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

PUBLIC MEETING MINUTES

FEBRUARY 26 - 27, 2015

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

February 26 - 27, 2015
DOE BASIC ENERGY SCIENCES ADVISORY COMMITTEE
SUMMARY OF MEETING

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) was convened on Thursday and Friday, February 26 - 27, 2015, at the North Bethesda Marriot Hotel and Conference Center in North Bethesda, MD, by BESAC Chair John Hemminger. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act. Attendees can visit http://science.energy.gov/bes/besac/ to learn about BESAC.

Committee members present:

John Hemminger, Chair	Roger French	Mark Ratner
Simon Bare	Bruce Gates	Anthony Rollett
William Barletta	Ernie Hall	Gary Rubloff
Gordon Brown	Sharon Hammes-Schiffer	Maria Santore
Sylvia Ceyer	Bruce Kay	Matthew Tirrell
Yet-Ming Chiang	Max Lagally	Douglas Tobias
Frank DiSalvo	William McCurdy, Jr.	John Tranquada

BESAC Designated Federal Officer:
Harriet Kung, DOE Associate Director of Science for Basic Energy Sciences (BES)

Committee Manager:
Katie Perine, DOE BES

THURSDAY, FEBRUARY 26, 2015

WELCOME AND INTRODUCTION

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) was convened at 8:20 a.m. EST on Thursday, February 26, 2015, at the Bethesda North Marriott Hotel and Conference Center by BESAC Chair **Dr. John Hemminger**. Committee members introduced themselves. Dr. Hemminger reviewed the agenda.

PERSPECTIVES ON SCIENCE AND ENERGY IN THE U.S. DOE

Dr. Lynn Orr, Under Secretary for Science and Energy, U.S. Department of Energy (DOE), highlighted the value of BESAC to the DOE and U.S. Federal government.

DOE is focused on climate and energy challenges. There is no shortage of primary energy sources to include sun, wind, geothermal, fossil fuels, and nuclear sources, but the conversion into energy services is what it is all about. The energy system takes a primary source and extracts energy services and waste heat. This needs to be done more efficiently to minimize waste heat. The President understands this and has committed the Nation to reducing levels of greenhouse gases by 2025.

In recent years, the DOE Secretary restructured the science and energy programs. Orr is responsible for both and is looking for appropriate links between the fundamental science and applications. Examples of this are well known and show the benefits of solving specific problems in the energy sector. The idea of a fully-stocked portfolio is important and should foster productive conversations. BESAC has contributed to this and influenced DOE.

Over the past year, DOE has worked to present a budget that represents cross-cutting teams in areas that demand cross-agency, lab and university program expertise, and are useful ways to bring people together as DOE strengthens underpinning disciplines.

Orr mentioned the Quadrennial Technology Review that is looking at the status of technologies and areas of research across the energy landscape.

DOE has been experimenting with formats for research. Examples are the Hubs, Energy Frontier Research Centers (EFRCs), the Advanced Research Projects Agency – Energy (ARPA-E), big science facilities, and individual investigators that expand DOE's portfolio and bring people together in productive ways.

Relating to the FY 2016 budget request, the Office of Science (SC) is the largest federal sponsor of basic research in the physical sciences. DOE supports about 22,000 researchers at 17 laboratories and 300 universities. The Presidential Budget Request includes $5.3B for SC, an increase of about 5 percent. DOE has support from the President and evidence of bipartisan support for research as an essential function of the Federal government.

BES is an appropriate sponsor of facilities and its record is good. The Secretary was at Brookhaven National Laboratory last week to dedicate the National Synchrotron Light Source-II (NSLS-II). Its will be a critical tool for materials science and other fields. The BES report on future light sources provided good guidance.

BESAC's vision is being translated to help push forward the Linac Coherent Light Source-II (LCLS-II). It will give unparalleled spatial and temporal resolution that will be useful in many ways.

Looking back at BESAC over the years, Orr recalled the many grand science challenge reports that show how much the science and energy landscapes have changed in that time. Wind deployment is up six-fold, solar photovoltaic prices are down about 80 percent, LED lighting technology is now commercially viable, and there are dramatic increases in battery costs. The electric vehicle did not previously exist, the use of coal is down, and natural gas use is up. Changes have been faster than the scale of the energy system might suggest. Major transitions in the energy systems of the world are nearing. It is also useful to reflect on work set in motion in 2001 when BESAC identified the fundamental 21st century challenges and an impressive range of disciplines and areas of research, many of which have advanced tremendously over that time.

Basic needs workshops fed in to the grand challenges workshop that fed into the ERFCs to address those challenges. DOE seeks to hold a competition every few years. Another model is the hub model. There are two BES hubs doing impressive things.

Discussion

Orr shared with **Hemminger** that there is potential for collaboration with the National Nuclear Security Administration (NNSA) to address fundamental challenges that cut across national security and environmental management. It would be useful to leverage expertise in national security laboratories in the non-classified world where appropriate.

Simon Bare asked about the interactions between labs and industry. **Orr** shared that an Office of Technology Transitions is being stood up to build productive relationships and streamline the ways that labs interact with industry. Around $20M per year will be used to promote promising energy technologies for commercial purposes. The technology commercialization fund operates as a tax on applied research. The office is being led by Jetta Wong, and the Secretary is very interested in this.

Anthony Rollett asked about engaging industry in basic research and pre-competitive arrangements. **Orr** noted that user facilities host many industrial users who have sponsored instruments and there is plenty of interaction. There is the CRADA mechanism (cooperative research and development agreement) for national labs, and opportunity to look at what has worked and been fostered. To change energy worldwide, laboratory capabilities need to be leveraged.

Max Lagally asked about the status of nuclear energy going forward. **Orr** sees the situations in the U.S. and worldwide as different. There was a long period where no new facilities were started. The U.S. has four in various stages that are going forward. Cost is an issue in the competitive landscape. There is an important role for base-load low-carbon electricity generation. The spent fuel issues have not gotten simpler. Yucca Mountain has proponents but the Blue Ribbon Commission report concluded that DOE would not make progress without moving to a consent based approach where local residents are drawn into the conversation early. There is some money in DOE's budget request to explore interim storage and to consider a separate facility for highly-enriched uranium from weapons research, separate from civilian spent nuclear fuel.

Bruce Gates noted language in BESAC reports that justifies basic research and asked how well SC is communicating that message. **Orr** shared that basic research needs continued promotion. SC highlights links from basic to application to show the public the value of basic research. He noted that many forget the application side when doing basic research. Discovery is important and SC should not give up on the idea that a fundamental investigation of the universe is essential. There is some support for that idea in Congress even with strong ideas about energy research applications and areas.

REPORT BY THE BESAC SUBCOMMITTEE ON TRANSFORMATIONAL OPPORTUNITIES

Hemminger and **George Crabtree** presented the draft report "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science." The subcommittee authoring the report is addressing a charge from the Director of the Office of Science asking for a progress update since identifying grand challenges in a 2007 BESAC report, new areas of research and knowledge gaps, an assessment of the balance of funding modalities, and areas of research that may not be adequately supported or represented.

BESAC responded to the last part of the charge independently in early 2014 due to a direct request from SC. Community input was generated through www.besac2014.com and the subcommittee is continuing to solicit and review input received through the site.

The draft report will be presented at a town hall session at the American Physical Society March Meeting, and Harriet Kung will share information at the American Chemical Society national meeting in March 2015.

The timing of the report is useful as SC begins formulating the FY 2017 budget.

The draft report describes the results that have been generated as a result of pursuing the grand challenges. The report also describes transformational opportunities.

