BASIC ENERGY SCIENCES ADVISORY COMMITTEE

MEETING MINUTES

Bethesda North Marriott Hotel & Conference Center

5701 Marinelli Road, North Bethesda, MD 20852

July 26 - 27, 2012

PARTICIPANTS

BESAC members present: Simon Bare William Barletta Nora Berrah Gordon Brown Sylvia Ceyer Yet-Ming Chiang George Crabtree Beatriz Roldan Cuenya Frank DiSalvo **Roger French** Allen Goldman Laura Greene John Hemminger, Chair Bruce Kay Kate Kirby Max Lagally William McCurdy, Jr. Mark Ratner John Richards Rohlfing John Spence **Douglas Tobias** John Tranquada

BESAC members not present: Peter Cummings Bruce Gates Ernie Hall Sharon Hammes-Schiffer

Also participating:
William Brinkman, Director, Office of Science
Patricia Dehmer, Deputy Director for Science Programs, Office of Science
Linda Horton, Director, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division
Harriet Kung, Director, Office of Science, Basic Energy Sciences
Katie Perine, Office of Science, Basic Energy Sciences, Committee Manager
Eric Rohlfing, Director, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division
Gary Rubloff, University of Maryland
John Sarrao, Lawrence Livermore National Laboratory

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

MEETING MINUTES

Thursday, July 26, 2012

The meeting was called to order by Basic Energy Sciences Advisory Committee (BESAC) Chair **Dr. John Hemminger** at 9:05 a.m. Dr. Hemminger led an introduction of the BESAC members and discussed the schedule for future meetings. A Committee of Visitors (COV) for the Office of Science (SC), Office of Basic Energy Science (BES) Scientific User Facilities Division will be held in 2013. There will also be a COV for the Energy Frontier Research Centers (EFRCs) and the Fuels from Sunlight Energy Innovation Hub solicitation. An additional COV will cover the Workforce Development for Teachers and Scientists (WDTS) program, BESAC members may be asked to participate in the COVs.

Dr. Hemminger reviewed the agenda, highlighting the review of the mesoscale science report.

Presentation: News from the Office of Basic Energy Sciences

Dr. Harriet Kung, Director, BES, gave an update on recent progress and budget developments.¹ For Fiscal Year (FY) 2012, BES received an appropriation of \$1.688B. This is an increase of approximately \$10M over FY 2011 but is short of BES' request for a \$200M increase. This presents budget challenges including operating user facilities below optimal levels. The increase includes specific language to support major item of equipment (MIE) projects. Overall core research is down about \$25M compared to FY 2011.

BES continues to deliver exciting results. The 46 EFRCs have led to the publication of more than 2,000 peer-reviewed publications since 2009. The Centers have made strides in patent publication and invention disclosure. Nine start-ups have benefitted from EFRC contributions.

The EFRCs are accelerating the scientific process, based on midterm reviews conducted between January and April 2012. The reviews were held at lower cost regional cities near major airport hubs and clustered according to both topical and regional considerations. The reviews found that the centers are taking on higher-risk challenges and working on more difficult questions for results that are transformational. The review also looked at training and workforce elements, and each review included the examination of documentation on strategic vision, scientific plans and programs, technological accomplishments, and management strategies. Reviews resulted in recommendations and action items with some positive and negative financial consequences.

BES launched two research opportunities in computational and chemical sciences research in FY 2012 that have benefitted from BESAC and BES workshops. The first is in predictive theory and modeling. An expression of interest in February 2012 drew more than 500 pre-applications and 140 full proposals. Proposals are funded up to \$13.5M per year for three to five years and include \$4M for equipment. The second opportunity is a Scientific Discovery through Advanced Computing (SciDAC) call with colleagues in the DOE Office of Advanced Scientific Computing Research. DOE is getting ready to issue seven awards at \$6M per year in topic areas that reflect BES' priorities for this area of research.

