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

PUBLIC MEETING MINUTES

July 12-13, 2018

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

DEPARTMENT OF ENERGY BASIC ENERGY SCIENCES ADVISORY COMMITTEE
SUMMARY OF MEETING

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) convened on Thursday and Friday, July 12-13, 2018 at Bethesda North Marriott Hotel & Conference Center, 5701 Marinelli Road, Rockville, MD. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act. Information about BESAC and this meeting can be found at http://science.energy.gov/bes/besac/

BESAC Members Present:
Persis Drell, BESAC Chair, Stanford University
Helmut Dosch, DESY
Cynthia Friend, Harvard University
Yan Gao, General Electric Company
Sharon Hammes-Schiffer, Yale University
Marc Kastner, Science Philanthropy Alliance
Bruce Kay, Pacific Northwest Laboratory
Stephen Leone, University of California, Berkeley, Lawrence Berkeley National Laboratory (LBNL)
Monica Olvera de la Cruz, Northwestern University
Abbas Ourmazd, University of Wisconsin, Milwaukee
Ian Robertson, University of Wisconsin, Madison
Anthony Rollett, Carnegie Mellon University
Gary Rubloff, University of Maryland
Esther Takeuchi, Stony Brook University
John Tranquada, Brookhaven National Laboratory
Stephen Wasserman

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

Committee Manager:
Katie Runkles, BES Program Analyst

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

Thursday, July 12, 2018

BESAC Chair, Persis Drell, called the meeting to order at 9:30 a.m. Eastern Time (ET) to an audience of approximately 100 people. Drell asked BESAC members to introduce themselves and opened the meeting.

NEWS FROM DOE OFFICE OF SCIENCE

Steve Binkley, Deputy Director for Science Programs, Office of Science (SC) focused on three topics: DOE leadership, appointee status, and the fiscal year (FY) 2019 budget. Dr. Christopher Fall was nominated for the Director of the Office of Science in May 2018. The Senate hearing for Dr. Fall was held June 26, 2018 and SC is awaiting Senate confirmation. Dr.

Fall is currently the Principal Deputy Director of the Advanced Research Project Agency-Energy (ARPA-E). Most recently he served with the Office of Naval Research and in the White House Office of Science and Technology Policy (OSTP). Dr. Fall holds a BS in Mechanical Engineering, MBA from Kellogg School of Management, and a PhD in Neuroscience.

SC's FY19 budget request is $5.39B; the House mark is $6.6B and the Senate mark is $6.65B. FY19 priorities include cutting-edge, early-stage research and development (R&D), achieving 40% funding for research, maintaining investment in Exascale Computing, continuing operations of the national laboratories, maintaining all on-going construction projects, and starting new construction projects. SC's FY19 investment in Quantum Information Science (QIS) is $105M. Binkley concluded that in the coming weeks and months Congress will deliberate on appropriation decisions for FY19 and SC will be ready to execute on October 1, 2018 if appropriations are made on time this year.

Discussion

Dosch asked about a national program to address the impact of the major data influx at user facilities. **Binkley** said while the issue is clearly recognized there is no national program in place. The volume and velocity of data generation shows a need for a system-wide approach. Equally important to SC's view is to develop the tools and knowledge to handle such quantities of data. SC is looking at machine learning (ML) and artificial intelligence (AI) techniques and deep neural network approaches for process, management, and scientific discovery. There are also ongoing discussions at the interagency level.

Ourmazd asked about efforts to establish the algorithmic side of the Exascale Computing Program. **Binkley** said Advanced Scientific Computing Research (ASCR) is focusing on the underlying applied mathematics in computer science, software development activities are embedded in BES for quantum chemistry and materials, and Biological and Environmental Research (BER) is specifically focused on computational problems for climate and ocean dynamics. The applications are best developed in the science programs. Large data analytics and infrastructure is the next generation development in these areas.

Drell inquired about ITER status. **Binkley** indicated that the ITER appropriation for FY18 was $122M, enough funding to support the two highest priority U.S. contributions (Central Solenoid Magnet System and the Tokamak Cooling Water System). The U.S. is on target to deliver those component sub systems to meet the first plasma milestone in 2025.

NEWS FROM OFFICE OF BASIC ENERGY SCIENCE

Harriet Kung, Director, Office of Basic Energy Sciences (BES) discussed BES staffing, budget news, solicitations, and program highlights. BES welcomed Stefan Vajda; backfilling for two positions was approved, one of which will be an external posting.

The enacted FY18 budget for BES was $2.09B; the FY19 President's budget request for BES is $1.85B but the House and Senate marks are higher, $2.129B and $2.193B, respectively. BES priorities include support of the Core Research Areas, Energy Frontier Research Centers (EFRCs), Energy Innovation Hubs, Computational Materials and Chemical Sciences, 12 scientific user facilities; QIS; and facility upgrades.

BES's budget from FY17 to FY19 Request has kept research at or near 40%, facilities support between 43% and 47.5%, and construction projects between 12.1% and 17.7%. Kung described the growth in BES funding from 2000-2018 and the BES construction profiles between

1984 and 2019. FY18 funds allowed BES to pull forward several key priorities in research and construction.