Accomplishments since 2007 include the creation of the EFRCs, the SC Early Career Awards program, and Single Investigator and Small Group Research (SISGR) funding. The grand challenge report helped focus a lot of research in the community, and the research landscape has changed. Some of the transformational opportunities identified in the new report reflect the changes that have occurred and include new possibilities that were not clear at the time of the prior report.

One theme is control. **Hemminger** shared that researchers may think that we are in charge of the scientific revolution and have control over the rules of nature to control and invent things. That is an overly enthusiastic view of nature and life.

One grand challenge was the control of material processes at the level of electrons. Progress has been made in the areas of exciton fission, ultrafast multi-step catalysis, and multiferroic spin valves. The latter allows for influencing ferromagnetic or anti-ferromagnetic properties in a material. This material was predicted before being made.

A second grand challenge was designing and perfecting atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties. Progress has been made in areas related to the materials genome, directed self-assembly at a nano-level, and *in situ* characterization.

Emergent phenomena highlight the third grand challenge, asking how properties of matter energy emerge from complex correlations of the atomic or electronic constituents and how these properties can be controlled. Electronic liquid crystals, predictive vortex simulation, and charged polymers are areas of recent progress that hold the potential for new functionalities and applications.

Mastering energy and information at the nanoscale to create new technologies that rival living things was the fourth grand challenge. New molecular motors, folding polymers, and self-regulation are areas of recent progress. Thermal self-regulation can be achieved with catalysts in the ends of a material to stimulate an endothermic reaction when a material gets hot allowing the material to cool itself. It has the kind of level of complexity that is akin to what is seen in biology.

Unconventional precipitation, charge transfer dynamics, and the arresting of thermal runaway are areas of recent progress that highlight the fifth grand challenge, to characterize and control matter away from the equilibrium.

Hemminger presented a graphic that demonstrates the grand challenges and five transformational opportunities that can be explored. **Crabtree** described the transformational opportunities and how more than one challenge can contribute to and inform the opportunities.

One opportunity that has emerged since 2007 is mastering hierarchical architectures and beyond-equilibrium matter. Advances are needed in predictive models that allow for understanding non-equilibrium and excited states. The mastery of synthesis and assembly of hierarchical structure for multi-dimensional hybrid matter is another exciting opportunity. *In situ* characterization of spatial and temporal evolution during synthesis and assembly is complex and an area for discovery.

Another emerging opportunity is understanding defects in materials, including the critical roles of heterogeneity, interfaces and disorder. This area is important to better understand materials degradation and lifetime prediction, and the correlations of physical events to material degradation.

A third opportunity is harnessing coherence in light and matter. There were no free electron lasers in 2007 but now we can study electrons on ultrafast timescales to understand material function. There are also forms of matter than depend on. Quantum computing requires qubits and understanding that was lacking in 2007.

Two additional cross-cutting opportunities were identified. Revolutionary advances in models, mathematics, algorithms, data and computing allow for transforming science and discovery. The ability to simulate and measure something in a short timeframe allows for quicker analysis and confirmation of earlier predictions in order to develop new ones. Embedded within this opportunity is advancing theory to predict dynamic structures and understand how functionality occurs. Instead of designing materials, one can look toward designing for functionality.

A second cross-cutting opportunity is exploiting transformative advances in imaging capabilities across multiple scales. Multi-imaging and multi-mode imaging help us understand and control functionality.

The 2007 report identified a number of needs, including a more highly trained and diverse workforce. This need continues but with new knowledge about how to make this happen. The 2007 report also proposed the development of fundamental theory to nurture understanding leading to more effective research. A third proposal identified the need for a balance of funding, and support of experimental and computational facilities in particular.

Instrumentation and tools is a critical area that needs a strong commitment going forward. The development of mathematical and computational capabilities can advance discovery science.

Synthesis should be expanded to give more predictive capability. This requires embracing computational materials science, materials genomics and inverse design. Needed is a science of synthesis and the capability to match the magnitude and sophistication of our computational resources.

Human capital is an important area for advancement. When early career awards conclude, awardees need opportunities along the career pipeline to continue to grow. Networks of scientists are needed to meet the grand challenges, and connections to strengthen and foster the next generation of multi-lingual scientists are vital. Multi-lingual means transferrable skills across multiple disciplines.

BES should maintain a balanced portfolio of investments. Every problem should have the right team to go after it, meaning that hubs and centers should have the right expertise in specific areas of engagement to maximize their potential. Some may focus on specific areas while others can be large and span the range from initial experimentation to technology transfer.

NEWS FROM THE DOE OFFICE OF SCIENCE

Dr. Pat Dehmer, Acting Director, SC, shared that the SC Fiscal Year (FY) 2016 request is $5,340M, about 5.4 percent higher than FY 2015. The largest increases are in Advanced Scientific Computing Research (ASCR), the Scientific Laboratories Infrastructure, Safeguards and Security, and BES.

ASCR will pursue the development of exascale node technology and systems, and support the Computational Science Graduate Fellowship to fund a new cohort. BER requested a substantial $18.7M increase to pair experiment, theory, and computation for the development of new climate models for exascale computers. Nuclear Physics (NP) received an eight percent increase for research for high-priority research areas, the result of a deliberate attempt by SC to inject more funding into the NP research budget.

Dehmer shared the request based on six areas. Facilities for ASCR, BER, BES and HEP are operating at or near optimal. In construction, LCLS-II and other facilities are going well, and some sites are seeing upgrades. In Major Items of Equipment (MIE), BES continues the Advanced Photo Source (APS) Upgrade and NSLS-II Experimental Tools.

Dehmer commented on the draft BESAC subcommittee report. The five transformational opportunities are excellent and the topics are understandable.

The transformational opportunities "Beyond Equilibrium Architectured Matter" and "Beyond Ideal Materials and Systems" encompass the themes of the 2007 report, and seem to use the original ideas to form the recommendations therein.

The coherence transformational opportunity is highlighted by LCLS, dating back to its start in 2009. The discoveries since have been revolutionary, driving work domestically and internationally. These changes support the recognition of this theme.

The crosscutting transformational opportunity on mathematical, computational and computer sciences research are reinforced by SC's implementation of three computing facilities. All include upgrades over the next four years. Since 2007, the National Energy Research Scientific Computing Center (NERSC) has nearly doubled its petaflop capacity. Overall, SC is at a factor of 1,000 times more computing power than in 2007.

The crosscutting transformational opportunity on imaging is reinforced by the new capabilities coming online at NSLS-II. NSLS-II was first considered around 2005 and first light was achieved in October 2014. The recommendations in the draft subcommittee report are driven by the changes that have occurred since NSLS-II came online.

Dehmer is pleased with the topical areas and believes that they are the right ones. The report will push BES and cause dramatic changes. It will help justify programs and explain what is new.

Discussion

Gates asked if the sense of the acceleration of science comes across clearly in the current subcommittee draft report. **Dehmer** believes that it is clear and fits with the report even if words like acceleration or imperative do not garner attention in Washington D.C.

Ernie Hall asked if the draft report gave enough guidance on balancing funding modalities, as was requested in the charge. **Dehmer** is comfortable with the current description and the Secretary of Energy Advisory Board is also looking at this issue to guide balance.

Bare was pleased with the SC budget, but asked how BESAC can help the NSLS-II maintain progress on instrument build-out on a timescale that is amenable to meeting goals that support science. **Dehmer** urged that BESAC talk with **Harriet Kung** about putting the next instrument MIE for NSLS-II into the BES budget.