¹ http://science.energy.gov/~/media/bes/besac/powerpoint/20120726/Kung.pptx Basic Energy Sciences Advisory Committee July 26 – 27, 2012 – Meeting Minutes

The SC Early Career Research Program is another opportunity that started in FY 2010 through the use of FY 2009 American Recovery and Reinvestment Act (ARRA) funds and has since made 206 awards.² Individual SC offices are responsible for the review and award selections and support the individual early career scientists' research programs. Awards in FY 2012 reach 19 U.S. states for BES and 25 for SC, with awards spread across 47 unique institutions. The FY 2012 awards will cover 24 BES program areas.

Early Career award successes include the work of Wei-Ren Chen at Oak Ridge National Laboratory who is studying soft colloids with the goal of combining tailored synthesis with neutron scattering to design colloids materials for energy conversion applications. Dr. Ozgur Sahin at Columbia University is using bacteria spores to design materials for energy applications. Dr. Xiangfeng Duan at the University of California, Los Angeles, is designing efficient photo catalysts. Dr. Gary Douberly of the University of Georgia is developing helium nanodroplet isolation spectroscopy to provide insight into combustion processes.

The construction of the National Synchrotron Light Source-II (NSLS-II) is progressing on schedule and on budget. The ring building construction is now complete. Favorable market conditions allowed for two laboratory office building (LOB) shells to be added to the scope. LOBs 1-3 were completed in June and LOBs 4 and 5 are scheduled to be completed by December.

Three new published reports support the BES communication plan. The BES 2011 Summary Report is in high demand and already in a second printing.³ The FY 2011 Research Summaries publication features more than 1,300 research projects across all three BES divisions. The "Science Serving the Nation" brochure has gone to Congress and high-level hearings conducted in recent months. The second BES "eat-and-learn" placement features an energy use theme and describes how science can impact energy objectives in important ways.⁴

BES' FY 2013 budget request is \$1.800B and is a \$111M increase over FY 2012. New opportunities proposed include joint R&D with the EFRCs and the DOE Office of Energy Efficiency and Renewable Energy (EERE). For core research, the House and Senate marks were supportive of the Materials and Chemistry by Design and Science for Clean Energy programs. Scientific user facility operations were also well received, as were high-priority projects in construction and instrumentation.

For the FY 2013 budget request, the House recommended that BES receive \$1.657B, \$37M below FY 2012 levels and \$142M below the FY 2013 request. Many activities can continue and the two energy innovation hubs will be supported at requested levels. The EFRCs will be supported at the base level of \$100M. BES' request of \$20M for joint work with EERE and the mandated state-based Experimental Program to Stimulate Competitive Research (EPSCoR) program were not supported in the House mark. On the MIE side, the House fully supported the Advanced Photon Source Upgrade and NSLS-II Experimental Tools project. Construction was

² Early Career Award Program homepage: http://science.energy.gov/early-career/

³ http://science.energy.gov/bes/research/

⁴ http://science.energy.gov/bes/news-and-resources/energy-flow/

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\$13.5M below the request. BES was reminded that the Committee provided funding in FY 2012 for two MIEs that were not continued by BES. Hence, the Committee recommended a rescission of \$23.5M due to SC termination of these two projects.

The Senate recommended a budget of \$1.712B, \$87.5M below the request. Funding is provided for basic research, for two energy innovation hubs at the requested levels, and a recommendation for EPSCoR support of \$20M. Construction projects were fully supported by the Senate. Mesoscale research efforts were not supported as the Committee felt that a sufficient plan is lacking that identifies specific scientific needs and justification for this research.

Looking at the rest of the SC, Fusion Energy Sciences (FES), ASCR, and Nuclear Physics (NP) received increases in the House mark. The Senate held flat on FES, gave increases for Materials and Chemistry by Design (ASCR) and Biology by Design (Biological and Environmental Research, BER). Across SC, BES is slightly better than average. There is general support for the facilities, while the research increases did not get as much traction as BES had hoped.

