reports be selected and shortened. **Cogliani** indicated the "75 Breakthroughs by America's National Laboratories" list has been used at hearings on energy innovation. **Lippel** said such highlights are great resources but they need one more level of distillation. **McDonald** added it is more convincing if the highlights are backward looking than forward looking. Because the one-page summaries are so good he suggested establishing a process for refreshing them on a regular basis.

Materials Decadal Survey (National Research Council), Matt Tirrell

Tirrell explained the current decadal survey was started in early 2017 and sponsored by BES, Materials Sciences and Engineering Division. The subcommittee held five meetings nationwide, received input from 40 speakers and panelists, and surveyed industry. Materials Sciences and Materials Engineering is a vast field stretching from the frontiers of fundamental science to industrial-scale manufacturing. The subcommittee examined the four previous decadal survey reports and found some prominent developments were not mentioned. These developments include graphene and topological insulators, vitrimers and polymers with dynamic covalent bonds, and Gorilla Glass.

The key findings and recommendations in the report focused on basic research as a fundamental science, integrated computational materials science and materials engineering

methodology, quantum materials science and engineering, quality and sustainability of Earth's environment, polymer materials, convergent research, and three key findings about infrastructure. The recommendations concentrated on funding, encouraging use, supporting new initiatives and remaining internationally competitive, sustainable manufacturing, environmental degradability, and fostering communication.

The report notes that the U.S. is competitive but not dominant in materials science and engineering. The decadal survey suggests the U.S. response to competitiveness should include sustained support, nurtured international collaborations, an environment to bring new technologies to market, and local production and technology transfer. Two recommendations include assessing the threat of worldwide competition and pursuing a permanent program focused on materials science and smart manufacturing.

Discussion

Gao suggested a stronger emphasis be placed on cross-agency collaboration. He explained most collaboration happens at the individual level, but a formal collaboration between the Department of Defense and BES user facilities can benefit defense materials.

Epps asked about competitive versus collaborative infrastructure. **Tirrell** said both exist and reinforce one another; he described the user facilities, especially DOE, as a good model. A strong endorsement of current practices are the discussions and considerations of ensuring the facilities maintain their capabilities after the upgrades.

Olvera de la Cruz said Europe includes soft matter physics in condensed matter physics, but such a culture does not exist in the U.S. She asked if Tirrell thought the cultural separation hurts the U.S. **Tirrell** agreed that soft matter physics, being done outside materials science departments, could be done in physics departments. He was unsure of the effect of the separation. Further, he stated that two of the three previous decadal surveys were styled as condensed matter materials physics, rather than the broader purview of this report.

Kastner adjourned the meeting for lunch at 12:00 p.m. and reconvened BESAC at 1:33 p.m.

HFIR History, Jim Roberto, ORNL

Roberto shared the historical context of HFIR, including the Advanced Neutron Source (ANS), the current landscape, and HFIR going forward. HFIR began in the 1960s at ORNL and Brookhaven National Lab (BNL). In the 1950s Seaborg wrote to the Atomic Energy Commission Chairman Lewis Strauss about the need for a "very high flux reactor". HFIR was completed in 1965 and still has the highest neutron flux reactor outside Russia.

In the 1980s, ORNL proposed the ANS in response to the Seitz-Eastman recommendations. By 1995 the ANS project was cancelled due to rising costs, unresolved Highly-enriched Uranium (HEU) / Low-enriched Uranium (LEU) debate, and lack of unity in the neutron community. In response to the ANS cancellation, a 1996 BESAC panel called for upgrades to the High Flux Beam Reactor (HFBR) and HFIR. In 1997, ORNL's bid for the Spallation Neutron Source (SNS) was accepted and completed in 2006. In 2007 HFIR completed neutron scattering upgrades and a new infrastructure. Today HFIR serves national missions including neutron scattering, isotope production, and materials irradiation. For example, HFIR is the only source in the world for heavy actinides such as tennessine.

