BASIC ENERGY SCIENCES ADVISORY COMMITTEE

MEETING MINUTES

Bethesda North Marriott Hotel & Conference Center

5701 Marinelli Road, North Bethesda, MD 20852

February 28 – March 1, 2013

PARTICIPANTS

BESAC members present:
Simon Bare
William Barletta
Gordon Brown
Sylvia Ceyer
Beatriz Roldan Cuenya
Frank DiSalvo
Roger French
Bruce Gates
Ernie Hall
Sharon Hammes-Schiffer
John Hemminger, Chair
Bruce Kay
Max Lagally
William McCurdy, Jr.
Monica Olvera de la Cruz
Mark Ratner
Anthony Rollett
Gary Rubloff
John Spence
Douglas Tobias
John Tranquada

BESAC members not present:
Yet-Ming Chiang
Persis Drell
Maria Santore
Matthew Tirrell

Also participating:
Patricia Dehmer, Deputy Director for Science Programs, Office of Science
George Crabtree, Argonne National Laboratory
Alex King, Ames Laboratory
Jim Murphy, Director, Office of Science, Basic Energy Sciences, Scientific User Facilities Division
Harriet Kung, Director, Office of Science, Basic Energy Sciences
Laura Biven, Office of Science Programs

Approximately 125 others were in attendance in the course of the two-day meeting.

MEETING MINUTES

Thursday, February 28, 2013

The meeting was called to order by Basic Energy Sciences Advisory Committee (BESAC) Chair Dr. John Hemminger at 8:45 a.m. Dr. Hemminger led an introduction of the BESAC members and reviewed the agenda.

Presentation: News from the DOE Office of Science

Dr. Patricia Dehmer, Deputy Director for Science Programs, Office of Science (SC), gave an update on the SC budget. She described the FY 2012 operating level, FY 2013 Request, and FY 2013 House and Senate markups for SC. Under the current FY 2013 continuing resolution (CR), SC operates at the lowest of these amounts for each program office. SC is currently operating at $4.6B which is $262M below FY 2012 and $380M below the FY 2013 request. Biological and Environmental Research (BER) in particular is operating at 10% below the FY 2012 level due to the low FY 2013 House mark. Under the CR, many construction projects are not fully funded and no new starts are allowed. If there is a full year CR, SC would operate at the FY 2012 level, and under the sequester, the SC budget would be reduced by an additional 5%. The sequester is set to take affect Friday, March 1, 2013. Under the sequester, SC expects to award fewer grants, no capital equipment, and no upgrades. Lawrence Livermore National Laboratory is looking at furloughs. The National Science Foundation announced 1000 new awards would not be made.

In looking at FY 2012 accomplishments, Dr. Dehmer highlighted two examples. First, in late 2012, three of the top four supercomputers in the world were from the Department of Energy. Number one was Titan from Oak Ridge National Laboratory, number two was Sequoia from Lawrence Livermore National Laboratory, and number four was Mira at Argonne National Laboratory. Second, Dr. Dehmer discussed the light sources and the major role they have played in Nobel prize-winning science. Across all of the SC facilities, there are approximately 25,000 facility users. Of that amount, ~10,000 use the light sources and ~4,000-5,000 use computing resources. In both supercomputing and light sources, the facilities are threatened by international competition. China and others want to get to exascale faster than the U.S. We have dominated these areas for decades, but this will likely wane in the next 5 years. The impacts of both of light sources and supercomputers have been shared with the Hill.

In other areas of SC, Fusion Energy Sciences is considering what its domestic program should look like in the era of ITER. High Energy Physics (HEP) just closed the Tevatron and is thinking about its future and is planning another long term planning exercise with its advisory committee. The Nuclear Science Advisory Committee just finished a report on the implementation of the 2007 Long Range Plan for Nuclear Physics (NP) and how they will deal with their three major facilities. Dr. Dehmer summed up these remarks by stating that the advisory committee inputs are important and play into the formulation of the budget.

Dr. Dehmer also discussed the SC Priority Goal which was worked out with the Office of Management and Budget. The SC goal is driven by the concern that SC has many operating facilities with large operations cost. SC is considering what facilities meet the current mission need, which can be deferred, and which need to close in order for new facilities to come online. All of the Federal Advisory Committees received the facility prioritization charge. By the end of March, each advisory committee must submit their response to the Director of the Office of Science.

Ten years ago, BESAC took on the charge to prioritize the facilities of the future. The top 5-6 facilities were included in the budget. At the time, BES aimed to ensure that the Linac Coherent Light Source (LCLS) was high on the list. It was and it got funded. The next facility is competing with all other ideas in SC. Management is taking into consideration impact, readiness to proceed, and cost-benefit. It is extremely difficult to pull budget authority out of research to start new construction. Currently ~$200M of BES' ~$1.8B budget is spent on construction and equipment projects.

In 1996, BES and Advanced Scientific Computing Research (ASCR) were 31% of the SC budget. Today they are 45%, reflecting demand for increases in those two programs. HEP has not done as well, closing two major facilities with no new domestic facilities. NP has also decreased as a percent of the total SC budget, but the program has a good strategic plan now for moving forward.