Dr. Kung took a retrospective view of past research initiatives to help inform BES' future planning. In the past 15 years, BES has built a forward-looking portfolio of facilities and research programs coupled with workforce development and training opportunities. Prior National Nanotechnology Initiative reports helped achieve increases for BES and launch five nanoscale science research centers. The EFRCs would not have been successful without the Basic Research Needs and Grand Challenges reports.

BESAC's engagement with BES in building its foundation, being forward-looking, and developing trend-setting planning activities every step of the way is clear. Dr. Kung hopes that BESAC will continue to guide the transformation of BES' research and help present a compelling case for mesoscale science. There are many unknowns in the current budget environment, yet BES continues to look forward and build on its core research and portfolio. The lesson learned is to determine what is right for the community and to stick to that as a guiding approach.

The Neutron and Photon Detector Workshop was approved for August 1-3, 2012. It will examine state-of-the-art detectors for existing and future facilities. The workshop also seeks to identify connections to data-intensive computing and high-speed networking capabilities. Also important is finding models to deploy lab-developed detectors and translate these technologies to industry partners that can leverage the investments.

There are new opportunities in BES and new staff members. Tim Maier from the Brookhaven Site Office is on assignment with BES. There are vacancies in the X-Ray and Neutron Scattering Facilities program and in the Fuels from Sunlight Energy Innovation Hub program.

Discussion

The EFRC review process has illuminated their successes but there is a lot undetermined in terms of renewals. The FY 2014 budget formulation is underway and renewal will be based on

discussions with the DOE and the Office of Management and Budget (OMB). The BES model of allowing the best researcher teams to go forward will drive consideration of renewals.

A continuing resolution (CR) is anticipated for three months or more, so the community does have an opportunity to voice their opinion on mesoscale science. BES has set its long-term vision and the current report will inform staff on how mesoscale can influence the BES portfolio. It is important for the community to voice its view on mesoscale science to Congress. The current message from Congress is that they are interested but want a plan and convincing argument for this investment. With regard to the timeline needed for such a plan, Dr. Kung noted that the normal internal budget process is taking place now. Dr. Hemminger commented that the mesoscale report is distinguished by the level of community involvement and outreach; opportunities to talk about mesoscale science have had a positive impact.

Dr. Bare has observed that the DOE does a good job upfront getting facilities established but wondered about the struggle with getting continued operational budgets. Dr. Kung sees both Senate and House mark-ups as supportive for operations. The Senate increase is largely for facilities operations and language therein that will allow for operation at a near-optimal level. The overall funding constraint has limited the extent of both Senate and House support.

In looking at the movement of equipment to NSLS-II or buying new top-of-the-line equipment, BES has been conducting pre-operations reviews of NSLS-II to look at its operations transition plan. Starting in FY 2013, BES has requested pre- and early operations funds to move instrumentation. There are various other sources such as the National Institutes of Health (NIH) and others for some beamlines that support other organizations. This dialogue will continue to take place over the next six to twelve months.

Congress seems to be more supportive of construction than research, prompting questions about communication of BES research. Past history shows that the bar always seems to be high for any research increases. Large funding requests in FY 2007 and FY 2008 were met, due to BESAC and community-unified efforts. This support continued into FY 2010 and the budget profile reflects this jump after several years of hard work to gain traction and community mobilization.

The recent mesoscale report presents an opportunity to convince staffers of the importance of research investments. In 2000, BESAC got a great response when it went to the House. Dr. Berrah believes that the report needs to be distilled to a 10-page report with illustrations to describe the connection to real applications. There is a need to go to Capitol Hill; university and industry partners should also contribute to share this important issue with Congress.

Presentation: News from the DOE Office of Science

Dr. William Brinkman, Director, DOE Office of Science (SC), gave an update on recent progress and budget developments.⁵ The FY 2013 House and Senate marks show disagreement over FES and BER. A compromise is expected, while SC continues work on the FY 2014 budget request.