NEWS FROM THE OFFICE OF BASIC ENERGY SCIENCES

Dr. Harriet Kung, DOE, Associate Director of Science for BES, provided an update. Kung shared staffing changes to include **Tanja Pietraβ** starting as the Director of the BES Chemical, Sciences, Geosciences and Biosciences Division. A current opening is the program manager for facilities upgrades and MIE projects and another for geosciences.

The FY 2015 appropriation language included funding of $100M for the EFRCs, and funds for the Batteries and Energy Storage Innovation Hub, and the Experimental Program to Stimulate Competitive Research (EPSCoR). The appropriation confirmed the closure of the Lujan Neutron Scattering Center and supported the transition to safe storage.

The total budget for FY 2015 is $1,733M. BES has done well within the flat SC budget with an increase of $20M over FY 2014, yet total funding is $73M less than the FY 2015 request for BES. Bright spots in the appropriation include construction and instrumentation, with all projects funded at the request levels. Credit for this comes from prior BESAC reports.

In 2011 and 2012, we had ambitious research initiatives in the request that were not received well on the Hill. Appropriations for research have been flat in recent years. The request for facility operations has increased with growing discrepancy between request and appropriation levels. Construction requests and appropriation levels are aligned in 2015. LCLS-II has received strong support since the BESAC Light Sources report. Funding growth in BES can be linked to BESAC support and that of the community. One clear challenge is in the area of facility operations and the communication of lost opportunities when funding is inadequate. All of the areas that have been well-funded have strong strategic planning support, strong community support, and respond to clear and compelling needs. The past decade of BES research has captured the opportunities at the forefront of science. The new BESAC subcommittee report shows areas where BES can strategically move forward, retain an edge in Federal investment, and maintain pace against competitors.

The EFRCs underwent a recompetition in FY 2014 and a management review process for new EFRCs will be undertaken in 2015. The reviews will help identify effective practices to help maximize the EFRCs' overall scientific success.

The first term for the BES Joint Center for Artificial Photosynthesis (JCAP) will end in September 2015. It seeks to develop a solar-fuel generator. The latest review recommended that JPAC submit a renewal proposal and capitalize on its development of a prototype for producing hydrogen. The proposal was reviewed in January 2015 and an decision is expected in the coming months.

The Joint Center for Energy Storage Research (JCESR) has helped to advance energy storage science and created a new paradigm for battery development.

Kung introduced the Computational Materials Sciences effort in support of the Materials Genome Initiative. This will be a companion piece to the DOE's investment in high-performance computing hardware to provide materials-related software. The computational materials sciences effort will deliver research codes for the design of functional materials. The approach uses integrated teams. An FOA was posted in January 2015 with full applications due in April. The influence of a Presidential initiative has helped to support this new start. There is opportunity to accelerate the lifecycle from discovery through deployment at a much lower cost and harness the discoveries being developed by multiple teams. The strategic plan of the Materials Genome Initiative was released in December 2014.

The full funding requirement is an issue discussed at past BESAC meetings. Multi-year contracts of $1M or less must be fully-funded. Across SC, directors and program managers have tried to use all mechanisms available to maintain the overall quality and topical balance within portfolios, and not decimate the success rate. There has been a drop in the new grant success rate and renewal grant success rate over the past decade. The steady state is unlikely to come for several years. BES is working to ensure the strength of the overall portfolio.

One change noted for BES scientific user facilities is the merger of the e-beam microcharacterization centers with the Nanoscale Science Research Centers. This will provide some efficiency gains in user support and interface. All facilities are striving to provide excellent user support and more than 16,000 users were supported in FY 2014. The development of new capabilities and refurbishment of older capabilities is a priority for BES. **Kung** noted the industry partners who have benefitted from engaging facilities.

BES communication efforts are directed at the general public and the community. A new brochure document describes discoveries and critical areas of research. The research summary provides specific investment details.

The FY 2016 budget request is $1,849M, an increase of $116M over the FY 2015 appropriation. Highlights include an increase for the EFRCs of $10M, a new investment in mid-scale instrumentation for ultrafast electron scattering, and an increase of $4M for Computational Materials Sciences. FY 2016 funding will allow for facilities to operate at near optimal levels.

Construction funding has constrained the BES budget in past years. BES is managing the roll-off of projects and phase-in of new projects. In 2013, sequestration forced a five percent reduction. BES benefitted from a roll-off of NSLS-II construction which shielded research from the severity of cuts. The construction budget line of less than $150M is still troubling. BES hopes that FY 2016 will get closer to an optimal level of $250M.

The EFRCs are a very compelling investment for BES. In FY 2014, 32 EFRCs were funded via a very competitive review process. The EFRC competition was every five years but will shift to an every two-year review starting in FY 2016. A mid-term progress review will take place in FY 2016 and identify tasks that are maturing or under-performing. BES may use that funding for a FY 2016 solicitation. Topics for FY 2016 will be more focused and cover areas that may currently receive limited funding support in other areas of the portfolio.

Computational Materials Sciences funding in FY 2015 included $8M in new awards. The FY 2016 request of $12M will continue support for the 2015 award and support additional awards. The U.S. trails competitors in computational codes for materials discovery and engineering.

For midscale instrumentation, the FY 2016 request includes $5M to develop instrumentation to enable ultrafast electron characterization for BES chemical and materials sciences research activities. This is also an area that highlights the need for workforce training and ensuring support for instrumentation to enable scientific innovation.

The LCLS-II is the highest priority for BES and will reach its peak funding level in FY 2016 at $200M. APS-U is also underway and $20M is proposed for FY 2016 to support R&D, design and limited prototyping.

Kung summarized the FY 2016 President's budget request. BES hopes that further engagement with the community will result in intellectual support for all of the investments being made.

Kung highlighted work at Stanford University uncovering new states in single antenna protein molecules. The process devised a tool to detect transition states in the native environments of molecules. Another research example used diffraction and spectroscopy tools at LCLS to probe photosystem II and detected a transient state. At Brookhaven, a group has discovered through analyzing biomechanical pathways a link between lipid synthesis and degradation leading to an increase in oil content in leaves.

Materials science research at Sandia National Laboratories looked at exposing materials to different radiation dosage and studied the resultant stresses in the materials. This level of understanding is critical for understanding end of life conditions for nuclear reactors.

Another example of materials science research is in stress corrosion cracking. As a crack opens, there is accelerated diffusion along the grain boundaries. The results showed chromium depletion at the grain boundary. Insights inform ways to prevent stress corrosion cracking.

Another example is the work on twin-bunch two-color x-ray free electron laser at LCLS. This work is a demonstration of how BES can stay ahead of competitors and can push existing facilities both in hardware and software. The experiment was innovative as it showed how to generate a twin-bunch that are separated by five picsoeconds.

Kung thanked the subcommittee for its report and providing timely and compelling direction for BES and SC to chart its future. The report is part of community-based input on the direction needed and investments required.

Discussion

Kung shared with **Bill Barletta** that about 20 to 30 percent of facility users are students.

Sharon Hammes-Schiffer asked about the plan for EFRC FOAs. Will BES do a more specific call for topics in FY 2016, a more general call every four years, or just a call every two years? **Kung** shared that the goal is two equal sized cohorts rotating on a regular basis but that the decision is driven by available funding. Growing in the second partnering years would make the transition easier. A few cycles may be needed to reach this equilibrium.

Yet-Ming Chiang asked if there is a good balance between the number of proposals and funding levels requested, noting that university departments are driven by funding. **Kung** shared that BES has more meritorious proposals than it can support. The only data that shows a link between funding received and future employment comes from the EFRCs. One indicator of demand could be the number of proposals received over time and success rates. BES has not seen a decrease in the number of proposals overall in its core program.

Kung told **Hemminger** that the number of white papers received are procurement sensitive.