Discussion

Dr. William McCurdy asked if the Hill is also concerned about the proliferation of SC facilities. Dr. Dehmer responded that everyone is concerned about facilities crowding out research, especially under constrained budgets. We want to ensure that we don't start new construction that would crowd out research in the future. Dr. Simon Bare asked what BESAC can do to help achieve that balance. Dr. Dehmer responded that $200M is a reasonable steady-state investment in construction and instrumentation projects. BESAC has been charged to look at both facilities and science in the past and BES integrates that advice when it formulates the budget. The basic research needs and grand challenge reports have resulted in significant increases in budget authority for BES research. Dr. John Hemminger asked how the other SC offices are doing in balancing facilities. Dr. Dehmer responded that ASCR has a good plan for moving forward, NP is looking at tough times but the federal advisory committee has presented a path forward, HEP will be going through a major community workshop then will look at setting priorities again. The BES corollary to the HEP process is the light source charge to be addressed later this summer. Dr. Beatriz Cuenya asked how sequestration affects ongoing BES projects. Dr. Dehmer responded that there is a set funding profile for ongoing projects that have reached critical decision-2 and BES will do its best to mitigate the impact on projects.

Presentation: News from the Office of Basic Energy Sciences

Dr. Harriet Kung, Director of Basic Energy Sciences, gave an update on program activities. First, Dr. Kung highlighted new hires since the last BESAC meeting including Dr. Jim Murphy as Director of the Scientific User Facilities Division and Dr. Jim Rhyne as program manager for neutron scattering facilities. Dr. Eric Rohlfing is on detail to the Advanced Research Projects Agency – Energy (ARPA-E) as Acting Deputy Director for Technology. Dr. John Miller is Acting Division Director for Chemical Sciences, Geosciences and Biosciences in his stead. There are two vacancies in BES. One is program manager for the Nanoscale Science Research Centers and Electron-beam Microcharacterization Centers. The other is program manager for the Fuels from Sunlight Energy Innovation Hub. BES is recruiting for these positions.

Dr. Kung gave an update on the Energy Frontier Research Centers (EFRCs). The EFRCs are a relatively new funding modality, started in 2009. They have had tremendous productivity and high scientific impact, including more than 3,400 peer reviewed papers with many in high impact journals. The EFRCs have attracted many early career faculty, filed over 200 patent applications and more than 60 patent/invention disclosures. At least 60 companies have benefited from EFRC research. This summer, BES will conduct a Committee of Visitors to evaluate the efficacy and impact of the EFRC and Energy Innovation Hub programs.

A research highlight was described from the Argonne National Laboratory Center for Electrical Energy Storage (an EFRC). In this research, the researchers coated the anode of a lithium-ion battery with thermally responsive polyethylene microspheres. When the internal temperature of the battery reached 110°C, the microspheres melt and shut down operation of the battery to prevent further damage.

Another research highlight from the Non-Equilibrium Energy Research Center EFRC at Northwestern University and University of Michigan showed that surface functionalized gold nanoparticles will selectively bind mercury or cadmium. This could be a sensitive and portable way of measuring environmental toxicity with impact in many fields.

The Energy Innovation Hubs are Secretary Chu's signature initiative. BES' first hub was the Fuels from Sunlight Hub, the Joint Center for Artificial Photosynthesis (JCAP). The renovation of Jorgensen Lab for JCAP recently received LEED Platinum certification. Recent organizational changes include a new full time director and founding director/chief scientist. BES is planning an on-site review in mid-April covering both scientific productivity and management of the Hub. As a research highlight, JCAP worked with the Stanford Synchrotron Radiation Lightsource to develop a high throughput x-ray diffraction tool. JCAP's goal is to screen 10,000 samples per day and this could be broadly deployed to other facilities.

The second BES Energy Innovation Hub for Batteries and Energy Storage was recently awarded to the Joint Center for Energy Storage Research (JCESR). JCESR secured $5M

from the State of Illinois for infrastructure. BESAC was provided a JCESR fact sheet earlier in the day and Dr. Kung requested comments.

BES hosted over 15,000 facility users in FY 2012. The users help push frontiers in technique development and source reliability. A recent highlight from the Linac Coherent Light Source (LCLS) showed a novel beam splitting scheme using diamond crystals to allow two experiments to be performed simultaneously. This could help expand the usage of LCLS before LCLS-II comes online. At the Advanced Photon Source (APS), the first high energy superconducting undulator was installed as part of the APS Upgrade project. And at NSLS-II, construction is proceeding well with booster commissioning to begin later this year.

BES continues its efforts to improve our communications. BES completed a variety of recent outreach publications. Now you can also find science highlights on the BES website which are a good way to communicate highly impactful basic research.

Turning to the budget, Dr. Kung described the status of the FY 2013 appropriation. Both the House and Senate did provide marks on the budget, but Congress passed a 6 month Continuing Resolution for funding through March 27th. BES started the fiscal year operating at conservative level. BES will not need to pull any money back from laboratories or universities. We are not expecting SC federal staff furloughs or layoffs in FY 2013, but the final appropriation level for the remainder of FY 2013 is unknown. Looking at the BES funding history, the gap between request and appropriations makes it challenging to formulate and execute the budget. Facilities have been largely flat funded, resulting in reduced user support and deferred maintenance which impacts all users.

Dr. Kung described the current charge to BESAC. It is a short fused charge with a three month turnaround that needs to be reviewed and approved by BESAC at this meeting. A BESAC subcommittee was formed with expertise related to all of the facilities, but not representatives of each facility. The charge covers 14 existing facilities and 4 projects. For the projects, the APS Upgrade and LCLS-II are at CD-1, Approve Alternative Selection, but close to achieving CD-2, Approve Performance Baseline. The Next Generation Light Source and Spallation Neutron Source Second Target Station are both at CD-0, Approve Mission Need.