⁵ http://science.energy.gov/~/media/bes/besac/pdf/2012-0726-brinkman-besac-asgiven.pdf Basic Energy Sciences Advisory Committee July 26 – 27, 2012 – Meeting Minutes Budgetary concerns include the potential for funding only about half of the current EFRCs and a few new ones, despite their success. Another issue is managing NP and three major facilities needs – the Continuous Electron Beam Accelerator Facility, the Facility for Rare Isotope Beams, and the Relativistic Heavy Ion Collider. SC has an agreement with OMB on an optimal budget profile for FES' major project: ITER. DOE also has large responsibilities to support exascale research and to sustain U.S. high energy physics competitiveness.

Global average temperature increases prompted many to work in the DOE. Dr. Brinkman is encouraged about recent news that CO_2 emitting sources of energy are predicted to stay flat. Coal is being replaced by natural gas, offering apositive advance albeit a "50 percent solution" since it emits 50% less CO_2 . Advances in electric cars and efficient design are encouraging, led by Tesla which offers a powerful yet efficient high-end vehicle. Toyota has addressed the middle of the consumer market with the Prius, but addressing the top of the market can expand the market space and drive prices down. Tesla has a loan from the DOE to build a plant in North Carolina. The Fisker car company also has a DOE loan.

Dr. John Rogers of University of Illinois at Urbana-Champaign created a company producing highly-efficient solar cells and panels. The product is 33 percent efficient which is a record for a commercially-available product. Cells are being made with silicon. Their market position is good.

Enhanced oil recovery (EOR) through carbon capture utilization and storage is a big issue. The U.S. is the largest producer of oil with EOR. At the four corners section of the U.S., there is available CO_2 in the ground. A pipeline sends CO_2 to Texas for EOR. This produces a more fluid material and produces more oil than traditional pumping. The CO_2 can be reused. A challenge is that CO_2 transport costs the oil industry \$10 per ton. This could be applied to coal plants but Dr. Brinkman does not know if CO_2 can be sequestered from flue gas and shipped for \$10 per ton. The costs may be more around \$60 to \$80 per ton. He does not see legislation that will change these dynamics but believes that CO_2 capture from coal plants is very important. A future plant could also look at hydrogen capture.

There is a push for small modular nuclear reactors. These would be built on an assembly line and shipped anywhere. They would be less expensive, producing 100-200 MW of power. Building a new power plant to produce several gigawatts could run \$6B to \$7B.

Discussion

Concern was expressed about the pace of the Next Generation Light Source (NGLS) development timeline. Dr. Brinkman noted that SC would like to do more but it is difficult to support NGLS and LCLS-II at the same time. He believes that the community needs to keep Congress continually aware of the importance of these facilities and maintain their visibility on the Hill.

Many people can take the mesoscale message to Congress and strike a balance between short-term investments and returns and long-term scientific work. Dr. Brinkman believes that SC

cannot go overboard in making claims but has come a long ways in delivering results with examples such as the EFRCs and the biofuel centers. He looks forward to seeing the mesoscale report and how it can be used.

There is concern about OMB's policy on scientific conference expenditures. Dr. Kirby has heard a lot about this issue from members of scientific societies. SC is doing what it needs to do in this regard, Dr. Brinkman responded. Conforming to the new requirements takes time and much work.

Dr. Spence brought up efficient aircraft turbines and asked why they cannot be used in coal plants. He expressed that this seems like a good way to reduce CO_2 emissions.

Presentation: News from Advanced Research Projects Agency - Energy (ARPA-E)

Dr. Eric Toone, Principal Deputy Director, ARPA-E, gave a progress update. ARPA-E grew out of the "Rising Above the Gathering Storm" report from the National Academies. The agency was first funded by \$400M in ARRA funds in 2009. The current budget is \$175M. When the agency was first funded there were no employees.

ARPA-E's mission is to reduce energy imports, improve energy efficiency across all sectors, and reduce energy impacts including greenhouse gases. ARPA-E has made 181 project awards with less than half in academia and 12 percent in industry.