HFIR and SM-3 in Russia are the highest power high-flux reactors in the world. HFIR provides the highest steady-state thermal neutron flux, high-end aspects of isotope production,

and the adjacent Radiochemical Engineering Development Center (REDC) for radioisotopes. Going forward HFIR will provide continued leadership for high-flux applications for steady-state neutron scattering and HFIR/REDC will continue to grow the importance of isotopes. Future considerations include HFIR life extension, a D_2O reflector, and a second guide hall.

Discussion

Robertson asked about HFIR's lifetime extension and replacement plans. **Roberto** explained everything in the reactor can be, and most has been, replaced. The major activity is replacement of the pressure vessel. ORNL developed a replacement plan when the ANS project failed and is continuing to think about replacing the pressure vessel.

Gao inquired about the test reactor at Idaho National Lab (INL), which includes materials irradiation. **Roberto** noted there is a difference in mission space for HFIR and INL. HFIR's materials irradiation is for small instrumental samples for research, whereas INL irradiates materials for large assemblies for engineering science.

Friend asked about plans and funding to reopen HFIR. **Roberto** indicated ORNL is working closely with DOE SC, and an internal investigation has been completed. The failure has been traced to failure of fuel plates. There was no release of radiation. ORNL understands how the failure happened, and aims to resume operations by the end of FY19.

Kastner asked who in DOE is responsible for isotope production. **Roberto** explained there are several customers for isotope production including specialized isotopes such as californium-252. Nuclear Physics (NP) runs a very vibrant isotope program which utilizes parts of HFIR and REDC.

McDonald inquired about measuring the remaining use of the main pressure vessel. **Roberto** said ORNL believes the pressure vessel will be conservatively viable through mid-century. HFIR will continue operation for the long term and ORNL is considering replacing the pressure vessel earlier to capture new capabilities.

Louca asked about accommodations for neutron users affected by the HFIR shutdown. **Paul Langan** explained that ~3,000 users per year are accommodated by neutron sources and 15% of the proposals focus on collecting data from both HFIR and SNS. To the extent possible ORNL is accommodating HFIR users at the SNS for appropriate projects. Currently 400 users have been impacted by the HFIR shutdown.

American Physical Society (APS) Report on Neutrons for the Nation, Julia Phillips, Retired Sandia National Laboratory (SNL)

Phillips explained that the APS report was motivated by four questions concerning the importance of neutron sources for the future, important characteristics and their production, the global landscape, and policy issues. The report contains six key findings and four recommendations. The key findings concentrate on the importance of neutron sources, the U.S. capability in neutron research and development (R&D), high performance research reactors (fueled by HEU), risk of reactor fuels containing HEU, and complementary capabilities of spallation facilities, research reactors, and high-performance instrumentation. The four recommendations focused on support for the diversity of neutron R&D capabilities, increased investment, commitment to high density LEUs, and new generations of LEU-fueled High Performance Research Reactors (HPRR).

Commissioning a new HPRR has a long lead-time and a decision is required sooner than later. Developing very high density LEU fuels appropriate for converting existing HPRRs has

taken much longer than originally anticipated. The recommendations led to three questions: can all uses of HPRRs be met without the use of HEU, can or should all of the current uses of HFIR be met in a single HPRR, and are there other approaches to meet the needs of HEU-fueled HPRRs.

Discussion

Hsu asked if reactor activity in Europe or Asia has remained constant over the last 20 years. **Philips** explained that while there have been studies in Europe about replacing and converting reactors, outside of Russia only one reactor has been built that does not use HEU.

Louca asked if the APS study compares productivity between the 48 instruments in the U.S. to the 100+ instruments in Asia and Europe. **Phillips** stated that at the time of National Academies' (NAS) 2016 study "Reducing the Use of Highly Enriched Uranium in Civilian Research Reactors", the Institut Laue–Langevin (ILL) was the most productive facility. While the National Institute of Standards and Technology (NIST) reactor is competitive on a world scale, it is only one reactor.