Dr. Kung noted that the BESAC subcommittee should focus on the charge, not on whether funding is available. The charge is to review (1) the ability to contribute to world leading science in the next decade and (2) readiness for construction. BES is also not looking for an overall ranking of the facilities. Prior to the subcommittee meeting, each facility was asked to provide a white paper and presentation in advance that addresses the charge.

Dr. Kung described the second charge to BESAC about light sources specifically. The light sources have a huge user community and broad science impact. U.S. leadership is being fiercely challenged by worldwide competition. The charge asks whether current facilities are impacting grand science challenges and what additional capabilities are

needed to steward the field. Looking back, the Leone report was direct and unambiguously pointed at hard x-ray, which led to LCLS as one of the highest priorities for new construction. There are a lot of options now and greater worldwide competition, but also high funding constraints.

Discussion

Dr. Ernie Hall asked about the future of the EFRCs. Dr. Kung replied that BES has rigorous review and monitoring of the current EFRCs. We have seen early success of this new funding modality which gives us a lot of confidence that it has demonstrated accomplishments commensurate with what we expect. All of the above are taken into consideration during budget formulation. We are hopeful that the results to date will result in positive response on the Hill. In the last few years, budget requests did not stick, so we need to continue to communicate the importance of this kind of long term investment.

Dr. Bruce Gates asked how the facilities are operating under flat funding when the cost of operations increases. Dr. Kung replied that we track the level of operations (percent optimal). To achieve near 100% optimal operations, a facility may cut back on staffing, procurement of replacement parts, or maintenance.

Presentation: Batteries and Energy Storage Hub Overview

Dr. George Crabtree described the recently awarded Batteries and Energy Storage Hub, the Joint Center for Energy Storage Research (JCESR). The JCESR challenge is denoted as "5-5-5," representing a goal of developing a battery with 5 times the energy density at 1/5 the cost in 5 years. Lithium ion batteries have only achieved 5% energy density improvement per year, therefore the focus is on new storage concepts beyond lithium ion. The Hub will develop innovative tools and build prototypes. A new paradigm for battery development is sought by integrating discovery science and prototypes in one organization.

The two biggest energy uses are poised for transformational change. Transportation can be addressed through electrification of cars. Electricity can move to generation by renewables like wind and solar. For both transitions, the bottleneck is storage.

JCESR seeks to establish three legacies: fundamental knowledge at the atomic and molecular level of battery phenomena, two pre-commercial battery prototypes (one each for the grid and car), and a new paradigm for battery development.

Conventional battery R&D is isolated. The science community holds workshops, attends conferences, and produces knowledge while the engineering community works separately on incremental improvements to technologies. JCESR aims to break this convention with end-to-end integration. JCESR is beginning with three concepts for making batteries (not three batteries): multivalent intercalation, chemical transformation, non-aqueous redox flow. No manufacturing is planned but intellectual property will be handed off to the

commercial community. JCESR wants them on the team from the beginning. Private sector partners include JCI, the biggest producer of batteries in the world, mostly lead acid; Clean Energy Trust, which promotes entrepreneurship; and Applied Materials, a potential supplier of battery materials.

The JCESR team has earned 206 R&D 100 awards, began 142 startups, earned $1.3B in licensing revenue, awarded 718 battery patents, and more. There are 40 JCESR affiliates, which include the Energy Frontier Research Centers, venture capital firms, other universities, and companies. The planned annual workshop will involve the affiliates with what JCESR has done and what is planned.

JCESR identified ten fundamental science challenges under the three concepts that guide the research program. For multivalent intercalation, the aim is to replace Li+ with Mg2+ or Y3+ to increase energy density of the battery. For chemical transformation, the concept is for all atoms to store and release energy through chemical reactions. In non-aqueous redox flow, solid electrodes are replaced with liquids so you can pump them around. There are many different options for redox couples resulting in low cost options which are important for grid applications.

The Electrochemical Discovery Laboratory will be the hub of the Hub. Here the electrolyte and materials genome efforts provide ideas for synthesis of new materials which will be first synthesized in single crystal or thin film. The materials will then go through various characterization steps and those with appropriate performance move to cell design and prototyping. The focus of the materials genome effort is to discover new classes of functional materials and save time by only synthesizing the most promising candidates. For the electrolyte genome, JCESR can look at, for example, tailoring organic electrolytes through ligands on organic molecules and again choosing the most promising candidates for synthesis.

The techno-economic modeling effort will build a battery on the computer to find how well it works. It will evaluate technical performance and manufacturing cost to determine which are the best to promote to cell design. Ones that aren't promoted will go back to science for improving the part that is not working well.

JCESR will also utilize translational development teams which integrate science with engineering. Their goal is to make and break the prototype. JCESR will start with two teams on day one to design and prototype cells related to non-aqueous redox flow and magnesium intercalation.

The JCESR intellectual property (IP) plan was signed by all partners before proposal was submitted. JCESR industrial partners may get better terms than non-partners. Argonne National Laboratory will be licensing agent for all IP so it is only one stop for industry.

The science at JCESR is phenomena driven, while the development and demonstration are performance driven.