BES budget priorities for FY19 include QIS ($32M), Ultrafast Science ($10M), and Computational Materials and Chemical Sciences ($26M), Materials and Chemical Science for Future Nuclear Energy, and priorities identified by BESAC and Basic Research Needs (BRN) reports. In FY18, funding was increased by $1.7M at the Linac Coherent Light Source (LCLS), decreased by 0.5% at all other light sources, increased by $13.8M at neutron facilities, and increased by $7.7M at Nanoscale Science Research Centers. Kung shared the House and Senate appropriations language; the largest deviation is for facilities.

The EFRC recompetition in 2018 resulted in 42 awards (31 new/renewal and 11 2-year extensions). BES ran two roundtables on QIS in October 2017. FY 2018 Funding Opportunity Announcements (FOAs) included two on QIS, Ultrafast Science, Computational Chemical Sciences, and DOE Established Program to Stimulate Competitive Research. BES highlights on the progress at the National Synchrotron Light Source-II, development of the Helical Superconducting Undulator, and research from the Nanoscience Centers concluded Kung's presentation.

Discussion

Kay asked about the money associated with the 2-year extensions for 11 EFRCs. **Kung** said BES was still negotiating budgets; the goal is to free up $10M from the $100M included in the recompetition. BES aims to have a recompetition every two years with two equal size cohorts and provide a smoother transition for students.

Hammes-Schiffer inquired if funds for computing overall are going to DOE supported super computers and computing facilities. **Kung** said ASCR funds the hardware and hardware development. ASCR provides the computing hours and resources for the BES research community.

Dosch asked about U.S. private sector QIS efforts and neuromorphic computing. **Kung** stated BES will run QIS in concert and collaboration with the private sector, ensuring funding aligns with BES core competencies in areas where BES can make a difference. One EFRC focuses specifically on neuromorphic computing and BES invests in this through core research as well.

Drell adjourned BESAC for a break at 9:54 a.m. and reconvened the meeting at 10:20 a.m.

BES AT 40 PRESENTATIONS AND PANEL DISCUSSION

Marc Kastner, Science Philanthropy Alliance, led a panel discussion on the 2018 BES report entitled "A Remarkable Return on Investment in Fundamental Research: 40 Years of Basic Energy Sciences at the Department of Energy." The panel consisted of Monica Olvera de la Cruz, John Sarrao, George Crabtree, Al Hammond, Philip Lippel, and Leland Cogliani. Kastner explained that the panel would share the presentations they gave to Congressional staffers with BESAC.

Binkley provided history on DOE and BES's origins. DOE evolved out of the Atomic Energy Commission (AEC), which evolved out of the Manhattan Project. Contemporary to those changes were shifts in government thinking about the role of science in the national context. Vannevar Bush's 1945 publication "Science The Endless Frontier" encapsulated the new thinking. There was recognition that basic science underpins innovation and therefore has long

term consequences to the health and vitality of the U.S. economy. The conscious effort at the end of WWII to preserve and harness the scientific vitality in other directions factored into the AEC and SC's roots. Eisenhower's speech in December 1953 at the United Nations codified using atomic energy for peaceful purposes and the Atomic Energy Act amendment launched efforts focused on the civilian side of nuclear energy. The predecessor organization for BES, the Division of Physical Research, was a significant in establishing the research base for fission nuclear energy and the National Labs. Responding to the 1973 and 1979 oil shocks the AEC morphed into the Energy R&D Administration and then the Department of Energy; the Division of Physical Research became the Office of Energy Research (OER). Scientific User Facilities were recommended by the Seitz-Eastman (1984) report "Major Facilities for the Materials Research and Related Disciplines." In 1998 OER was renamed the Office of Science and now operates 26 user facilities.

Kastner talked about shared scientific research facilities. The Stanford Synchrotron Radiation Lightsource (SSRL) and the High Flux Isotope Reactor (HFIR), originally built for other things, began being used by the materials science community for x-rays (SSRL) and for neutrons (HFIR). National Synchrotron Light Source (NSLS) at Brookhaven National Lab (BNL) and Intense Pulsed Neutron Source (IPNS) at ANL were the first user facilities built for the materials science community. The facilities began to provide free access for scientific research and paid access for proprietary research by industry.

Dosch commented that user facilities foster interdisciplinarity in science. **Kastner** added the educational component, huge numbers of fellows and post-docs, is a point made in stories.

Olvera de la Cruz discussed nanoscience and focused on nanodots' impact on common devices such as TVs, solar cells, light emitting diodes (LEDs), batteries, and nuclear waste. Nanodots convert light into different colors and reduce energy usage. Using nanodots on a TV, for instance, can save 20% of energy use. Solar cells can be made more cheaply by multi-layering nanodots. Nanodots for LEDs currently reduce energy use by 1/3 and are projected to reach 85% by 2035. Microsized batteries can be created using nanoinks and are used in devices such as hearing aids. Nanoscience allows the platinum catalyst to be placed on the surface of a lithium battery making fuels cells much cheaper by using less material. Finally nanoscience is exploring the removal of cesium from nuclear waste by making specific molecules that can bind cesium which is radioactive for many years.