Kastner asked about LEU requirements for converting existing reactors versus the LEU criteria for a new reactor. **Phillips** said reactors had to operate at 90% performance for conversion from HEU. New LEU reactors allow for some of the requirements to be relaxed. **Kastner** inquired if the conditions are relaxed enough to build a new reactor with LEU fuels. **Phillips** commented that a HPRR could be built using existing LEU fuels, but she was unsure about performance compared to HFIRs capability.

Roldan Cuenya asked about current LEU fuel technologies for new reactors. **Phillips** explained qualified, high density LEU fuel is being used in some reactors. Germany has one HEU reactor whose capabilities could be replicated with LEU.

SNS Proton Power Upgrade (PPU) Project Update, John Galambos, ORNL

The PPU doubles the SNS proton beam capability from 1.4MW to 2.8MW, and increases the proton beam energy and current by 30% and 50%, respectively. The increases can be completed largely on existing accelerator technology and the project leverages built-in upgrade provisions. The PPU scope is to install seven new cryomodules, upgrade injection and extraction, upgrade the existing linac radio-frequency (RF), and install new RF equipment for the new cryomodules. A stub in the transport line between the ring and the existing target station will be provided yielding a seamless tie-in for the Second Target Station (STS) project without interrupting operations of the first target.

Most of the installation will occur at normally scheduled maintenance outages, with one exception in 2023. As the superconducting cryomodules are installed they will be used. The beam energy and power will gradually be increased between 2022-2024 timeframe. Favorable budgets over the last two years have allowed the project to move forward quickly in accelerator systems and target systems. Over the next 12 months the cryomodule and high power RF designs will be formalized and procurements initiated. Target gas injection development will be finalized, the klystron gallery final design will be completed, and construction initiated.

Discussion

Kastner asked about the physics behind the gas injection reducing damage. **Galambos** explained gas acts like a shock absorber and it makes the fluid compressible. A very short pulse of protons hitting the mercury creates a shock wave. By making the fluid compressible the

injection and operation is 0.1% volume of helium. The strength sensors' dramatic drop can be measured in the instantaneous pressure pulse. The target is damaged by either fatigue or a shock wave that causes cavitation damage. Reduction in the pressure pulse reduces the fatigue damage. The nose of the target has been cored out and has shown a dramatic reduction in the cavitation damage. **Louca** added that the gas injection was not in the original design; it was a solution to mitigate the problem with the target, and it resolved the problem.

Ourmazd inquired about modifying the software to reduce the required signal to noise ratio. **Galambos** indicated while an area of scrutiny, software was in the operations scope. The PPU scope is aimed at doubling the power.

Kastner called a break 2:37 p.m. and reconvened the meeting at 3:02 p.m.

Advanced Light Source Upgrade (ALS-U) Project Update, David Robin, LBNL

The motivation for the ALS-U was based on a BRN need to understand, predict, and control emergent materials and chemical properties. Properties such as high chemical material contrast, nanoscale spatial sensitivity, and broad temporal sensitivity to nanoscale motion are needed to understand materials. The combination of capabilities is currently lacking at light sources and thus created the need for high soft x-ray brightness and coherent flux.

ALS is a 3rd generation light source and has been in operation for 25 years. It is optimized for production and use in the soft x-ray space. The scope of ALS-U is to replace the existing storage ring with a new 2 GeV, high-brightness storage ring fed by a new full-energy accumulator ring, to add a suite of two new and two upgraded world-leading undulator beamlines and two new full-length undulators, and realign the existing beamlines. The project received CD-0 in 2016, CD-1 in 2019, is now in the design phase and anticipating CD-2 in 2020. Early finish will be in the second quarter of 2026.

The ALS-U accelerator scope will be keeping the linear accelerator and booster, replacing the storage ring, and adding a new accumulator ring. The accumulator ring is for full-energy swap-out injection and recovery of bunch trains. The plan is to install the accumulator ring early for the dark period to minimize risk and duration. Experimental systems include MAESTRO and COSMIC upgrades, a new soft x-ray beamline, and a new tender x-ray beamline. Strong budgets in FY18 and FY19 have allowed the acceleration of the project.