Discussion

Regarding the electrolyte genome effort, Dr. Monica Olvera de la Cruz noted that this hasn't been done for liquids and the solvation spheres will be different for doubly charged ions. It will be a challenge to understand the structure and dynamics for moving from solution to intercalation.

Dr. John Hemminger asked if the Hub is focused on grand challenge problems. Dr. Crabtree responded that they are looking at them indirectly. The electrolyte genome is an example. In addition, the EFRCs can work on problems that JCESR can't do; they can take an interesting science opportunity to understand the basic science. The Hub will not emphasize basic science.

Dr. Anthony Rollett commended JCESR for dealing with IP issues upfront. He followed up by asking about degradation. Dr. Crabtree responded that cost is related to lifetime (longer lifetime, lower cost). JCESR wants to know how things fail and will be looking at this in the techno-economic modeling and during prototyping.

Dr. Max Lagally asked if there is any violation of the rules of thermodynamics in the first 5 of 5-5-5, representing 5x the energy density. Dr. Crabtree responded that the best possible scenario or theoretical limit is a factor of 10. A factor of 5 doesn't push the limits. Most systems get 1/10 of theoretical limit.

Presentation: Critical Materials Hub Overview

Dr. Alex King presented a summary of the Critical Materials Hub, the Critical Materials Institute (CMI). The CMI partnership includes many national laboratories, academic partners, and industrial partners. Dr. King noted that the success of the Hub will result in nothing happening; technologies will not fail because of lack of materials. He described a critical material as any substance used in technology that is subject to supply risks and for which there are no easy substitutes. In lay terms, it is stuff you need but that you can't always get and that you can't make. Critical materials depend on whom, where, and when you ask. For example, Ford and General Motors might say steel is the most critical material. If you ask an automotive manufacturer in Korea, they might say magnesium.

What matters also depends how far into the future you are looking. The rare earths that are the critical materials today may not be in the future. The price of rare earths has dropped in the last two years, but the crisis is not over. Price is only one indicator. China stopped exporting rare earths then stopped producing all together, yet prices continues to fall. This is because you can't buy futures of rare earths; you just go and negotiate them. The price spike in 2011 was due to speculators in china who were buying rare earths. The price fell when we started clearing out those stocks.

The revolution in Zaire caused the price spike in cobalt in 1980. Since then, many things have happened. New mines become attractive once the price spikes and other technologies emerge.

The mission of CMI is to eliminate materials criticality of clean energy technologies in the US, not including batteries. A supply risk is considered high for there are only one or two suppliers. CMI will focus on 7 critical or near critical elements to start (Y, Nd, Eu, Tb, Dy, Li, Te). These were identified in the Department's Critical Materials Strategy published in December 2011. The three pillars of DOE's strategy are: diversify global supply chains; develop substitute materials; and enhance recycling, reuse and efficient use of materials. An additional goal is to learn to anticipate materials criticality.

If mining is the solution to eliminate materials criticality, it takes about ten years on average to build a mine. And hence if a technology is at risk today, this is not a good solution. CMI will not be doing prospecting as part of the Hub.

One of the elements that CMI will begin with is neodymium (Nd). Traditional uses are in tiny magnets (gram quantities); emerging uses are for traction motors (~7 lbs of Nd) and wind turbines (~700 lbs of Nd). Recycling Nd from existing technologies won't provide enough material in the long term. ARPA-E is looking at new materials. We will be looking at diversifying supply.

One approach to diversifying supply is looking at separation processes in mines. The current approach of classical froth flotation utilizes air bubbles which adhere bastnaesite. This is skimmed off and further purified. However, monazite contains higher atomic weight rare earths but currently goes to the tailings heap. CMI will investigate collector molecules that will bind monazite to air bubbles.

Terbium and europium are used in lighting technologies. LEDs use less of these elements per lumen than a fluorescent tube. If we then look at the timescale for when LEDs will take over lighting market, best approach for these elements is recycling.

Looking at mining revenues, Nd provides value for a mine. If we substitute Nd in various technologies, the price of Nd will drop, reducing mine revenues and potentially challenging the supply of europium, terbium, and yttrium.

CMI will be managing projects by technology readiness levels (TRLs), with a plan to move to higher TRLS from year 1 through year 5 of the Hub award.

Discussion

Dr. Max Lagally asked if the raw materials are disappearing. Dr. King responded that the Deputy Director of the Hub is a mineral economist and considers these questions. The raw materials are always available if you're willing to pay the price. Helium is the one exception. Rare earths are concentrated in a few places around the world. In fact, Nd is more dispersed in a phone than it was in the earth and therefore it's more expensive to recover from a phone.

Dr. Bruce Gates asked about the general basic science challenges that the Hub will address. Dr. King responded that the 4f electrons are not well understood. Density

functional theory doesn't get it right. Basic research is needed on 4f electrons, and we have a small component of the Hub on crosscutting research such as this area.

Dr. Tony Rollett asked if the Hub has looked at extracting metallurgy. Dr. King replied that the Hub has every extractive metallurgist in the country working with them (there are two in the U.S.). Historically, we have not had to worry about availability of materials.

Presentation: International Light Sources Survey

Dr. Jim Murphy, Director of the Scientific User Facilities Division, Basic Energy Sciences, presented an overview of U.S. and international light sources. Dr. Murphy started by describing 1st and 2nd generation light sources which utilize synchrotron radiation. For these sources, we only use ~0.1% of the bandwidth at any given time. The 2nd, 3rd, and 4th generation sources utilize undulator radiation which results in a much narrower bandwidth which is dependent on the number of periods in the undulator.