Sarrao discussed the Tough Stuff story which talks about the role BES's fundamental research has played in national security and nuclear deterrence. Microstructure models developed by BES are used to certify the reliability of the U.S. nuclear stockpile and to explain the behavior of materials in extreme environments. BES' fundamental research helped reconsider processing methodology for the development of new nuclear devices. Both coal fired power plants and nuclear reactors require an understanding of how to extend their life and have operational confidence in very high extremes and at very high temperatures and pressures. Tough Stuff is the materials as well as the nature of the challenge – predicting and controlling materials in extremes.

Crabtree talked about the history of superconductivity; discovered in 1911 in mercury. In the 1950s Bardeen, Cooper and Schrieffer explained why metal loses its resistivity at 4°Kelvin and published their BCS-theory. The first device that used superconductivity was the SQUID (Superconducting Quantum Interference Device) which measures magnetic fields with very high sensitivity and precision. It was used to map neurons firing in the brain without putting any electrodes on the skin. In the 1960s superconducting wires, niobium titanium wires, were used

for research magnets. In 1986 high temperature superconductivity was discovered and superconducting transition temperature increased rapidly from 20K before 1986 to 30K, then in 2015 to 200K – close to room temperature. Superconducting filters are used in every cellphone to prevent conversations from interfering with each other.

Kastner talked about quantum computing pointing out first that most financial transactions are protected by encryption-based security based on factoring a number into its prime numbers. Around 1990 Peter Shor proved a theorem that a quantum computer could factor prime numbers much faster than a conventional computer. Huge investment is seen globally because whoever gets the quantum computer first has enormous power. Industry leaders are building devices up to 50 or 70 qubits. The fundamental qubit device is built on the fundamental materials research that BES has invested in since the 1980s.

Cogliani, co-chair of the Energy Sciences Coalition, the lead advocacy group for SC, described his observations from the presentations to over 30 congressional offices. Two broad observations that resonate well with Congress are a community driven process with consensus around scientific issues and world leading unique science facilities that allow the U.S. to lead, host, and attract the best scientific minds. Cogliani recommended developing a one-page summary of the report encapsulating the possible types of research and applications with the overall findings.

Lippel, Assistant Director of the MIT Washington Office, characterized the meetings with Congressional staffers. The first meetings with key staffers asked what kind of report would be beneficial. Representatives from both parties attended the roll-out event held at Lewis-Burke. The Senate Energy and Natural Resources Committee was appreciative of the report and said it provided the kinds of things useful to them. People who had less technical expertise than those on the key authorizing subcommittees were approached. The group had thoughtful discussions with Frank Lucas of OK and Randy Weber of TX. The message, through the stories, was the science and technology benefits were based on long, consistent investment in research that ultimately led to things that effect their lives.

Hammond, the report author, offered his perspective on the report and its reception. A report like this is the foundation of a communication strategy and not just as an object in its own right. The processes that lead to basic research effectiveness are not very well communicated and have put the enterprise at high risk. Shorter versions of the stories, user-friendly websites for non-technical people, and communications staff in DOE are necessary. Communications needs to be a larger part of everything BES does to be effective.

Kastner asked Cogliani to expand on the one-page summary. **Cogliani** suggested a one-page summary for the entire report and also for individual stories. The 1-page summary for the entire report could include a list of technologies and findings that Congresspersons or staff could draw from for different purposes, including speeches and statements supporting continued funding for BES.

Discussion

Drell asked if Secretary Perry and Under Secretary Dabbar were briefed on the report. **Kastner** had a meeting with Dabbar before the roll-out and an appointment with Michael Kratsios in OSTP. **Olvera de la Cruz** added that Dabbar encouraged the subcommittee to talk about expected materials and future developments. **Crabtree** said that Dabbar was telling the panel how to cast the stories and suggested things to emphasize. He and everyone else wanted capsule statements, one sentence that really hit home. **Olvera de la Cruz** mentioned that those

with less science connection were interested in the process of choosing which subjects to fund and why; how DOE and BES operate.

Rubloff asked how much people were attracted by things BES sees in the future. **Sarrao** said the average person knew about the big facilities in their district, they may have heard of the EFRCs, but this report drives home the notion that the much of the portfolio is being generated by individual performers and small teams.

Dosch mentioned a strategy is needed to keep the scientific agenda in Congress. **Lippel** noted that this report is purposefully different in that it tries to encapsulate things that happened over a long period of time and add up to something collectively. One of the ways the report can be useful is as an anchor to more local science news stories or events to relate them to ongoing work. **Drell** stated that a really good communication strategy is to say the same thing over and over again. One of the strengths of this report is using it to make the case to Congress. Using similar stories can have a lasting impression but it requires everyone to play a role. **Kastner** recommended that BESAC ask Hammond to create the one-page summary for the entire report and for each of the stories.