ARPA-E seeks to fund technologies that will put new technologies on a new learning curve, as opposed to pushing existing technologies. Industry and others can take existing technologies to the marketplace. The agency funds projects for around three years aims to support disruptive technologies. Early automobiles were not disruptive, but the less expensive Model T revolutionized the market.

Program directors (PD) come to ARPA-E and an environment where there are no set activities. PDs stay for three or four years and have latitude to identify projects to create impactful programs and start new technologies. They make a pitch to the Director three months into their tenure and once approved can solicit applications and make selections.

The agency takes on technical risk that many agencies would not assume. Rather than being conservative by asking if something will work, ARPA-E considers the impact if something will work. Projects are carefully managed and PDs work with principal investigators to set annual milestones with hard go/no-go decision points. PDs review projects three or four times during the first year and if things go off track, projects are shut down. This is not a sign of failure as some things are good ideas that just did not work. In its first year, ARPA-E made 37 awards and later shut down eight projects.

Current ARPA-E projects include the Agrivida start-up in Massachusetts that is creating dedicated energy crops for conversion into biofuels. It is also supported by private sector funds. The enzymes used to break down lignin and other components are inserted directly into the plant cell wall. The enzymes are modified with proteins and spliced in locations where it is needed.

This results in an active protein and an enzyme that respond to changes in temperature, pH and other factors.

FORO Energy in Colorado has developed a drill with a 50 kilowatt laser that drills through the hardest rock on earth for geothermal applications. The rock is fractured by the laser in advance of the bit and the drill can go through ten times faster than traditional methods.

APRA-E funded 37 projects and \$150M in funding for its first funding opportunity. A scan of the technology landscape identified investments in specific areas.

One project supported by ARPA-E at the University of California-Los Angeles is developing electrofuels. It builds on energy-dense organisms that can convert fuels and uses direct electromagnetic current.

The Batteries for Electrical Energy Storage in Transportation (BEEST) program looks for a new generation of batteries beyond lithium ion batteries. A new set of metrics has been set that go far beyond what can be achieved with lithium ion batteries.

The Innovative Materials and Processes for Advanced Carbon Capture Technologies (IMPACCT) program has a goal to reduce the cost of CO_2 capture to around \$15 per ton. Under this program, Codexis is developing new and efficient forms of enzymes known as carbonic anhydrases to absorb CO_2 more rapidly and under challenging conditions found in the gas exhaust of coal-fired power plants.

The Building Energy Efficiency Through Innovative Thermodevices (BEETIT) program focuses on new approaches and technologies for building cooling equipment and air conditioners. One recipient, ADMA Products, is looking at separating dehumidification from heating and cooling to create a high-efficiency system. Several projects have received follow-on support from the Navy.

The Grid-Scale Rampable Intermittent Dispatchable Storage (GRIDS) program looks at gridscale energy storage for integrating renewable energy. The U.S. uses the equivalent of about six Hoover Dams of energy per day. GRIDS is looking at flow batteries, compressed air energy storage, and other innovative approaches for large-scale energy storage.

The Agile Delivery of Electrical Power Technology (ADEPT) program focuses on advanced, energy efficient power conversion technologies. A lot of energy use goes through power electronics and there have been few advances in the past century. One ADEPT project is developing solid state converters and shrinking them to the size of a shoe box.

The Green Electricity Network Integration (GENI) program looks at hardware and software advances for the distribution of power on a grid. There are a number of approaches that are looking directly at power flows versus dumping power on the grid. A project by GE Global Research focuses on hardware solutions for the direct transmission of high voltage power from renewable sources to the grid.

The High Energy Advanced Thermal Storage (HEATS) program is a storage effort that is looking at thermal energy storage technologies in several different ways. It is balancing approaches at various scales—from small thermal batteries used to heat a car that could also extend the range of an electric vehicle, to combined heat and power systems that store heat and reduce energy consumption, up to large solar installations for solar-electric conversion.