Kung told **Rollett** that it will take about five years for forward funding of proposals to work through the system. There should be some relief in FY 2015 and she is encouraged by BES' funding numbers but things could be painful in the next few years.

Gates wondered if researchers who are not funded have the resilience to stay in the field, noting the loss of a generation amidst current fiscal challenges. **Kung** hopes that her presentation of full funding data will calm some and acknowledged that the overall funding constraint is a concern, especially with the chance of sequestration in FY 2016.

NSLS-II UPDATE

John Hill, Director, NSLS-II at Brookhaven National Laboratory, described the vision for NSLS-II: to be the brightest synchrotron in the world; enabling world-leading programs in imaging and dynamics with unprecedented resolution; and providing impacts in condensed matter physics, materials physics, chemistry and biology. The vision highlights imaging, dynamics, and synergy as key strengths of NSLS-II.

The NSLS-II is a 3 GeV machine. It contains damping wigglers. The bright beam in NSLS-II enables understanding the complexity and dynamics of materials with self-organized phases through to intrinsically heterogeneous systems. The facility can also look at *in-operando* or real life scenarios with sample cells that can be used on different beamlines or instruments. These capabilities provide for a wide impact across a range of fields.

The construction of NSLS-II is now complete after 10 years of work. An independent scope review in December 2014 ensured that all promised deliverables were met. A review for CD-4 was completed in early February 2015. Secretary Moniz joined a dedication ceremony in February.

The accelerator is performing well and has provided 1,300 hours of operation to date. Insertion devices have been commissioned and front-ends are conditioned for 50 mA operations. Horizontal beam emittance has decreased to less than 1 nm-rad and has demonstrated excellent stability.

The NSLS-II will ramp up to 300 mA by the end of FY 2015 and near 500 mA by FY 2017. User hours will also increase from 2,087 to 3,517 over the same time.

There are seven project beamlines that have been delivered as part of the construction project. Each are being commissioned and will be commissioned for 25 mA operations. The technical commissioning of the beam line is progressing with early users taking place this week.

The first spectroscopy data was attained at NSLS-II in November 2014 and diffraction data by December. Benchmarking measurements have been conducted on reference samples. NSLS-I and II comparisons have been conducted and show II's superiority and quality.

Coherence and stability have been tested. Hill showed an image of a butterfly antenna taken at about 1.5 microns to shown clarity and definition. An image was taken of a metal oxide to show a speckle pattern rather than a broad spot. These results indicate that the beam and accelerator are stable.

The schedule for the coming months will include a shutdown around May through July. The first real general users will begin their work around the end of the summer in 2015.

The user program is open and proposals are being accepted. Eighty-one proposals were received for the first run. Hill is working to create the expectation among users that the beam is just getting underway.

One of the first experiments looked at dynamic mesoscopic electronic phases to study the physical properties of complex oxides. Other experiments are combining techniques. One is a correlative experiment with photons and electrons. The SRX beamline will be used for an experiment looking at catalytic mechanisms in a micro-cell in operando.

Five years from now, the NSLS-II aims to support a robust, diverse user program as a world-class synchrotron with bright stable beams. Its focus will be on imaging and dynamics with an impact on energy storage, catalysis, materials problems, and life sciences. NSLS-II will develop next generation data management and analysis. By 2020, NSLS-II will host 28 operating beamlines.

Future experiments over the next year include understanding electronic correlations in the cuprates. One challenge is storing the data from experiments and the ability to do analysis. New York State has committed $15M to support data management.

Looking ahead, one challenge is to transition from construction to full operations and to build a thriving, robust user science program.

Discussion

Gary Rubloff asked is the facilities and the other synchrotrons will emphasize *in situ* synthesis. **Hill** confirmed that this a big trend now and experimentation is planned.

Hill confirmed for **Max Lagally** that NSLS-II will emphasize imaging, dynamics, and inelastic scattering. He wants to grow the community and attract more and new users. They are in early discussions about a guest house for visiting users.

SOFT X-RAY WORKSHOP REPORT

Roger Falcone, Director, Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory, described the Soft X-Ray Workshop held in October 2014.

The discussion noted that coherent soft x-rays were important to research. Soft x-rays are differentiated from hard x-rays by talking about electrons, chemical bonding, the electronic structure, and how magnetism works. At times, the areas overlap and all light sources have a range of capability to address research needs.

In the light source areas, there are synchrotron rings and linear devices such as FELs. There is a complementary nature between the two.

BES supports four synchrotron ring x-ray sources. There is overlap in the science that each provides and yet each has distinctive capabilities. Each source has distinct characteristics, range from 2 GeV up to 6 GeV, so there is a factor of three differences in the electron energy that comes out. The spectrum is different and this defines the centroid of the peak performance of each facility.

Brightness and coherence are enabling properties. Brightness is a well defined physical parameter, and can be thought of as temperature for an equilibrium system. A laser has great surface brightness. Coherence, specifically transverse wave coherence, has uniformity in its wave front. A laser generally produces uniform wave fronts resulting in laser “speckle.”

Brightness and coherence have increased by many orders of magnitude over the past decades, as much as 10 orders of magnitude per decade. Looking at coherent x-ray sources of the future and at the spot that comes out of the light source, the goal is a point source.

The fundamental limit of source size and divergence depends on the wavelength of light. Diffraction-limited storage beams have circulating electron beams small enough that the spot size and divergence of emitted x-rays are dominated by the fundamental diffraction of light, and not by the electron beam. The technology that enables this is multi-bend achromat magnets. More magnets and bends lead to more highly coherent beams. A less coherent beam can’t be focused to a tiny spot. Coherent waves lend you to the tiniest spot possible. The challenge is that sample damage can occur.

Soft x-rays let us light up any element in the periodic table. We can probe the valence band where the chemistry is occurring. Resonances can be seen with each element but are less visible with the heavier elements.

The workshop held in 2014 looked at unraveling phenomena in condensed matter, including interactions between different degrees of freedom, charge, spin, orbitals and lattices. Charge is the key in a transistor. Spin and charge are important for magnetic properties. Topological insulators cover spin, charge, and orbital coupling. Thinking about spin, charge and lattice informs thinking about superconductors. Condensed matter physics looks at couplings in all of these different degrees of freedom. Soft x-rays are a useful probe to sort out various couplings.

The charge for the workshop to consider transformational research opportunities possible via storage-ring-based, ultra-high-brightness soft x-ray beams. Soft x-rays will enable frontier science in materials and energy.

Probing deep in to the nanoscale will allow for moving move beyond current measurement limits. Another challenge will be working with inherently heterogeneous materials. Coherent scattering allows for this work. Heterogeneous materials benefit from the coherency of the light. The high brightness beams would allow us to probe natural or spontaneous dynamics. All of these challenges benefit from higher coherent flux and soft scattering of x-rays.

The workshop identified six scientific opportunities that can have societal impacts to include enabling directed chemistry, materials to enable low power processing, and the ability to address global biological and environmental challenges.

One of the first of the six opportunities is imaging spatiotemporal catalytic correlations. With the revolution possible with soft x-ray experimentation, multi-center catalysts that achieve efficient synthesis could benefit from in situ tools with chemical specificity and spatiotemporal resolution to understand kinetic correlations in heterogeneous catalysis.

Another challenge is looking at transport across complex interphase regions. There was discussion of surface chemistry in aerosols, and imaging intercalation in battery electrodes. These opportunities share common needs such as *in operando* analysis tools with chemical contrast to probe nanoscale transport. The coherence soft x-ray rays can make movies of the system that can enable understanding.