Discussion

Musumeci asked about the design of the two different rings and ALS-U's stance in international competition. **Robin** stated the accumulator ring allows for much higher performance and recovery of the beam. Compared to other facilities, ALS will be the brightest soft x-ray source in the world.

Ourmazd inquired about the software chain and the application program's interface. **Robin** stated that was outside the scope of the project but still very important.

Roldan Cuenya asked for examples of taking advantage of the enhanced resolution. **Robin** explained that in the lithium example he showed it was charged at a rate they could measure. The goal is super charging; something not yet possible. **Roldan Cuenya** mentioned industrial interests in long term operation. **Robin's** understanding is industrial interests focus on sources of damage and impacted rate.

Stack asked about expanding the field of view. **Stephen Streiffer** (Argonne) stated any increase in brightness can be partitioned in different ways and ALS will expand the field of view.

Advanced Proton Source Upgrade (APS-U) Project Update, Bob Hettel, Argonne National Laboratory (ANL)

APS is a 4th generation storage ring light source focused on hard x-ray. The project motivation is higher brightness, higher coherence, and higher energy penetrating x-rays. APS-U will replace the existing double-bend lattice with a 7 bend achromat (BA) incorporating reverse bending. Most of the existing undulators will be replaced with 9 superconducting and rebuilt permanent magnet (PM) undulators. APS-U will have 9 new high performance beamlines and 15 enhanced beamlines. A collaborative effort is addressing the challenge of preserving coherence through the beamlines.

The U.S. remains the leader in high-energy x-ray science, however, the international landscape in high-energy (6 GeV scale) machines is reinforcing the APS-U project. APS-U is on schedule and received CD-2 in December 2018. CD-3 is expected in FY20 with a dark time in 2022-2023. The recent enhanced funding allowed the CD-3 date to move forward to FY19.

Discussion

Gao inquired about high performance computing (HPC) capability and the AI experimental control and data analysis effect on users. **Hettel** explained HPC is being covered by operations. **Streiffer** added that an experimental workflow, including advances in computing power and analysis methods, has been mapped out for each beamline. APS-U operations is using that as a roadmap to ensure the analysis packages are ready for the users at a defined level. AI and HPC are very important in data analysis. For example, by using machine learning techniques coherent fraction imaging data can be analyzed at a 1000x factor faster than direct inversion. HPC can help to evaluate the collected data against completion criteria or signal-to-noise criteria.

Ourmazd asked about the applications provided to users and stressed the importance of user engagement in algorithm development. **Streiffer** indicated the operating system is mostly instrument control systems. However, the project is importing Bluesky and standardizing it across beamlines, giving users a standard operating system. Light sources are becoming involved in data analysis allowing the user to leave with results in hand rather than experimental data they must analyze.

Stack asked about strategies to handle increased beam damage. **Streiffer** explained the situation is well-understood by the free-electron lasers (FEL). One strategy is to determine what the radiation damage actually is while another is to design experimental protocols.

Louca inquired about increases in the number of users and experiments following the upgrade. **Hettel** expressed that the experiments and turnaround time will be much faster. **Streiffer** stated that the APS-U expects the number of users to be constant, but the experiments and the range of parameter space the individual user investigates will be larger.

Presentation of new BESAC Charges (on same recording as previous)

Kastner introduced two new BESAC charges on neutrons and international competitiveness, asking for comments about each question in the two charges.

Related to the upgrade paths for HFIR, **McDonald** asked about the experience of ILL. **Langan** explained that ILL began construction in 1970, changed its pressure vessel in 1994, updated systems within the pressure vessel, and built a second guide hall. **Kastner** noted some of the subcommittee members will need to understand the current state of nuclear fuels development.