Ourmazd offered two suggestions: 1) create a one-page summary of the process, recommendations, and lessons learned in rolling out the report, and 2) to determine the arguments to use with those who do not have a stake.

Gao reminded BESAC to communicate that benefits from the scientific research can take 20-30 years. The community must emphasize that research is an investment for the future. **Drell** endorsed Gao's statement about the benefits not being realized for 30 years. **Cogliani** commented that members of Congress understand SC has a broad portfolio, and many politicians are tilting towards science that does not have a clear, immediate application. Overall Congressional support is about maintaining a strong base capability in STEM fields, energy, national security, broader DOE mission space, and the support DOE provides to other agencies.

Drell adjourned BESAC for lunch at 11:41 a.m. and reconvened the meeting at 1:32 p.m.

LIGHT SOURCE UPGRADES & INTERNATIONAL LANDSCAPE – FOLLOWED BY A PANEL DISCUSSION

The panel consisted of Stephen Streiffer (ANL), Steve Kevan (LBNL), Mike Dunne (SLAC), Tetsuya Ishikawa (SPring 8), and Helmut Dosch (DESY).

Streiffer said the approach of the Advanced Photon Source Upgrade (APS-U) was to focus on science outcomes particularly in high energy x-rays to penetrate *in situ* and *operandi* environments. The APS-U will enable multiscale, three dimensional explorations of complex materials and chemical systems by 2026. The APS-U scope includes investment in the new storage ring and long beamlines. The accelerator side is completing its final design; APS is executing long lead procurements and has received the production magnets which are being evaluated now. A CD-2 review will occur in October 2018, earliest first light in 2023, and upgrade completion in 2026.

Kevan discussed the Advanced Light Source Upgrade (ALS-U) which will maintain U.S. leadership in soft x-ray science and address critical needs as outlined in BRN reports. ALS-U tools will provide combinations of spectral, spatial, and temporal resolution. The ALS-U accelerator design includes new high-performance undulators, accumulator ring, and a new storage ring. Providing high brightness and coherent flux is necessary to enable understanding of emergent material and chemical properties.

Dunne shared updates on the X-ray Free Electron Laser (XFEL) projects LCLS-II and LCLS-II-High Energy (HE). The two upgrades will increase beam pulses from 120 pulses per second to 1 million pulses per second. LCLS-II is currently 70% complete and LCLS-II-HE had its CD-1 review in June 2018. LCLS-II addresses dynamics in materials and chemical science systems, and LCLS-II-HE will enable structural dynamics at the atomic scale.

Ishikawa explained synchrotron radiation (SR) and XFELs in Asia-Oceania. There are 19 SR sources in Asia-Oceania with an additional 9 in construction or planning phases. SPring-8 has a planned multi-bend achromat (MBA) upgrade to create SPring-8-II. Greenfield construction for MBA storage rings is underway in Japan, China, Thailand, and India. There are currently three room-temperature linac-based XFELs, a superconducting linac XFEL is planned in Shanghai, and Japan is exploring the possibility of making 10kHz machine using room-temperature technology.

Dosch explained that the European landscape of x-rays and lasers includes two European flagship facilities, the European Synchrotron Radiation Facility (ESRF) and the European XFEL. 15 national facilities also serve European user communities. National funding agencies request that new National facilities and upgrades take the European landscape into account but currently there are insufficient standards and cooperation. A new consortium, League of European Accelerator-based Photon Sources (LEAPS), has coalesced as a new voice in Europe. Challenges in the 21st century are ambition of the facilities, strategy, organization, roadmaps, and integration.

Discussion

Kastner asked if a sociological challenge will arise with x-ray lasers because of the limited number of users that can access them. **Dunne** said that going from 100 Hz to MHz will increase capacity substantially and will open new opportunities for higher risk experiments serving a broader community. XFEL is fundamentally a different world from synchrotrons, but XFEL sources should be viewed as a portfolio of capabilities for the community. **Streiffer** noted that even with larger capacity the demand for synchrotrons still outstrips supply. **Dosch** mentioned that careful selection of applications, suggestions of different facilities in which to run experiments, and mitigation strategies will help with any user frustrations.

Kastner asked Dosch about international benchmarking. **Dosch** indicated a template is being used for road mapping and there is an advisory board. **Kevan** added that soft x-ray beamlines are pushing the limits of oversubscription. FELs and storage rings have the same challenges but FELs are handling it better because the installations are newer and more automated. Some solutions include better automation and computer-assisted experimentation.

Friend asked about integrating strategies to most effectively use the facilities and noted that FELs have a higher access barrier than synchrotrons. **Streiffer** stated that there is increased coordination in technique and algorithm development and between the light sources. There is also exploration of the role of coordinating bodies such as the Society for Scientific User Research Facilities. **Dunne** indicated two ways to address the barrier to FEL access, 1) to offer standard platforms allowing users to bring their sample and quickly begin interrogating the system of interest, and 2) the presence of a capable internal scientific workforce to help design the experiment to get the most out of it. **Dosch** noted two problems 1) that mathematicians and informatics scientists are needed to help get the knowledge, not just the data, out of the sample and 2) as user facilities open up to new audiences an option to submit a problem and be directed towards the appropriate facility will be needed.