A third challenge is imaging low power charge and spin processing. One area of interest were skyrmions that are nanoscale spiral spin textures for low power memory. Another are memristors that provide a platform for 3D high density digital memory and low power neural processing.

The fourth challenge was imaging complex electronic textures and symmetries. There is a desire to identify band gaps in materials down to the few nanometer scale, and create nanometer spatial resolution. Strengths of soft x-ray are high coherent flux and emerging diffractive optics enables soft x-ray spectromicroscopy with low-nm spatial resolution.

A fifth challenge was the ability to probe soft (low energy) modes to optimize functional systems. Probing the crossover between dynamic and kinetic regimes can be understood through the use of coherent soft x-rays. Looking at systems is a great challenge.

A final challenge discussed was imaging functioning biopolymers and biopolymer complexes. It looks at coupled membrane-protein motion through small angle scattering. The field is gaining in importance.

One example of work being done is 3D imaging of particles to create a chemically-resolved particle map at 18 nanometers resolution.

RIX spectroscopy is strengthened by the use of brighter and brighter sources, opening up the possibility for looking at a variety of angles and wavelengths. The result can be an increase in throughput with multiplex detection.

This science is being advanced internationally. People are upgrading to brighter sources. NSLS-II is a bright source. Other sources are the MAX-IV in Sweden and SIRIUS in Brazil, which are 3 GeV rings coming online in 2016. Upgrades are thought of as more effective options as new facilities are expensive to build. Every synchrotron ring globally is driving toward brighter sources with greater coherence.

Discussion

Lagally asked if one could do Raman spectroscopy with such a machine. **Falcone** shared that RIXS increases the scattering process to allow for the right sources. There are higher order Raman effects that probably will not happen at synchrotrons but are being pursued. At the milli-volt level, this might be more interesting.

Bill McCurdy noted that the workshop examples did not show multi-pulse spectroscopies superimposed on the pulses from the synchrotron. He wondered if a coherent source with a diffraction limited upgrade and the advantage of doing this at that type of facility. **Falcone** shared that they deferred ultrafast measurements to FELS. The interest here is focusing on *in situ* spectroscopies, specifically. At higher pressure, the higher brightness source can support gas-solid interface studies.

McCurdy asked about fourier transfer spectroscopy and **Falcone** shared that the mirror would need to be moved a little translationally. Scanning is still easy if stability is maintained.

Hemminger noted that the U.S. synchrotron user community has experienced recent trauma with the shutdown of NSLS prior to NSLS-II coming online. What would be the downtime for an ALS upgrade? **Falcone** shared that the shutdown at ALS while upgrades are occurring would last about one year. The European Synchrotron Radiation Facility has received funding and upgrades should be complete by 2020.

DISCUSSION OF THE BESAC SUBCOMMITTEE REPORT

Hemminger shared suggestions received on ways to improve the report Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science.

BESAC discussed the five transformational opportunities. The opportunities listed are fine but are not necessarily explicit to readers in the report's current form.

The term "transformational" is not necessarily clear or well-defined. A lesson from industry is that advancing work relies on taking the best from pure science and making it useful, hence the use of the term "transformational."

McCurdy felt is what striking that there is a focus on materials yet molecular aspects are ignored particularly in the first two opportunities. Chemistry was the start of the nanoscale revolution and self-assembly. The challenges are all chemistry and yet are not presented that way. Synthesis is listed as an urgent need, as an example, yet only looks at things from a materials aspect. **Hemminger** agreed and noted that this will be updated in the report.

Gordon Brown recalled a quad chart on synthesis that does not appear in the report, and recommended revisiting the 2007 report as it effectively addressed synthesis.

Lagally suggested dropping "beyond equilibrium matter" and focusing on synthesis instead.

Maria Santore suggested that there are other ways to manipulate matter and many words tied to synthesis. She asked if the five opportunities are the right ones, noting that the differentiation or relationship between the previous five challenges and current ones is unclear. **Hemminger** noted that this can be clarified in the introduction.

Hemminger shared that SC and Dehmer are the first audiences for the report. BESAC should agree on the science and that the report is a good tool for SC. Dehmer likes the current draft. The Grand Challenge portion can be a separate insert that allow for those interested in a technical document to review the Grand Challenges to read more. **Hemminger** shared that the report needs additional editing.

Roger French noted that the synthesis was addressed in the Grand Challenges report and that the subcommittee felt that it did not need to do this again. There are overarching things in the new topics and the new report.

Doug Tobias shared that the report should highlight fields' status and move the Grand Challenges to the front to set the context. **Hemminger** noted that the charge asked for updates since the 2007 report. The subcommittee felt that putting updates and progress reports at the end felt like giving them short shrift. He noted that the executive summary could be redone to give a short recap of the challenges.

Barletta supported the idea of including synthesis. He also noted the opportunity to integrate multiple advances to create new imaging and visualization techniques.

Barletta suggested writing the executive summary in plain language.

Chiang asked about the distinction between beyond equilibrium and non-equilibrium. **Hemminger** shared that they are the same thing.

Ernie Hall shared that opportunity two is the most relevant to the charge received. The first is contained somewhat in the 2007 Grand Challenges. He asked about elevating tools as opportunities. Tools include models/math, imaging capabilities, and even coherence.

Simon Bare commented that the report does not address changes to the landscape since the 2007 report. It should explain why things are so different now and why the new report is needed.

Bare added the the first cross-cutting opportunity as expressed does not say what will be done in that area. It needs a verb in the title. **Hemminger** noted that it should start with active verbs like the other opportunities.

Gates commented that "acceleration of science" is a key phrase. Dehmer used this in her talk but it is not in the report and it should show that science has accelerated.

Lagally warned not to suggest that something is new that is not new. Beyond equilibrium is not new but the acceleration is new, as is doing more and doing it better. **Hemminger** added that that could be said about the prior report. It is a matter of the choice of words.

McCurdy offered that "why now?" should be asked with each opportunity and seems to be missing. The third opportunity speaks to coherence in light sources and was voiced by Dehmer. It is an essential thing that has happened, with coherence in condensed systems as an example. **McCurdy** noted that computing has grown in the past 15 years and not just in hardware, with theory and the impact of the accessibility to large-scale computing codes as an example. This aspect should be cross-cutting as it touches many disciplines. The fifth opportunity speaks to imaging and progress could be addressed by a collection of good examples such as imaging of vortices in helium droplets.

Frank DiSalvo added that it might be sensible to say that synthesizing materials is hard to do and that there have not been advances in the field of synthesis especially in branches of chemistry that are not molecular. It is hard even when making a stable material. The tools are lacking even though there are things in nanoscience that address this. **Hemminger** agreed noting that there is success in some areas of complex materials synthesis and directed self-assembly.

Lagally suggested thinking of synthesis in a broader sense and the assembly of things that are mesoscale or higher. All of these hierarchical structures are forms of synthesis.

Gates urged talking about synthesis beyond what is covered in opportunity two. Control of defects and interfaces is needed.

French noted the need to get a larger view of what is happening. The tree graphic shows how the first two opportunities are beyond, that the third exists, and that the cross-cutting opportunities come from these advances. **Hemminger** noted that the graphic was meant to be an evolutionary device. We can modify some concepts and the words.

McCurdy added that moving synthesis up in the discussion and out of the last chapter creates a hook for chemistry and springboard for the first two opportunities. **Hemminger** shared that one mistake of the draft is that the synthesis concept is not integrated in all the chapters. Synthesis is not the only thing in chemistry, but the report needs to include more of it. **Hemminger** shared that the word "mastering" in opportunity one was a replacement for synthesis that sounded better and a lot of what that is about is the hierarchical ways to make these things.