The three most common types of light sources are storage rings, energy recovery linacs (ERL) and free electron lasers (FEL). Around the world there are many storage rings, a few ERLs at low energy (none at x-ray wavelengths yet), and some FELs. The light sources are a tremendous resource that serves a vast user community.

We still have premier U.S. facilities but challenge is to maintain leadership amidst fierce world-wide competition. There are four BES projects to maintain our lead in light sources: National Synchrotron Light Source-II (NSLS-II), Linac Coherent Light Source-II (LCLS-II), Advanced Photon Source Upgrade (APS-U), and Next Generation Light Source (NGLS).

The U.S. facilities and comparable international facilities are:

- Advanced Light Source: Swiss light source
- Stanford Synchrotron Radiation Lightsource and National Synchrotron Light Source: MAX IV will finish in 2015 and Brazil light source in design stage
- Advanced Photon Source: ESRF, SPRING-8, PETRA II
- Next Generation Light Source: FLASH
- Linac Coherent Light Source: Swiss FEL, XFEL Desy, XFEL Korea, SACLA Japan

The photons at a light source inherit the electron properties from which they are generated. Therefore, in order to make good photons, we must make good electrons. We want to maximize the brightness of the photons. The diffraction limit is when electron beam emittance is roughly equal to the light emittance. We have already achieved low vertical emittance. Now we need to work on horizontal emittance; 1 nm is the current ceiling. There are no operating rings below 1 nm horizontal emittance. The diffraction limit is wavelength dependent. At one Angstrom, it is ~8 pm. Damping wigglers at NSLS-II aim to bring emittance down from over 1 nm to about 0.5 nm.

For FELs, there are normal conducting linacs, such as at LCLS (copper linac), and superconducting linacs. The FEL at Desy is a pulsed superconducting linac with 3000 pulses at 10 Hz. In FELs, the key driver to performance is the injector; improvements to the injector improve the FEL. For resolution, LCLS is at one angstrom, the goal for NGLS is ten angstroms. NGLS would also have a high rep rate (1 MHz). The MHz pulse rep rate results in high average brightness. For an XFEL-oscillator ERL, the energy would be higher (6-10 GeV versus 2.4 GeV for NGLS) but it would also have high rep rate and one angstrom resolution.

Looking at average brightness, ESRF, PETRA, and Spring8 are already competing with APS. NGLS has a high average brightness because of its rep rate. In self-amplification by stimulated emission (SASE) FELs, we inject a seed to boost brightness. For peak brightness, FELs are 8-9 times brighter than storage rings. NSLS-II increases its brightness in the 10-20 keV range versus NSLS, but APS remains the focus for hard x-rays. For the APS Upgrade project, SPX (short pulse x-ray) aims to increase the number of photons in a pulse.

In summary, international competition is compromising a little on capacity but less on performance. As the performance gap narrows, science will have to set us apart. The BES R&D program helps deliver revolutionary new sources while ensuring an evolutionary path for existing sources.

Discussion

Dr. John Spence asked what possibilities there are at LCLS or FELs for many monochromatic frequencies in order to make molecular movies. Dr. Murphy responded that the focus so far has been to narrow the band width. SASE is the widest bandwidth and two color frequencies are currently being looked at. Perhaps in the future we could have 7 color frequencies. It is an R&D project for the future, but wouldn't rule it out.

Dr. John Hemminger asked how facilities handle end stations and their funding, or funding of equipment. It seems more robust abroad. Dr. Murphy responded that we try to fund operational budgets to do as much facility R&D as possible. BES counts on facility directors to allocate the funds for optimum for user support. BES has asked facilities to take over more operations of end stations.

Presentation: BES Facilities Prioritization Subcommittee

Dr. William Barletta, co-chair of the BES Facilities Prioritization Subcommittee, presented the draft report to BESAC. Dr. John Hemminger, BESAC chair, noted that the timeline for this report is compressed and it must be approved at this meeting. The charge to the committee is to look at all present and proposed BES facilities and assess their ability to contribute to world-leading science and their readiness for construction. The subcommittee is to provide a report that categorizes the facilities with justification, but not to rank order the facilities. Dr. Barletta briefly described the committee's findings related to each of the BES facilities.

Advanced Light Source: strong user demand, high productivity, strong international competition, important to U.S. world leading science

Advanced Photon Source: leading U.S. source for hard x-rays, large user demand, strong international competition, absolutely central to U.S. world leading science

National Synchrotron Light Source: operations end September 2014, lower priority for U.S. world leading science

National Synchrotron Light Source-II: large, ultra-low emittance ring; infrared to hard x-rays; absolutely central to U.S. world leading science

Stanford Synchrotron Radiation Lightsource: mid-energy facility, high user satisfaction, operational synergies with LCLS, important to U.S. world leading science

LCLS: first hard x-ray FEL, highly over-subscribed, absolutely central to U.S. world leading science

Spallation Neutron Source: world's highest power spallation source, U.S. neutron science suffers from low capacity (35% of Europe), absolutely central to U.S. world leading science

High Flux Isotope Reactor: nation's highest flux facility with continuous neutrons, exceptional resource for materials irradiation, important to U.S. world leading science

Lujan Neutron Scattering Center: strongly leverages NNSA investment in LANSCE, extra capability and capacity is helpful, accessories not at other facilities are important but not essential, lower priority for U.S. world leading science