Hsu asked about data on LEU fuels compared to HEU fuels. **Roberto** indicated there are qualified LEU fuels, approved by the Nuclear Regulatory Commission (NRC), which can be used in reactors up to 20MW. Research is taking place in Europe, however, no qualifying fuels can operate at HFIR today. The issue is fabricating the LEU fuel in the right geometry with the necessary density to meet HFIR requirements. **Phillips** said fuel elements for all high performance reactors are intricate assemblies. When the NAS (2016) study began, the previous report (2011) projected the LEU issue would be solved by 2014. By 2016 the timescale had been pushed out to 2030.

McDonald asked if replacing the pressure vessel gives as much geometry flexibility as starting from scratch. **Roberto** explained the easiest way forward is to find a fuel that matches the form factor of existing reactors rather than making big changes. **Kastner** commented that the choice is use LEU with a recommendation to start from scratch, or keep HFIR operating and work on LEU development.

Kastner explained the second charge on international competition and directed the committee to the third question about attracters and deterrents, especially in the context of the foreign talent memorandum. **Gao** stated that the process of innovation relies on talented people and policies and strategies. He recommended BES consider ways to motivate and keep top talent at the beamline because they develop new capabilities at user facilities. He also said there is a need to encourage both individual and shared use of data for innovation.

Tirrell said the second charge focuses on who is drawing talent and resources away from the U.S. and how BES should address the issue. **Musumeci** mentioned Europe has other award levels that provide incentives to innovate; ECA is not enough and BES should consider extending awards.

Stack noted a recent Nature paper about small teams being more innovative than large teams. Conversely, economists have been saying that innovation gets harder as fields mature, making larger teams necessary.

Roldan Cuenya suggested opening more positions for young people. **Olvera de la Cruz** expressed that innovation requires a willingness and ability to move away from one's comfort zone. **Takeuchi** stated the single biggest concern for an academic or national lab career is that funding will dry up; graduate and post-doctoral students want and need job security. She was concerned about providing opportunities to succeed.

Epps discussed funding cycles, awards, and small and large teams. He explained that the 3-year funding cycles do not match the PhD graduation cycle creating a difficult situation for new faculty members and playing into students' anxiety. He suggested a mid-career award might be an incentive beyond the ECA and funding ending after five years. And he recommended BES cautiously interpret the benefits and challenges of small and large teams; there is a social dynamic at play in teams that affects innovation.

Ourmazd suggested the sub-committee adhere to the structure in the charge, stating answering the questions secures money, heads off criticism, and allows BES to retain talent.

Friend pointed out that all mid-career scientists should be supported to do innovative work. She noted that early career individuals in other areas generally do not expect job security and suggested BES focus on making people feel more agile in their work.

Ayers noted there is lack of support beyond early career and significant fluctuation in one's research direction. In the U.S., to continue to receive funding, one must focus on the "hot topic" of the moment.

Santore stated that part of being a leader is to be agile.

Robertson noted there has been no evaluation on the impact of early career awards on future success. He called for data about conversion rates on the performance of early career recipients as they move forward, stating the data may indicate universities need to do more.

McDonald stated the focus of funding should be on doing science, not looking good in a competition.

Hsu mentioned that young people want to feel in control of what they do and suggested BES could afford to offer funding for small and large group collaborations.

Tirrell explained the international competition data is complicated. While there were no economic experts on the decadal survey committee, data was gathered and some basic comparisons were made. For example, in China, the rate of growth is very rapid but it is on the industrial side. While Chinese government funding is going up it is not necessarily going to the universities. These situations and the reasons for them need to be understood. **Kastner** suggested the subcommittee include expertise in international competition.

Musumeci said the user facilities are one of main attractions to the U.S. He recommended finding a balance between facilities development and research.

Roldan Cuenya suggested the labs refrain from using soft money to fund employees and find a mechanism to shift people to permanently funded positions. She explained Europe has a rule that a PhD holder cannot be on soft money more than six years. **Stack** asked if the model of hiring someone on hard money after six years impacts hiring and adaptability. **Roldan Cuenya** said for those who do not find a permanent position in a lab, they go to industry or pursue another option. **Hsu** added that U.S. universities are moving towards more soft money than tenure track positions.