Rollett noted that the grand challenge on synthesis is an enduring challenge.

Gates voiced earlier comments about synthesis being a big challenge and being careful to avoid overextending the opportunity beyond what can be accomplished. Failing to show the essential need for synthesis skills means promising research in ways that cannot be sustained. **Gates** clarified that we need to include synthesis and emphasize the magnitude of the challenge.

McCurdy noted that this changes the emphasis of the report and not just the details.

DiSalvo added that there are characterization tools but nothing to study. Investment in tools is enormous comparable to investment in synthesis.

Crabtree shared that synthesis was shown as a gap in 2007 and asked what opportunity exists now to make synthesis better than it was. **DiSalvo** proposed asking the community.

Ratner shared that synthesis was listed as a grand challenge in the last report, and that it cannot be put into a box. The draft seems to talk about synthesis in sidebars or in every chapter. **Hemminger** commented that it would be interesting to expand where it could be described.

French added that synthesis should be throughout the report, believing that the first opportunity is about synthesis and function.

Hemminger shared excitement about noting the making of things throughout the report.

Bare noted success in synthesizing materials but a lack of the functions needed in the synthesis. The report could emphasize synthesizing the functions that are needed.

John Tranquada read many of the opportunities as inclusive of far-off ideas that may not happen soon and that fit the grand challenge concept. The former challenges were very inclusive. He would be concerned if the new things mentioned in the current draft are the only new things and opportunities that are expected. Getting too detailed might get away from being inclusive of many opportunities that should be cited. **Hemminger** responded that this comes back to how the report will be used. BES urges principal investigators to read DOE reports and their proposals should be responsive, in some sense.

McCurdy moved to approve that BESAC is comfortable with the five opportunities in the draft report. The move was seconded and BESAC approved the motion with none opposed.

Hemminger shared that Dehmer was not pleased with the chapter on enabling success, adding the need to limit the number of items to emphasize specific things. He asked if there are things missing from the draft.

McCurdy commented that BESAC has never talked about the principles of investment in the portfolios. Prior reports discussed core programs and research but do not identify that core research is done differently in DOE compared with other agencies. DOE program managers have a strategy. BES is a steward of facilities that support research for DOE, other agencies, and industry. BESAC frequently skirts the education mission, but we steward the people who work in these areas.

McCurdy suggested not skirting whether the research should be at a particular level and urged making maps of the strategy or investment for a long march. **Hemminger** suggested not writing a report that is counterproductive. Writing about an educational mission would not likely be damaging but if Congressional leadership felt that DOE should not be involved in education then they could be displeased.

DiSalvo commented that the report should address how DOE is doing things right rather that how it is different from other agencies. He added that discussing workforce development rather than education is the right approach and terminology.

Hemminger asked for feedback on the concept of stimulating instrumentation science. This resonated well with attendees of subcommittee meetings. There could be a supplemental funding program that supports building new instruments, coupled to research. It shouldn't be a new call for proposals specific to instrumentation development.

Sylvia Ceyer supports the idea but is afraid of calling it a supplement. DOE should value instrumentation development and give it time to be developed within the whole proposal.

Barletta urged describing the science that needs to be done first then building the tool, rather than building tool first. Instrumentation development on its own ends up second or third place. The goal needs to be to try and solve a hard scientific problem.

Chiang suggested shifting focus in chapter five to current knowledge rather than past history. **Tobias** added that material could be shifted and put at the end of the current chapter five.

Tranquada cited a concern about the sustainability of scientific programs where new core research funding is only in EFRCs. These basically support students and postdocs but may not be the only thing. **Hemminger** agreed that this is not sustainable and mentioned comments from SC and BES that research funding should be kept at 40 percent. **Kung** added that there is a portion within that that supports the researchers. There is concern about conveying that the EFRCs only support students and postdocs, and that is not the intent. BES wants to support a sustainable portion of a PI's time. This is a dynamic balance and BES needs to work with PIs to establish that balance. The new report proposes a compelling agenda for materials sciences funding and can be presented to the community to catalyze growth.

Hemminger asked BESAC to consider the amount of time that they could devote to revising the report between now and the publication of the report in June 2015.

PUBLIC COMMENT

None

ADJOURNMENT

The meeting was adjourned by **Hemminger** at 5:08 p.m.

FRIDAY, FEBRUARY 27, 2015

The BESAC meeting was convened by **Chair John Hemminger** at 8:07 a.m. EST.

PRESENTATION OF THE SPALLATION NEUTRON SOURCE

Dr. Paul Langan, Associate Laboratory Director, Neutron Sciences Directorate, Oak Ridge National Laboratory (ORNL), gave an update on the Spallation Neutron Source (SNS). ORNL runs two advanced neutron scattering user facilities, the High Flux Isotope Reactor (HFIR) and SNS. SNS operated at world-record power levels in 2014.

Users conduct high-impact science due to the unique qualities of neutrons. They are a highly complementary probe to others such as photons, able to differentiate between isotopes allowing for the study of systems. Their energies are well matched to study the dynamics of materials. Neutrons have spin and are sensitive to magnetism which is important for the study of superconductivity.

One study at ORNL examined the suppression of thermal conductivity in SnTe and PbTe. Both are highly efficient thermoelectric materials. Results suggest that new materials could be designed with nested phonon dispersion through doping.

ORNL is investing in data analysis and modeling for real time analysis and feeds instantaneous decision making while the experiment is being conducted. Computing capabilities and visualization are essential to the scientific process at HFIR and SNS.

Researchers have identified evidence for fluctuating charge-stripes through inelastic neutron scattering experiments at SNS. Results verify the existence of new physical phenomena in matter that may play a role in superconductivity.

Recently, nanothreads were synthesized from benzene under pressure at room temperature and found the structure to be diamond-like. This shows the potential for discovering a new class of tunable nanomaterials, and opportunities for industrial applications in transportation or aerospace manufacturing.

Researchers from the Center for Nanophase Materials Science studied the optoelectric properties of polymers for photovoltaic devices. The studies exploited isotopic substitution to probe the difference between materials. Neutrons are good for studies of soft matter.

Neutrons can visualize hydrogen atoms to see the chemistry in biological structures. The enzyme DHFR has been studied for decades and this technique allowed for mapping of the enzyme's mechanism.

The number of instruments available to users has doubled and yet the facilities are still oversubscribed at a rate of two to three times capacity.

Neutron sciences is positioned at ORNL in anticipation of future needs. Recent reports describe next generation science and reflect recent workshops held at ORNL. Significant technical and conceptual advances are needed to meet the challenges described in the reports.

Multidisciplinary teams are working to develop and demonstrate the capabilities required. These include higher flux on sample, improved detectors, polarized beams, and computation. These are described in the document "Emerging Instruments for Next Generation Science."

The second target station (STS) would deliver transformative capabilities for complex and mesoscale systems. Building on community engagement and the advent of a strategic science plan, ORNL's vision for advanced neutron scattering has taken shape.

Maximizing resources and the impact of HFIR and SNS is part of the near-term focus. Long-term focus is on developing a second target station at SNS to double capacity and expand capabilities by two to three orders of magnitude.

Discussion

Langan shared with **Rollett** that future work in scattering will provide real time analysis as data is collected to advance decision-making.

Gates asked about the study on DHFR and what new information was obtained from the neutron experiments. **Langan** explained that the experiment allowed the researchers to observe the transfer of hydrogen between cofactor substrate solvent and enzyme. High resolution x-rays were used, but researchers were unable to identify where hydrogen atoms were bonding. Finally, users were able to answer specific questions about protonation. The neutron crystal structure was collected as well.