Rollett asked if there has been enough discussion and cooperation around the increases in data due to the higher brightness and bigger detectors. **Dunne** indicated that the five light source Directors in the U.S. charged their respective data teams to come up with common solutions to tackle the data issues. Dunne divided the issue into three phases 1) intelligent data gathering and intense data reduction, 2) online, real-time data analysis of the system while taking the data, and 3) an overlay of intelligence across the whole system to help identify the subtleties of the data and feed back into the system, as well as the long-term deep dive into the data.

Ourmazd recommended imposing a code of collaboration on users to share data in a pre-competitive phase and to acknowledge that the user needs data science expertise. **Dosch** agreed that each beamline needs a data officer. He cautioned about the code of collaboration being imposed on users because competition of the best ideas must be allowed.

Takeuchi asked the panelists to contrast funding from government and industry between Europe, Asia and the U.S. **Ishikawa** said in Japan a new rule requires the government and industry / local government split the cost of construction 50/50; however operation is mostly funded by the government with ~5% from industry. In China, the city or local government funds 80% and central government funds 20%. **Dosch** said in Europe the percentages vary by country, but Switzerland is the leading country for private sector investment at 5%. **Streiffer** stated the APS has averaged 4% from industry. **Kevan** indicated the Extended Ultraviolet Lithography Consortium at ALS invests in operating and building beamlines. **Gao** specified there is a lot of education to do for industrial people and facilities need to enable more *in situ* testing and materials processing so industry will benefit.

Drell asked all panelists to give a 15-second statement on what is next, their best guess in terms of technical facility or scientific need. Increase interdisciplinary user consortia (**Dosch**), make everything small (**Ishakawa**), use coherence and ultrahigh brightness to drive nonlinear processes (**Dunne**), a lot more automation on the floor to improve the user experience and throughput (**Kevan**), and make FELs common place (**Streiffer**).

Drell adjourned BESAC for a break at 3:05 p.m. and reconvened the meeting at 3:30 p.m.

NEUTRON SOURCE UPGRADES & INTERNATIONAL LANDSCAPE– FOLLOWED BY A PANEL DISCUSSION

The panelists Paul Langan (Oak Ridge National Lab (ORNL)), Dimitri Argyriou (Ames Laboratory), and Collin Broholm (Johns Hopkins University) discussed neutron source upgrades.

Langan leads operation and development of two BES funded neutron sources. ORNL operates two world-leading neutron sources that form a center of neutron scattering, HFIR and SNS. Researchers are using these two sources to do forefront science in priority areas for BES. SNS Upgrades have been split into two projects, will double accelerator power capability, will allow increased flux, and sets a platform for a second target station.

Argyriou stated China has recently started commissioning its 100kW spallation source and started collecting data on its first 3 instruments. Japan Proton Accelerator Research Complex (J-PARC) is a multi-use facility with a goal of a 1MW spallation source in 12-18 months. Australia commissioned the Open Pool Australian Lightwater (OPAL) reactor, a medium to high flux facility that is fully instrumented, serves the Australian and Southeast Asian community, and plans to extend the facility with an additional guide hall. The top three frontline sources in Europe are ISIS Neutron and Muon Source (ISIS) in the United Kingdom, the Institut Laue–Langevin (ILL) in France, and the Forschungs-Neutronenquelle Heinz Maier-Leibnitz Zentrum

(MLZ/FRM II) in Munich. ISIS commissioned a second target station which increased the instruments from 20 to 30; ILL is updating their instrumentation to next generation; and MLZ/FRM II has commissioned a new guide hall that will host an additional suite of 5-10 instruments. The European Spallation Source (ESS) in Sweden is a new type of source constructed by a Consortium of 16 European countries with an investment value of €2B.

Broholm said for quantum magnets the planned Second Target Station (STS) at SNS will do high efficiency polarized inelastic scattering in extreme sampling environments and go beyond conventional ways of collecting data to time evolution beyond equilibrium. For soft matter, STS will cover, on a single instrument during a single experiment, the entire range of 4, 5, 6 orders of magnitude in energy or time and lengths scale. Inelastic diffraction will be possible in materials chemistry by probing materials as they are applied in technological systems such as batteries, engines, and turbines. STS will allow scientists to follow cell structure and dynamics in living biological systems.

Discussion

Gao asked when neutron flux will be sufficient to do experiments as can be done today with a synchrotron. **Langan** said next generation spallation sources will be game changing and there will be improvements in instrument performance to result in game changing science. It's not all about flux. There are parameters such as peak brightness and peak shape that can move towards new frontiers of science. **Argyriou** stated neutrons are never going to go to Ultrafast. The dynamics of regular pulse as well as non-equilibrium processes can be examined by collecting dynamic elastic and inelastic in a single pulse over a large domain. The discussion should be about utilizing other parts of SC to develop or investigate new concepts for neutron sources. **Broholm** explained that neutron scattering can measure the cross-section of absolute units over 6 orders of magnitude of energy. STS expands that dynamic range. Even with existing sources, performance has increased dramatically, by at least 2 orders of magnitude.