Center for Nanoscale Materials (ANL): exploits hard x-ray nanoprobe, excellent access to environmental nanoprobes, absolutely central to U.S. world leading science

Center for Functional Nanomaterials (BNL): world class TEM capabilities, important to U.S. world leading science

The Molecular Foundry (LBNL): strong cross-disciplinary portfolio, chemical synthesis and characterization are integrated, absolutely central to U.S. world leading science

Center for Nanophase Materials Sciences (ORNL): excellent theory and scanning probes, well coupled to computing, important to U.S. world leading science

Center for Integrated Nanotechnologies (SNL/LANL): growing number of discovery platforms, unique capability for user platforms, absolutely central to U.S. world leading science

Advanced Photon Source Upgrade: maintains U.S. capabilities in hard x-rays and offers exciting possibilities for short pulse x-rays, hardware approach for 2 ps pulses needs to be vetted this spring, absolutely central to U.S. world leading science and ready to initiate construction

Linac Coherent Light Source-II: maintain LCLS leadership in ultra-short pulse science, broaden spectral range, increase average brightness, increase capacity, absolutely central to U.S. world leading science and ready to initiate construction

Next Generation Light Source: high rep rate soft x-ray source, could be absolutely central to U.S. world leading science and significant scientific/engineering challenges to resolve before initiating construction

Spallation Neutron Source Second Target Station: increase power beyond 2 MW, new instruments help with capability and capacity, important to U.S. world leading science and has scientific/engineering challenges to resolve before initiating construction, instruments need to be identified

Future light sources: absolutely central to U.S. world leading science, all options have significant scientific/engineering challenges to resolve before initiating construction, look forward to the BESAC workshop this spring

Discussion

If any BESAC or subcommittee member had a conflict of interest with a facility being discussed, those members were asked to exit the room during the discussion of that facility.

Dr. Max Lagally asked how presenters were chosen and how the presentations influenced the process. Dr. Barletta responded that every facility was invited to give testimony to the subcommittee. Invitations were extended to the laboratory directors and they could designate someone else. The nanoscale science research center directors were also invited. Each facility provided written material in advance of the meeting.

This charge is very similar to the Orbach facility prioritization process in 2003. The outcome from that process was a letter report. As in that case, the Director of the Office of Science is our audience.

The subcommittee expressed their support for the additional BESAC charge related to the next light source and will include a statement of enthusiasm in the subcommittee report. A new light source is important for U.S. competitiveness.

Dr. Bruce Gates asked if the subcommittee considered the holistic view of emerging and existing capabilities during deliberations. Dr. Barletta responded that yes, these were considered. Facilities tend to be nimble about what endstations can be built and users will

build where the science is. For the ultra-bright sources, endstations are expensive (~$10-20M).

For the National Synchrotron Light Source (NSLS), the current plan is to turn it off when NSLS-II comes online so the subcommittee rated NSLS as lower priority. Dr. Bruce Gates asked how existing NSLS users will be absorbed by other facilities. For users of VUV, ALS and NSLS-II were discussed as options. NSLS-II is working on a transition plan for users. Additional needs of specific user communities can be considered in the next BESAC charge on light sources.

Dr. Robert Dimeo stated that the U.S. has a significant capacity issue for neutron science. We are at ~35% capacity of Europe by instruments, publications, and users. There has been an explosion of research in macromolecular structures and dynamics and polymers. The Spallation Neutron Source Second Target Station is one opportunity to seize this opportunity. The High Flux Isotope Reactor (HFIR) could also do this with their cold neutron source and they have capacity for a second neutron source too. For HFIR, Dr. William McCurdy, Jr. pointed out that if we shut down a reactor source it'll likely be the end of reactor sources for our lifetime. This should be a strong statement in the letter report. There are the unique things that HFIR does, in addition to the needed capacity for neutron research. While this BESAC report focuses on the BES research at the facilities, the Director of the Office of Science is required to meet with other agency representatives.

Dr. John Spence asked where leading soft x-rays would come from if not from the Advanced Light Source (ALS). He noted that the best scientists will drive developments. Angle resolved spectroscopy instrumentation development is one area where ALS does well but it is highly competitive.

On the nanoscale science research centers, Dr. John Hemminger noted that some nanocenters had unique capabilities that don't exist anywhere else in the world. The Center for Nanophase Materials Sciences at ORNL was impressive but didn't have truly unique capabilities.

Dr. John Hemminger reiterated that this was the opportunity for BESAC to critically review the subcommittee's work. BESAC needs to approve the categorization for each facility and the process for writing the final letter report by the end of the meeting. We can circulate a draft for wordsmithing. BESAC agreed to socialize the categorizations and read materials overnight and vote the following day.

Public Comment

Dr. Michael Kreisler from NNSA asked how the subcommittee made its decisions. Dr. Hemminger replied that the subcommittee received written material from each facility addressing the subcommittee charge in advance and then heard a full day of testimony from each of the facilities before meeting in closed session to reach its conclusions.

With no additional public comments, Dr. John Hemminger adjourned the meeting.

Friday, March 1, 2013

Dr. John Hemminger, BESAC Chair, began the BESAC meeting began at 8:35 am.