Langan told **Hemminger** that other ORNL divisions are involved in SNS. There are several directorates and each has control over their LDRD budget. ORNL can be a leader in soft matter and related biosciences.

Langan described the STS for **Hemminger**. SNS has a high repitition rate and is optimized for high energy or small wavelength neutrons. STS will be optimized for long wavelengths and extends the reach of neutrons into complexity. The STS was planned in the original SNS design.

Hall asked about the time frame for STS construction and if it might disrupt SNS operations. **Langan** shared that the STS will take six to seven years to build. Most of the construction can be done without impacting SNS. The accelerator tunnel will be built to accommodate extra cryomodules. SNS might be down for about 6 months to knock through some walls.

Bare asked where SNS and STS fit in the global landscape of neutron sources. **Langan** shared that in Japan there is a complex with a neutron scattering facility that will reach 1 MW sometime this year. It has a lower frequency and will be highly competitive to ORNL's work in complex soft matter. A source is being built in Sweden with a long pulse length that will deliver neutrons in 2019. It will compete on complex systems. One important parameter for all is the peak flux.

Langan told **Tobais** that ORNL has tried to stay at its goal of 1.4 MW operations.

UPDATE ON COMMITTEE OF VISITORS FOR THE MATERIALS SCIENCE AND ENGINEERING DIVISION

Linda Horton of DOE described the Committee of Visitors (COV) that will take place in March 10-12, 2015 in Germantown, MD. The COV will be chaired by Gary Rubloff and will consist of 17 members.

This will be the fifth review of the Materials Science and Engineering Division (MSE). The top recommendation from COVs since the beginning of the process is how the reviews are conducted. SC now uses the Portfolio Analysis and Management System (PAMS). The COV process will be conducted using folders assembled from electronic or scanned information. There is a PAMS module that will be available for a future COV that will facilitate electronic review.

The COV will examine the MSE processes used for the laboratory and university programs to include applications and funding, the DOE EPSCoR Program, and the FY 2012 Ultrafast Materials and Chemical Sciences Funding Opportunity Announcement.

This COV will look at the MSE core program and not include other MSE investments such as the EFRCs. Horton reviewed the agenda developed by Chair Gary Rubloff

Discussion

Horton commented that moving to an electronic process has not been routine. The COV will be able to see subsets of folders from specific programs, and then be able to dig deeper as desired. BES will discuss the impact forward funding.

Horton noted that one variation for this COV will be the electronic review of laboratory files. All files will be on the same computer.

UPDATE ON THE BES NANOSCALE SCIENCE RESEARCH CENTERS

Jeff Neaton, Director, Molecular Foundry, shared an update on the five BES Nanoscale Science Research Centers (NSRCs). The facilities are eight to ten years old and one of the outcomes of the National Nanotechnology Initiative.

Staff spend about half of their time doing research to bring about new capabilities for users. The other half is spent working with users. The NSRCs are a uniquely collaborative environment that is a model for other research centers. As an example, the CAMERA activity is being developed based on this model.

Users are domestic and global. Sixty-one percent in FY 2014 were from academia; 38 percent were faculty or research scientists.

Cumulative FY 2014 funding for the NSRCs was around $100M. In 2014, more than 1,600 proposals were submitted with 2,243 users and 1,256 publications. Thirty-one percent of all publications appeared in high-impact journals.

The creation of peptoid polymers is one example of research taking place. Peptoids can be stitched together into polymers. They represent a new class of materials that is attracting user interest before it is widely available. Users have used these new materials in new applications. Theorists are also interested, and developed a force field for them.

Another example is a new way to do atomic force microscopy by driving the tip at multiple frequencies at once which allows for scanning over a substrate and staying on resonance in real time. A user looked at $LiCoO_2$, as an example, and could see where all of the lithium ions were. This instrumentation development is patented but currently found only at the NSRCs.

Users come to the NSRCs to find capabilities that cannot be found elsewhere and to access new communities that are developing novel instrumentation and new ways of doing synthesis. An example is a user that worked with two centers to discover a novel form of porous carbon with high supercapacitor performance.

Research conducted at the NSRCs was highlighted by the President's Council of Advisors on Science and Technology in their 2014 report on the National Nanotechnology Initiative. This work was published in Nature magazine.

The Centers are a multi-disciplinary research venue. There are many scientific and technical challenges that require this approach with input from multiple sciences, synthesis, and characterization to include imaging and spectroscopy, and advances in theory in a coordinated manner. All of these areas are housed within each of the Centers. There is also access to supercomputing.

Each Center is unique due in part to their co-location with other facilities and the expertise within each. When a user applies for time at an NSRC they can apply to do work at a co-located facility at the same time.

The NSRCs have merged with the Electron Microscopy Centers. This creates greater opportunities for users and expands operational efficiency through things such as a single proposal process. BES has recognized the need to take the next step in electron scattering, and organized a recent workshop in that area.

The National Nanotechnology Initiative Strategic Plan published in February 2014 proposes promoting broader accessibility for users and utilization of facilities, as well as driving greater connectivity with industry. In 2014, the NSRCs interacted with 45 companies who are doing public domain research that also feeds back into their own R&D.

Each NSRC has a publicly-available five-year strategic plan, and a budget review process is being done. The initial investments from 10 years ago are prompting the need to think about the renewal of instrumentation. There are strategies designed to leverage current resources but other aspects that will need new funding.

Even with these challenges, each NSRC is rolling out new capabilities and the investments of the past 20 months are bearing fruit. New investments include joint beam lines and advanced lithographic techniques.

Discussion

Brown asked about funding difficulties from some years ago at NCEM. **Neaton** shared that there have not been any detrimental impacts and some operational efficiencies have been gained. The real issue going forward is how to maintain world leadership in instrumentation associated with electron microscopy. BES is addressing this.

Hall asked about electron microscopy and feedback from users who access EM capabilities, noting that facilities for EM might be hard to find when included within the NSRC. **Neaton** shared that the NSRCs began working with the EMBCs about two years ago and have identified the benefits of having access to other facilities. There are communities that embrace this new model and the merger will create new communities and drive forward the use of EM.

Gates asked how the five centers have influenced one another, and what centers have stopped doing to avoid duplication or inefficiency. **Neaton** noted that centers have specific strengths. When users apply for one capability that may be stronger at another center, they are sent to that center. The Directors have a high level of interaction, to include creation of a portal that describes the expertise at each center. In terms of what to turn off, those decisions include a lot of factors to include a finite budget. Things are ending all of the time with new capabilities coming along. In the evolution of the NSRCs, they will continue to make greater use of the co-located facilities such as the light sources.

Ratner asked if the centers are in steady state or are in a growth mode. **Neaton** shared that staffing is at a steady state. Some efficiencies will increase to grow the number of proposals worked on. Demand is greater but at about the same capacity. In the past years, NSRCs have reached a steady state.

Neaton told **Rollett** outreach is an area that is being addressed. The best outreach is scientists giving talks and describing their work. Another form is more visibility to the program as a whole, and that has been initiated by the portal. Additional partnering with local facilities give visibility to the users coming in. There is a special symposium at the ACS meeting in 2015 where all of the NSRC directors will give talks.

Neaton told **Bare** that the portal is accessible via the BES site.

Bare asked about the 50/50 split of researchers' time. **Neaton** shared that this is the same model for the electron microscopy centers. In practice, it has worked well and lets researchers do their own research but with an eye on the user community. Staff can have a greater impact immediately and disseminate their research quickly. User facility scientists get to work on new and unanticipated discoveries. It is very vital in the nanoscience center framework particularly as the centers give expertise and that keeps it moving forward.