Kay commented on neutron experiments using deuterium in dynamic biological systems. **Langan** said living hosts are used to express deuterated material for neutron scattering experiments, but it has not impeded the ability to perform various metabolic processes involved in life. At the molecular level there is an effect which users take into account. An exciting development is manipulating the spin of hydrogen in biological systems to align those spins using dynamic nuclear polarization.

Dosch asked if there were any initiatives to determine how facilities providing access to structural materials fit together in different fields, how developments in one field influence science cases in other fields. **Drell** mentioned that different fields do that in a major way, for example the influence of accelerator physics and high energy physics in photon science. **Kastner** commented that a huge advance in cryo-electron microscopy came out of detector development for light sources.

Ourmazd noted that many processes in high energy physics can be duplicated in condensed matter, such as the Higgs boson, and asked if anything similar was being followed. **Broholm** said the quantum magnets can be thought of in their own universe and with different expressions of quantum field theories. Each of the quantum magnets have fundamental particles that form dynamic systems that behave exactly as the quantum field theory predicts. **Ourmazd** asked if the current experiments shed any light on high energy physics directions. **Broholm** said in principle field theorists are interested in what goes on in condensed matter physics and are interested in ways to illuminate that. **Argyriou** added multiferroics has echoes of some exotic

particles predicted in high energy physics. Using string theory to test the standard model to apply to condensed matter and solve the metabolic problem is being discussed amongst theorists. Concerning the different probes available to look at matter, Ames Lab uses every single tool available. Materials laboratories will always use an arsenal of techniques; the issue is the complementarity of which technique is going to provide the answer necessary to make progress. Coherent strategies are needed just as understanding use and synergies between them.

Friend suggested having a simple approach for integrating the neutron facilities with other BES facilities. **Langan** indicated that ORNL's neutron sources try to make access as easy as possible by informing and educating users of the benefits and unique complementary information available depending on the source. Joint application programs with light sources exist. **Broholm** added that in his view the younger generation may solve the issue of using different techniques and tools because they want to experiment with different approaches.

Rollett asked which disciplines are taking advantage of neutron scattering. **Langan** said at the SNS and HFIR quantum materials remain incredibly strong. Soft matter and catalysis are two areas of growth in the future. **Argyriou** said in Europe condensed matter is roughly 40%-50% of the users and soft matter and biology have increased to 30%-40%. Institutions like the European Molecular Biology Laboratory are building outstations next to neutron sources and those sources are coalescing with other disciplines.

MATERIALS SCIENCES AND ENGINEERING (MSE) DIVISION COMMITTEE OF VISITORS (COV) REPORT

Esther Takeuchi, Stony Brook University, discussed the COV report on the MSE Division. She described the COV charge and noted that it was helpful using the Portfolio Analysis and Management System (PAMS) online. For the first time Early Career Awards were covered in a COV. Seventeen participants were organized into 4 panels. The COV produced eight major findings, seven major recommendations, and three comments. The findings focused on white papers, portfolio turn-over rate, BRN reports, support in characterization and technique development, PAMS, Principal Investigator (PI) meetings, and funding cycles. The recommendations focused on travel, staffing levels, frequency of the COV, award extensions, communication with the scientific community, and using high impact journals as a metric of success. The comments were that the COV highly commended BES MSE Division personnel and leadership for advanced preparation and active participation in the process, and the Chair commended the panel leads and members for their participation.

Discussion

Rubloff was concerned about the ethical and disclosure issues related to journal impact factor and the money spent for publication. **Takeuchi** added other significant charges are associated with covers in journals.

Hammes-Schiffer expressed concern about the recommendation to reduce the number of full Early Career Award proposals because the exercise of writing proposals and getting feedback is useful to young investigators.

Ourmazd suggested the COV rephrase the second summary point to say "lack of travel over a long period will impair the program managers' ability to function effectively". **Takeuchi** agreed to alter the words.

Drell called for a vote from BESAC to accept the report. The COV report was accepted unanimously.

Public Comment Session

None.

Drell adjourned the meeting for the day at 5:05 p.m.

Friday, July 13, 2018

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

BASIC RESEARCH NEEDS WORKSHOP ON MICROELECTRONICS

Andy Schwartz, BES, discussed the Microelectronics BRN workshop planning process and status. The chair and co-chairs have been identified. The charge excludes quantum computing. A one-day roundtable was held in May 2018 to discuss goals, format, and output of the BRN to be convened in October 2018. At the May meeting topical areas were identified where fundamental research over 5-10 years could have a significant impact on microelectronic technologies. The output of the meeting was common themes in materials science, device physics, emerging architecture approaches, and cross-cutting areas (metrology, energy efficiency, manufacturability) and a list of questions to be addressed. The BRN workshop conveners are finalizing dates and locations and working on the scope and structure. Panel leads and participants are yet to be determined and a "factual document" is being planned.