Public Comment session

None.

Kastner adjourned BESAC at 4:38 p.m.

Friday, March 8, 2019

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

Linac Coherent Light Source-II (LCLS-II) Project Upgrade, John Galayda, SLAC

The LCLS-II is removing the SLAC copper linac from sectors 0-10, and adding a new cryoplant operating at 2keV using an existing electron bypass line which connects to a new transport line. LCLS-II will replace the original fixed-gap LCLS undulators and add two new x-ray sources. The LCLS-II upgrade began in 2013, CD-2 and CD-3 were approved in March 2016, the project is 81% complete, and CD-4 is anticipated in 2022. The copper linac will be replaced with niobium yielding approximately 3x increase in “quality factor” (Q) with nitrogen doped superconducting RF cavities, and dramatically reducing the cooling capacity for the operation.

The project is building two new undulator systems. Hard x-ray undulators are being prepared for installation by ANL, LBNL, and SLAC. FEL operations will resume in January 2020. The new hard x-ray undulators will be online February 2020, the cryomodules will be

installed and Cryoplant 1 commissioned by April 2020, and first light, using the SLAC linac, will be in March 2021.

Discussion

Ourmazd asked about development of the detectors. **Galayda** said the detectors are not being provided within the project, the detector program is led by the LCLS Directorate at SLAC.

Ong inquired about the improvement of the Q factor of niobium resonators. **Galayda** said the process involves diffusion of nitrogen gas into niobium by 5-25 microns during the firing process in the cavities. The improvement in Q was serendipitous; researchers at Fermilab were interested in developing niobium-nitride as an RF superconductor. The diffusion process was attempted to produce that compound. Scientists discovered that although Q was dramatically improved it was not because of the nitride.

Musumeci asked about the advantages and improvements in the operation of the copper linac with respect to LCLS operations. **Galayda** said the copper linac has been steadily developed over the years. The FEL process harvests a fraction of the kinetic energy of the electron beam. 6-millijoule pulses could be reached coming out of the SLAC linac. The bunch does not dismantle itself on its way to the undulators, and the electron's position is frozen as a result of the copper high-energy electron beam.

Hsu asked if there are any foreseen problems cooling the niobium cavities with liquid helium. **Galayda** explained this exotic technology is primarily used at accelerators. Cryoplants were designed at Jefferson Lab (JLab) which runs at 2.1 Kelvin. The two companies that can build the Cryoplants mostly build liquid methane hardware. A group of engineers and technicians will keep the Cryoplant operating. The Cryoplant should only require routine maintenance for 3-years or more.

Linac Coherent Light Source-II-HE (High Energy) Project Update, Greg Hays, SLAC

The LCLS-II-HE project's primary goal is to extend the photon energy range of LCLS-II. The project will add additional cryomodules to deliver photon energies beyond 12keV. LCLS-II-HE will use 300 meters of available space in the LCLS-II; CD-1 was approved in September 2018 and LCLS-II-HE operations are targeting the mid-2020s.

The scope of LCLS-II-HE is to double electron energy of the accelerator, install a second bypass line, and provide specialized instruments. Accelerator upgrades will enable hard x-ray high repetition rate and increase the experimental capacity. The existing end stations (XPP, DXS, CXI) will be upgraded and lead to five upgraded end stations.

The proposed collaboration is between SLAC, Fermilab, JLab, Cornell University, and LBNL. CD-1 was approved in September 2018, January 2020 is the goal for CD-2 and CD-3, and CD-4 will occur in October 2028. Over the next 12 months the collaboration will be formed and codified, cavity research will be ready for cryomodule demonstration, the HE prototype cryomodule will begin, CD-3a for cryomodule production will occur in FY19, and the cryomodule procurements will start.