Hemminger asked about examples of what partners bring into the facility. **Neaton** shared that at Argonne there has been some development by a user to bring in new equipment. The project was conducted and the equipment was left there. At a synchrotron, one might get outside investment. More of that could be done.

Rollett found the user portal easily and how to become a user. He asked what has happened that would not have happened without the centers. **Neaton** recalled examples made in high-impact areas. In terms of synthesis, one thing that people have been able to do is make standard best practices for doing synthesis. This work is making progress in ways that publications cannot always capture. Users can take these approaches back to their own laboratories.

DISCUSSION OF THE BESAC SUBCOMMITTEE REPORT

BESAC agreed on the overriding opportunities shown in the report. The task is to develop a report that will be effective.

Hemminger shared comments from BESAC members heard since day one and the discussion of the report. The structure would be altered to feature the Grand Challenges at the end of the report, and an executive summary and introduction section.

The discussion of synthesis will be more robust. **Hemminger** shared that there is a reasonable amount of discussion of synthesis but virtually all of it is around organic matter to include directed self-assembly. Missing is the discussion of challenges associated with hard or inorganic materials, and systems that have mesoscopic structure that drive functionality.

The current report has a strong materials focus without sufficient recognition of chemistry, which is a major focus of BES. Options for revision include replacing "materials" with "chemistry and materials," and using examples that are more chemical in nature.

Each section should include a "why now?" argument, and could be featured in sidebars.

Hall suggested that the Grand Challenges were done right and remain challenges. To begin by showing the Grand Challenges prefaces a description of what is new and "why now".

Hemminger shared that this can be done through a strong introduction and that these lead to the opportunities. **Brown** commented that these would solidify the "why now" argument.

Rollett asked if there are difficulties that should be presented such as purchasing midsize equipment as a foundation to opportunities. **Hemminger** wants to continue the concept of developing instrumentation scientists, and suggests that comments in instrumentation could include a description of the facilities for which BES is responsible. **Kung** noted that reinforcing mid-scale instrumentation and how it supports research is important. BES does have one challenge as anything above $2M has to be a budget line item. There is an effort to adjust that amount upward. BES is starting to formulate the 2017 budget and needs to know two years in advance what will be needed. BESAC could highlight the most critical equipment needs.

Ceyer commented that the cross-cutting material in chapters six and seven does not come across strongly enough and could be moved up to early chapters. **Hemminger** responded that it may be necessary to talk about the topics before addressing cross-cutting things. **Ceyer** noted that six and seven are thought about as enablers for these challenges.

Bare commented that pulling out synthesis from chapter eight will leave it as being thin. **Hemminger** suggested that doing synthesis well requires it to remain in chapter eight as a recommendation. There needs to be more example verbiage on hard materials in some other areas. The recommendation in chapter eight makes more sense remaining there.

Bare asked what is missing relative to the instrumentation scientist, noting that presentations have highlighted facilities' ability to nurture these experts. **Hemminger** shared that some of the experimental capabilities that have come about have originated mostly overseas. There are examples of instrumentation developed by scientists trained outside of the U.S. Graduate students and postdocs need the opportunity to participate in instrument building. **Ceyer** shared that another approach is the fundamental changes that occur in a single investigator group that has the funding and time to push the development of instrumentation.

McCurdy noted that that absence of chemistry and simply changing "materials" to "chemistry and materials" is insufficient. The chapters should be changed in a substantive way, emphasizing the importance of fundamental chemistry. At present, the report distorts the programs doing this work. Synthesis is referred to in a superficial way that does not identify how chemistry is foundational. **Hemminger** noted that **Ratner** is one resource on the subcommittee who can inform how chemistry can be highlighted. Subcommittee members could identify others who could guide the content. **McCurdy** pointed out that he and **Ratner** work in theory and may not be the best to comment on chemistry. **Hemminger** noted that **Ratner**, as an example, is someone who can reach to others, and he agrees with **McCurdy**. Others on the BESAC may be activated to support this portion of the writing.

Tranquada noted that chapter seven on imaging has great content with details focused on x-ray and electron capabilities. Examples on neutron scattering could be added. There are new scientific capabilities to include 4-dimensional imaging that could be included. The emphasis on synergy in chapter eight could also be strengthened.

Gates resonated with **McCurdy's** comments. Central to energy science is making and breaking chemical bonds, and not just synthesis. The report needs to mention energy, and there are topics that are missing. Central to energy science is the transformation of feedstocks, and materials are central to the transformation. We need to steer and control the chemical change. **Hemminger** noted that these are topics that need to be in the introduction and other places.

Hemminger noted verbiage that talks about the energy science workforce and that was met with disapproval from BES as it is an overused comment that no longer resonates.

Brown commented that an opportunity with the report is to stimulate greater connectivity between materials and chemistry, and now that is missing from the report.

Tobias noted **Ceyer's** comment to move chapters six and seven ahead to highlight the cross-cutting areas. **Hemminger** shared that a "why now" can be established for each and believes that the flow of the document should be examined.

DiSalvo shared that the report length will impact its effectiveness as the average person will not need lengthy details. Photos and graphics can help convey the message. This draft shows images that may not have meaning unless the reader has perspective or could provoke questions about the data shown. **Hemminger** noted that the 2007 report included non-technical graphics that were useful. This can be done in the current report on a topical basis.

French noted that starting the first two transformational opportunities with "beyond" helps reference the original grand challenges (beyond the grand challenges). Saying we need more synthesis might undercut our efforts to build on the grand challenge report. **Hemminger** shared that comments are pointing not toward the use of the word synthesis but the challenges associated with making inorganic materials. The substantive description of what chemists are interested is not just making materials but also things like dynamics on chemical systems and intermediates in photosynthesis.

Gates commented that part of looking at the challenges and progress since 2007 is the attraction of where progress has been made and trumpeting opportunities, and not talking about where progress has not been made. Synthesis falls in that category. **Hemminger** shared that synthesis is a huge challenge and with huge potential benefits.

Rubloff offered that thinking about how to shorten the report may be useful and suggested ways to restructure the content. **Hemminger** noted that the conclusion could highlight accomplishments and could also be a stand-alone document.

Brown noted that the advances being made for new and older light sources are not highlighted, and like synthesis, should permeate the report. **Hemminger** shared that facilities were not prominently featured as there was a recent BESAC report about what needs to be done about those, i.e. figuring out how to make them globally competitive. There should be recognition of facilities' successes. **Brown** suggested sharing how the facilities map onto the science. **Hemminger** shared that this is part of the "why now."

Ratner commented that the 2007 report included two chapters after the grand challenge descriptions that were ignored. The authors worked hard on those chapters. People get excited about the science and that focus should be maintained.

Hemminger shared that BES is already talking about opportunities identified by the community. BESAC needs to generate a report both for the community and decision makers. He would like to present a report to BESAC by July 2015. Some level of engagement will be needed by all on BESAC and each member at a minimum will need to review the draft.

Hemminger proposed engaging the executive committee of the subcommittee to identify those who could be actively involved in rewriting. **Hemminger** will report back to the BESAC on the progress and invite anyone who actively wants to be involved to participate.

PUBLIC COMMENT

Paul Lagnan volunteered to provide highlights on neutron 4D imaging for the subcommittee report.

ADJOURNMENT

Hemminger adjourned the meeting at 11:30 a.m EST.

NEXT MEETING

The next BESAC meeting will be held July 7-8, 2015

The minutes of the Basic Energy Science Advisory Committee meeting held on February 26-27, 2015 are certified to be an accurate representation of what occurred.

Signed by John Hemminger, Chair of the Basic Energy Science Advisory Committee on (date).

(Insert electronic signature)