Discussion

Leone asked how the BRN will ensure a focus on research for the future and avoid what industry is already doing. **Schwartz** said industry roadmaps will be reviewed but participants will focus on fundamental science questions that are relevant to our mission and impactful to solving problems.

Rubloff noted a wide range of applications integrate microelectronics beyond computing and stated it is important to adjudicate the distinction. **Schwartz** indicated that the BRN goes beyond computing to include things like sensing capabilities and the science needed for those application spaces.

Ourmazd raised questions on architecture, integration, and memory versus microcomputer speed. **Schwartz** said the topic of memory was one of the first conversations with the Chairs, the challenges of logic versus memory, whether the materials systems will be different, and how to run the workshop to cut horizontally and vertically; integration is key.

Rollett asked if the workshop will address the use of Graphics Processing Units (GPU) to work around Moore's Law. **Schwartz** said the workshop will focus on themes that impact multiple spaces rather than particular applications. The goal is to determine where SC investment will make the biggest impact.

Dosch inquired if the challenges and solutions to applications such as computing, communications, and sensing have been considered. **Schwartz** stated the charge allows the Chairs to have a conversation with SC about what makes more sense. The participants are asked to keep those application spaces and the real needs in mind.

Rollett suggested including the computational and physical data problem related to storage. **Schwartz** said BES, ASCR, and High Energy Physics (HEP) are interested in this space.

The storage problem is one of the strongest motivators from HEP because the lack of back-end capabilities is detrimental to future experiments.

Drell commented that this is not the first BRN that has combined multiple offices; as the trend continues there are real opportunities for getting fields together around common problems.

DOE ISOTOPE PROGRAM

Jehanne Gillo, Office of Nuclear Physics, discussed the DOE Isotope Program's 3-pronged mission, program production, facilities, program sites, and support for BES research. The mission is to produce and distribute radioactive and stable isotopes, to maintain infrastructure, and to conduct R&D on isotope production and processing techniques. The DOE Isotope Program has sole authority to produce and sell isotopes, it has revolving funding, and it monitors and anticipates isotope needs for missions, research, and industry. Distribution of isotopes is coordinated through the National Isotope Development Center at ORNL. There are two stewarded facilities, the Brookhaven Linac Isotope Producer and the LANL Isotope Production Facility (IPF). University facilities include University of Washington, University of Missouri, Duke University, Washington University, University of California Davis, and Texas A&M. Other isotope sites include Y-12 National Security Complex, ANL, Pacific Northwest National Laboratory, and Savannah River Site. Reactor facilities include the Idaho National Laboratory Advanced Test Reactor and HFIR at ORNL. Gillo shared examples of production and development including support of NNSA (^{236}U, ^{99}Mo, ^{99}Tc, ^{6}Li, ^{7}Li, ^{3}He), mitigation of dependence on foreign sources (^{82}Rb, ^{252}Cf, ^{241}Am), production development (^{227}Ac and ^{225}Ac), Iranian Heavy Water, Super Heavy Elements and Heavy Element Chemistry, and Isotopes for BES research.

Discussion

Dosch asked if ^{99}Mo is the responsibility of the Isotope Program. **Gillo** said the responsibility for ^{99}Mo is congressionally mandated to NNSA. The Isotope Program provides NNSA with technical support such as technical evaluation of their cooperative agreements, annual assessment with the Nuclear Science Advisory Committee on program progress, and to cover shortages of isotopes.

Tranquada commented that ^{3}He for detecting neutrons is of critical importance at the SNS and there are many applications with neutrons that rely on pure isotopes. **Gillo** clarified that the Isotope Program strongly encourages the use of alternatives to ^{3}He for neutron scattering detectors because there is only a finite amount of ^{3}He and many high-priority applications. Where there is no alternative the Isotope Program will make sure the ^{3}He is available.

Takeuchi asked about the size of operations. **Gillo** said that when the program came over to SC in 2009 there were $20M in appropriated funds and $20M in revenue from stakeholders to produce isotopes; now the program has ~$30M in appropriated funds and ~$80M in revenue.

Wasserman mentioned two videos on IPF and Eva Birnbaum produced at LANL for Congressional staffers. He suggested that this type of story, one that combines the scientific and the human perspectives, appeals greatly to the public.

Drell inquired if the medical community can ask for a particular isotope or can use new isotopes to investigate effectiveness. **Gillo** said the program asks NIH to provide a prioritized list of isotopes they want to develop and the Isotope Program goes down that list and makes them available. However, the landscape changes so quickly that the Isotope Program is always open to the community or a federal agency asking for specific isotopes to be developed.

Dosch asked who is responsible for the waste. **Gillo** stated that once the program sells an isotope the waste becomes the responsibility of the purchaser.

INTERAGENCY DISCUSSION ON QUANTUM INFORMATION SCIENCE

Jake Taylor, OSTP, covered the science of quantum information, how the current positioning leads to policy choices, and highlighted DOE's key role in the future of this space. QIS is a vast field covering many different topics: quantum sensing, quantum communications, quantum simulation, and quantum computation.