Discussion

Roldan Cuenya sought examples of new scientific challenges that can be addressed following the upgrade. **Mike Dunne** (Stanford) stated the reason to extend to high energies is to

provide atomic resolution. Extending performance to 13-20 kilovolts provides the ability to track electronic and nuclear structures involving chemical systems and material systems on the femtosecond timescales. **Roldan Cuenya** recommended that BES ensure there are enough funds to make the beamlines.

Musumeci asked about limitations and plans to address them. **Hays** explained x-ray performance is limited by emittance. The accelerator team is considering ways to design the optics lens for HE to improve the electron bunch brightness. Substantial improvement may be to change out the source; a brighter gun will be the best option to get better performance.

Ourmazd stated that user demands for process improvements led to LCLS-II and LCLS-II-HE, adding there is a lot of excitement about the qualitatively new experiments that will be possible with these machines.

Friend asked how the pulse duration will change in comparison to non-HE projects. **Hays** expected similar performance. **Dunne** said best performance will be at the 200 attosecond level in hard x-rays and a bit longer in soft x-rays. **Friend** asked about the durability of the nitrogen doped cavities. **Hays** said they are quite robust and there has been no degradation of performance. LCLS-II is the first machine built with this technology.

Kastner inquired about the effect of the upgrades on the detectors. **Hays** explained LCLS operations will be running the detector process. LCLS-II-HE will buy what is available through the R&D programs for the project.

Polymer Roundtable Update, Phillip Britt, ORNL

Britt briefed BESAC on chemical upcycling of polymers. The co-chairs are Geoff Coaste (Cornell) and Karen Winey (University of Pennsylvania). The charge is to assess fundamental challenges, and identify fundamental research opportunities for the science and design of plastics.

Upcycling is making higher value items from waste products. Some challenges to upcycling are sorting plastics to get a clean stream, additives and residue, layered materials, and deconstruction. Upcycling fits the BES mission because fundamental materials and chemical sciences are required; 80% of the polymer challenge is a chemistry challenge. BES understands the links between atomic and molecular scale organization, and has unique tools at user facilities to support atomic and mesoscale research in upcycling.

The roundtable will focus on four challenges: design chemical mechanisms and targeted molecular intermediates, create integrated depolymerization-reassembly processes, design next-generation polymeric materials, and investigate crosscutting opportunities for upcycling polymers. The goal is to gather experts, assess the current status, identify priority research opportunities, and prepare a report. The chairs have been confirmed, panel leads and participants are being finalized, the date and location have been selected, the factual document is being written, and a webinar will be held in advance of the workshop.

Discussion

Kastner asked for the definition of a roundtable compared to other approaches. **Kung** explained that traditionally BES has held a number of BRN workshops. BRNs are larger and require longer planning and report writing time whereas roundtables fit smaller scope and timeframe projects. The more focused scope and time frame for production of a report justified the roundtable approach.

Tirrell noted that catalysis is one of the key scientific fundamentals in upcycling and suggested diverse scientific disciplines need to participate. **Britt** agreed saying the chemists, the catalysists, the polymer scientists are needed to make new structures, and to understand structure, but there must be compelling properties that people want to use. Creative people must be involved and this is a great opportunity to explore and identify key bottlenecks and chart a path forward.

Epps stated depolymerization of biomass offers many lessons and asked about the Center for Sustainable Polymers and other sustainable polymer workshops' involvement. **Britt** said the goal is to learn and be inspired by what has already been done by others. **Epps** asked about input from policy regarding recycling single stream versus mixed streams versus leakage, and stated that people's behaviors must be considered. **Britt** mentioned the roundtable was focused on the science, but some of the solution is to change behaviors.

Leone asked if there will be discussions with economists and industry. **Britt** said industry people from the U.S. and Europe will attend the roundtable. The objective is to design processes and new chemistries that are energy efficient and translates into lower costs.

Olvera de la Cruz asked about working with a renewable energy laboratory. **Britt** explained opportunities in biocatalysis exist. The difference is the roundtable is focused on turning the polymers into high-value products rather than energy and CO_2. **Olvera de la Cruz** suggested the biomaterials community could learn about using enzymes. **Britt** noted that polylactic acid, which has some very nice properties for packaging, is easily depolymerizable.