Discussion of the Facilities Prioritization Charge

Dr. John Hemminger began the morning by reiterating that the text that goes with the recommendation in the report is very important. He elicited the help from BESAC members in drafting the letter report by the end of the following week. Drs. Bruce Gates, John Spence, Anthony Rollett, Douglas Tobias, Monica Olvera de la Cruz, John Tranquada, Gary Rubloff, William McCurdy Jr., and Max Lagally all agreed to contribute. Dr. Hemminger restated that the report will be public. Once it is submitted to BES, it will be posted on the BESAC website. Dr. William Barletta noted that facilities provide significant services for other (non-BES) users. These could be included in the draft report for the BES and Office of Science leadership.

BESAC reviewed the category assigned for each facility based on committee discussions:

- Advanced Light Source: important to U.S. world leading science
- Advanced Photon Source: absolutely central to U.S. world leading science
- National Synchrotron Light Source: lower priority for U.S. world leading science
- National Synchrotron Light Source-II: absolutely central to U.S. world leading science
- Stanford Synchrotron Radiation Lightsource: important to U.S. world leading science
- Linac Coherent Light Source: absolutely central to U.S. world leading science
- Spallation Neutron Source: absolutely central to U.S. world leading science
- High Flux Isotope Reactor: important to U.S. world leading science
- Lujan Neutron Scattering Center: lower priority for U.S. world leading science
- Center for Nanoscale Materials (ANL): absolutely central to U.S. world leading science
- Center for Functional Nanomaterials (BNL): important to U.S. world leading science
- The Molecular Foundry (LBNL): absolutely central to U.S. world leading science
- Center for Nanophase Materials Sciences (ORNL): important to U.S. world leading science
- Center for Integrated Nanotechnologies (SNL/LANL): absolutely central to U.S. world leading science
- Advanced Photon Source Upgrade: absolutely central to U.S. world leading science and ready to initiate construction with caveat on short pulse hardware
- Linac Coherent Light Source-II: absolutely central to U.S. world leading science and ready to initiate construction

- Next Generation Light Source: absolutely central to U.S. world leading science and significant scientific/engineering challenges to resolve before initiating construction
- Spallation Neutron Source Second Target Station: absolutely central to U.S. world leading science and significant scientific/engineering challenges to resolve before initiating construction. The write up should stress what capabilities will be improved in the potential suite of instruments, which is yet to be decided in consultation with the users. Since the specific instruments are not yet known, there could be scientific or engineering challenges related to them.
- Future light sources: absolutely central to U.S. world leading science and significant scientific/engineering challenges to resolve before initiating construction

Dr. Bruce Gates expressed his thank to the subcommittee. The discussions made him much more comfortable with the above decisions. Dr. Gates moved to accept the recommendations. Dr. John Hemminger asked for a show of hands on whether to accept the recommendations. There was full consensus. Dr. John Hemminger thanked Dr. Barletta for co-chairing the subcommittee. Dr. Simon Bare asked if the draft report will go to BESAC before submission to BES. Dr. Hemminger confirmed that the draft will go to BESAC for comments with a short turnaround time.

Dr. Ernie Hall noted that the electron beam microcharacterization centers were not included in this review. Dr. Hall asked how the e-beam facilities fit into the future plan. Dr. Harriet Kung responded that the TEAM project was regarded as a success. U.S. competencies in electron microscopy have been greatly increased. Since TEAM was completed, there has not been a concerted effort in looking to the next generation. We did receive funds for a TEAM-II project, but there were no successful proposals. Now that Dr. Jim Murphy is on board as division director for scientific user facilities, we should establish a roadmap for electron microscopy.

Presentation: Upcoming Committee of Visitors for the EFRCs/JCAP

Dr. Harriet Kung presented an update on the plan for the committee of visitors (COV) review of the Energy Frontier Research Centers (EFRCs) and the Fuels from Sunlight Hub, the Joint Center for Artificial Photosynthesis (JCAP). In addition, BESAC should expect a charge in the summer or fall to conduct another COV review of the Workforce Development for Teachers and Scientists program.

This will be the first COV review of the EFRCs and Hub. The COV process is not new; the first occurred in 2002. Past COV recommendations have addressed staffing, travel, and IT needs. The attention and support on these critical issues have been appreciated and helpful. Portfolio Analysis and Management System (PAMS) is one outcome, which is an exciting opportunity for us to take advantage of modern IT systems

The procurement process, monitoring, and management are different for the EFRCs and Hub awards. Both of these funding modalities have had a number of science reviews. The

COV will look at those reviews as well as the procurement process. The Batteries and Energy Storage Hub, the Join Center for Energy Storage Research (JCESR), will not be included in this review since the Hub was awarded in FY 2013. The COV covers up to FY 2012.

Dr. Kung expressed her appreciation that Dr. Persis Drell has agreed to chair the COV. Drs. Marc Kastner and Cynthia Friend will co-chair the EFRC panel and Dr. Michelle Buchanan will chair the JCAP panel. Dr. Drell will visit BES on March 15th to discuss the agenda and familiarize with the programs and process. Conference calls are expected in advance to prepare the panel chairs. The COV is schedule for Wednesday, May 29th, through Friday, May 31st.

Discussion

Dr. John Hemminger added that the summer BESAC meeting, July 25-26, will be important for discussion of two COV reports and discussion of the light source charge. Hopefully BES will also be able to share budget news.

Dr. Simon Bare asked if the COV will cover procurement and management of those that awards that were funded or also those that were declined. Dr. Kung replied that both are included. The COV will have access to all proposals (several hundred).