Quantum technology stems from fundamental promises in quantum mechanics. Quantum communications or quantum networking generates unique shared randomness using entanglement. Quantum simulation is the low-hanging fruit of controlled quantum systems. And quantum computation is pure information processing. From a policy perspective a key challenge is to understand the consequences of the new technology; asking questions such as how to operate within a post-quantum world and how to prepare for that eventuality. The next step is quantum simulation which requires a controlled quantum system known well enough to do reliable simulations; an area where a lot of immediate progress is being seen.

The deeper look into the policy space has to do with industrial and international engagement. On the 10 year horizon OSTP wants the corporations and government to be ready as the larger scale quantum computing devices come out. For OSTP QIS has overlapping categories – quantum sensing, networking, and computing. A National Science and Technology Council (NSTC) subcommittee on QIS has been formed; the goals are to create and maintain a national strategy for QIS, and coordinate current and future efforts across the agencies.

Discussion

Drell asked about the Office of Management and Budget's (OMB) position on QIS. **Taylor** said OMB has a deep interest in QIS and are part of the NSTC subcommittee. Taylor meets with OMB regularly.

Kastner asked what BES's participation in QIS will look like. **Taylor** saw lots of opportunity for BES in materials and engineering integration for quantum devices and quantum systems. International cooperation and collaboration space has opportunity as well.

Ourmazd inquired about connecting the dots between apparently disconnected things and funding mechanisms for risky ventures. **Taylor** noted three types of connections: program managers inviting each other to their reviews, formal coordination mechanisms such as NSTC, and cross-boundary efforts such as industry to government, academia to government, and between disciplines. Solutions to cross-disciplinary challenges require years of legwork and possibly government funds to seed the new area. Taylor said risk is a perception modified by the discussions, by convening and reporting. This is primarily a community engagement effort over the long term at all different levels; it has to be an integrated process.

Hammes-Schiffer noted the workforce issue in new cross-disciplinary areas and asked about graduate programs tailored to QIS, graduate fellowships, and federal agencies encouraging people to cross these boundaries. **Taylor** said some mechanisms are in place and BESAC can be influential via recommendations. There are opportunities in tracked fellowship approaches, but it starts earlier with the mentor in college or before.

Dosch asked if the correct mathematical tools are available for quantum information science. **Taylor** said the tools are strong; as mathematicians and computer scientists engage more deeply in QIS it has become apparent a lot of the machinery helpful for physics problems are not

right for explaining information problems. For quantum devices and sensing we largely have what we need.

RECOGNITION OF BESAC CHAIR

Kung recognized Drell's contributions to BESAC and the end of her tenure as the BESAC Chair. Kung shared that Drell stepped up to help with the transition from Hemminger at a very critical time. Kung was most impressed with Drell's thoughtfulness in approaching the Chair position, she infused a lot of her own ideas to bring the membership together including the switch from presentations to dialog-oriented meetings. Kung thanked Drell for her energy, wisdom, leadership, and positioning BES and BESAC on a robust and vibrant trajectory.

Binkley enjoyed working with Drell over the last decade and has witnessed her succession of major accomplishments. Drell also provided a dimension of service to science and the public within the U.S. that is taken very seriously. Binkley presented Drell with the Secretary of Energy's Award of Appreciation and read the inscription, "For your extraordinary service to the Department of Energy as Chair of the Basic Energy Science Advisory Committee. Under your visionary leadership BESAC has furthered its impact on shaping the federal research and scientific user facility portfolio and produced an inspirational report that celebrates past scientific accomplishments. Your distinguished service to the Department of Energy paves the way on a groundbreaking future for the Basic Energy Sciences program."

Drell stated that it has been an honor to be the BESAC chair because of the fantastic committee; wise, dedicated, selfless, and interested in the health of the U.S. scientific enterprise. Drell enjoyed getting to know the individual members of BESAC through dinners and conversations. She also now knows the 20 phenomenal individuals in BESAC and in the future she can get wise advice from friends she can call on. Drell thanked all of the federal officials who support BESAC and the scientific enterprise of the U.S. Drell personally thanked BES staff who helped her learn and grow over the last 16 years: Katie Runkles, Harriet Kung, Helen Kerch, Linda Horton, and Jim Murphy for their incredible advice and thanks to Jim "I could masquerade as an accelerator physicist," and Pat Dahmer for her mentorship. She ended by saying that the work BESAC members do is so important, set priorities, guide the national program, and have a profound influence on the future of the field. Thank you for what you do.

Olvera de la Cruz, "on behalf of all of us thank you so much, it was really a pleasure to have you lead us because you did a great job and made our job very, very fun." **Friend**, "you are an inspiring leader and inspired us all to go forward, so thank you Persis." **Ourmazd**, "I have personally learned from you and benefitted from your advice, not only on this committee but also in previous situations."

Public Comment Session

None.

Drell adjourned the BESAC meeting at 11:00 a.m.

Respectfully submitted,
Tiffani R. Conner, PhD, PMP, AHIP
Science Writer
ORISE/ ORAU
August 5, 2018