Ong asked if the education component will be addressed. **Britt** said promotion of the science and inspiring the next generation will follow the roundtable report.

Epps inquired about same-cycling asking how much of the focus on upcycling eliminates the possibility to same-cycle. **Britt** said while the ultimate goal is to make a better product, lots of successes will be discovered along the way.

Microelectronics Basic Research Needs (BRN) Report, Supratik Guha, ANL

Guha shared information on the motivation, status, and key results of the microelectronics BRN held in October 2018 with a final report due in April 2019. Two reasons for the timing of the BRN are that complementary metal–oxide–semiconductor (CMOS) scaling (Moore's Law) is ending, and data intensive and edge computing are emerging. New types of computing architectures are needed because of memory bottlenecks, data transport, and low power computing.

High performance computing and simulation underpins DOE missions and there DOE and vendor synergies in the deployment of computing technologies. The charge of the BRN was to assess scientific issues, identify critical challenges and opportunities, and examine CMOS beyond exascale technologies. There were four panels on big data collection, analytics and processing; co-design; power control, conversion and detection; and crosscutting themes. The five priority research directions (PRD) are all underpinned by principles of co-design. PRD1 is to flip the current paradigm: define innovative materials, device, and architecture requirements driven by applications, algorithms, and software. PRD2 is to revolutionize memory and data storage. PRD3 is to reimagine information flow unconstrained by interconnects. The last two PRDs focus on moving microelectronics to three dimensions. PRD4 is to redefine computing by leveraging unexploited physical phenomena, and PRD5 is to reinvent the electricity grid through new materials, devices, and architectures.

Discussion

Hsu asked how the report will be used. **Kung** said prior BRNs with similar multidisciplinary approaches have been recommended as well. BES is coordinating with Advanced Scientific Computing Research (ASCR) and High Energy Physics (HEP) in SC on how to take advantage of the PRDs. In future budget requests BES will be able to reflect some of these unique opportunities.

Bonnell asked about the timeframe imagined by participants to achieve solutions and solve challenges to reaching the next generation. **Guha** said the imagined timeframe was longer term, 10-30 years. **Bonnell** said there are potential disruptive technologies that seem to be constant; she asked about the recommendations if quantum computing and DNA were understood in the next 30 years. **Kung** said multiple approaches are being pursued. ASCR is aggressively pushing the exascale machines. Both HEP and BES are pursuing as many platforms as possible because of severe data needs for future science. **Guha** added that DNA was discussed, but the roundtable was not prescriptive. Quantum computing and classical computing will co-exist. Quantum computing is not ideal for a huge class of different approaches. The feeling was that non-conventional classical computing will continue but will require new types of architectures.

Discussion of New BESAC Charges

Kastner opened the floor for additional comments or discussion points.

Gao commented on benchmarking and comparing the economic impact of U.S. user facilities to Europe. He explained that over the last 10-20 years industrial participation at light sources has decreased, with exception of pharmaceutical companies. U.S. user facilities are part of BES whose mission is for fundamental science, whereas European facilities are independent companies. The U.S. facilities are tools that can be used for basic or applied research. The question is how to make the user facilities more helpful to the economy. The action item is to hold a workshop or roundtable with people from policy makers to researchers discussing the U.S. needs. **Kastner** asked BESAC members to send ideas to the subcommittee on international competition.

Tirrell asked for more information on the structure of the subcommittees. **Kastner** explained that the usual approach is to identify a chair, then put a committee of ~15 together with 50% from BESAC and 50% from other areas of expertise. Once the committee is created, they will hold meetings, workshops, and potentially conduct site visits.

Public Comment Session

None.

Kastner adjourned BESAC at 10:46 a.m.

Respectfully submitted,
T. Reneau Conner, PhD, PMP, AHIP
Science Writer
ORISE/ ORAU