Presentation: Upcoming Committee of Visitors for the Scientific User Facilities Division

Dr. Jim Murphy presented an update on the plan for the committee of visitors (COV) review of the Scientific User Facilities Division. Much of the COV process was covered in Dr. Kung's talk. This COV charge covers all operating facilities, 14 construction and major item of equipment projects, and accelerator and detector research for FY 2010-2012. The COV will be held April 24-26, 2013. This will be the first all-electronic review.

Discussion

Dr. Beatriz Cuenya asked if COV members will see the previous COV report. Dr. Murphy responded that yes, it will be available, and it is also available on the BESAC website.

Dr. John Spence asked if it might be time to move the COVs from every three years to every five years. Dr. Hemminger responded that BES launched the COV process and it rotates every year among the three divisions. In the future, it probably doesn't need to be that way and the committees could be smaller. Dr. Anthony Rollett asked if the purpose is to review process and ensure that is being carried out in an equitable way. If so, we could have longer times between COVs unless there are external pressures such as Congress. Dr. Hemminger noted that COVs have been helpful with resource allocations.

Dr. Simon Bare suggested conducting the COVs every 5 or 6 years and cutting the review down to two days.

Presentation: SC Data Usage Update

Dr. Laura Biven, Senior Science and Technology Advisor in the Office of the Deputy Director for Science Programs, presented an update on the Office of Science (SC) statement on digital data management.

SC is considering what our responsibility is for data usage. An SC policy has been drafted. It is currently in draft form and is consistent with OSTP guidance. It takes into account advice from all of the SC advisory committees.

The SC policy is focused on digital research data, data sharing and preservation. The requirements are for principal investigators and research institutions.

In developing this approach, we wanted an SC-specific policy with flexibility for research communities to tailor the implementation. We wanted it to be consistent with Administration guidance, but not overly burdensome on our research communities.

The SC policy has three principles and three requirements. The requirements are that proposals must include a data management plan, all data in publications must be digitally accessible, and facility users should consult the published data policy of that facility.

The SC policy will be effective October 1, 2013.

Discussion

Dr. John Spence asked if the SC policy will include a specific format for the data or how long data must be available. Dr. Biven replied that those details will not be detailed in the SC policy. The data management plan included in the proposal will be reviewed. The SC policy does not say that data should be maintained indefinitely.

Dr. Beatriz Cuenya asked if there are any copyright issues. Dr. Biven responded that she understands that it is not an issue. Journals maintain copyright for the specific formatted publication. Dr. William Barletta added that supplemental data provided as a link is not copyrighted. However, if you expect the publisher to do work on that data you need to ask the publisher about copyright.

Dr. Anthony Rollett asked if there was any discussion about a situation where an investigator does analysis on a large data set at a user facility. Dr. Biven responded that the investigator should use judgment on the proposed data management plan and cost should be taken into consideration on what could be provided.

Dr. Simon Bare asked if consideration was given to international competitiveness. Dr. Biven replied that those questions have been considered, and the benefits are deemed just too great. It's the right thing to do for science.

Dr. Beatriz Cuenya asked how SC will ensure that principal investigators are complying. Dr. Biven responded that the data management plan will be reviewed or assessed during progress reviews or at the time of initial funding.

BESAC Light Sources Charge Discussion

Dr. John Hemminger began the discussion of the BESAC light sources charge. The charge is pretty broad charge and reference reports are listed in the charge letter. BESAC's response is due by July 15th. A workshop was proposed for the spring to address the charge. Dr. Hemminger asked if there were other suggestions for process.

Dr. William Barletta asked if there is provision for engaging non-U.S. participants. Dr. Hemminger replied that he is hoping to reach out to international attendees. Dr. Beatriz Cuenya suggested holding the workshop after the COVs.

Dr. Gordon Brown asked why the report is due so soon. Dr. Harriet Kung replied that the report delivery is carefully timed to match the budget formulation schedule. In the current climate, there is tough competition for precious resources which means we need a plan by the end of July to support our budget request.

Dr. Max Lagally asked about what the suggestions are for the next grand challenge in this area. Dr. Hemminger replied that the Next Generation Light Source is furthest along with mission need having been granted. Proponents for other opportunities may want to step forward as well.

Dr. Simon Bare pointed out that before you get bogged down in what machine is needed, we should think about the science that needs to be done. He suggested organizing the workshop where each particular field drafts grand challenge questions ahead of time and then discusses the capabilities needed to address them at the workshop.

Dr. William McCurdy Jr. asked what is necessary to make this process converge. He noted that a lot of this work has already been done. He suggested that we organize the workshop around the science case for each of the options that Dr. Jim Murphy presented earlier. That's well known. Discussions could focus on how close we are to being ready to build it, technical challenges. Over 2 days with 4-5 alternatives, we can focus on the comparison. Otherwise we are going to think about the science and not on the convergence of the process.

Dr. Barletta added that the set of possibilities could be ordered by flexibility and cost, for example, a rep rate of 10 kHz is different and less expensive with a different science case than 10 MHz. The scientists and accelerator physicists need to be coupled around the science.

Dr. Bruce Kay suggested include compact lights sources, compact storage rings, and plasma sources. Dr. Barletta countered that compact sources have limited capabilities and the intent here is to look at a world leading capability. We should focus on world leading science.

Public Comment

None

The meeting was adjourned at 10:14 am.