The Rare Earth Alternatives in Critical Technologies (REACT) program is exploring costeffective alternatives to rare earths. An example is a synthetic approach to a new highly magnetic iron nitride alloy for electric motors.

The Plants Engineered to Replace Oil (PETRO) program is generating non-food crops that directly produce transportation fuel. The University of Florida is developing pine trees that generate up to 20 percent of their dry weight as sap. This source could be tapped while alive, like sugar maples.

ARPA-E has released two new solicitations. One is Methane Opportunities for Vehicular Energy (MOVE) that explores the use of natural gas for personal transportation. MOVE looks at developing innovative, low-cost natural gas storage technologies and methods at lower pressure in vehicle tanks that will help enable the widespread adoption of natural gas vehicles..

Advanced Management and Protection of Energy Storage Devices (AMPED) is looking at battery diagnostics. Currently batteries use only one quarter of their capability. AMPED explores novel approaches for real-time battery diagnostics to double the usable capacity.

ARPA-E also has an open solicitation. This is helpful for any technologies that do not fit into any of the existing programs. New ideas are received that might otherwise be missed. ARPA-E can also take a snapshot of the innovation landscape and recognize new directions. Thousands of applications have been received and review panels are assembling in the coming weeks with an anticipated announcement in September 2012.

Discussion

Lessons learned from failed projects include acknowledgement that the genetic tools needed to work with certain organisms and photosynthetic organisms do not exist. There is also a broad technology space for bioreactors. Lessons learned inform ARPA-E's decisions going forward.

It was pointed out that DARPA, by contrast, has supported program managers on assignment able to transfer to other agencies and further support the technologies initially funded at DARPA. The DOE does not have the Departments of the Navy or Army or other places for transition. Dr. Toone noted that ARPA-E has program managers with early stage translation experience. Unlike DARPA, ARPA-E does not have a customer but strives to move products toward the market. Translation is guided by Cheryl Martin, Deputy Director for Commercialization, and her team which thinks about moving things toward market. ARPA-E is acutely aware of these issues and is putting things into place to address this.

ARPA-E is situated in a logical space between basic science and applied programs and is an important DOE partner. It is the first point for demonstrating technology before things move to larger scale in applied programs and other places. ARPA-E is participating in the SunShot Initiative, on biofuel issues, and working hard to integrate with all parts of DOE.

Presentation: Integrated Multi-Scale Modeling of Structural Materials

Professor John Allison of the University of Michigan described his work on the DOE Software Innovation Center for Integrated Multi-Scale Modeling of Structural Metals.⁶ The effort is called Predictive Integrated Structural Materials Science (PRISMS).

The Materials Genome Initiative (MGI) has presented an opportunity for this field. The groundwork started in the late 1980s with discussions about materials science. The DOE Advanced Strategic Computing Initiative continued the conversation and by the late 1990s and early part of 2000 multiple efforts were underway. Work in recent years led to the MGI and has created a tipping point for this field.

The U.S. National Materials Advisory Board – Committee on Integrated Computational Materials Engineering (ICME) supported a vision to unite materials science with materials engineering and integrate materials more holistically in product development. The ICME looks to bridge manufacturing process simulation with constitutive models and engineering product performance analysis. This consists of chemistry thermodynamics diffusion fed through quantitative process-structure relations and structure-property relations. The goals are to drive this backwards to find new materials. This has previously been done in pieces but not together.

ICME is emerging as a transformational discipline. It has shown a return on investment of 3:1 to 9:1 in industry. The integration of domains around ICME will be important and be fostered by a cultural shift in sharing ideas and by the community embracing it as a discipline.

The PRISMS Center seeks to establish an integrated multi-scale modeling framework and open source software and develop advanced open source computational methods through tightly coupled with experiments and models. The Center will focus on specific materials to start and will establish an open source knowledge repository for the community.

PRISMS will look at fatigue and ductility of magnesium alloys based on Professor Allison's prior work at the Ford Motor Company. Since the Wright Brothers' flight in 1906, it took more than 90 years to get to the same point in alloy development. The science in this area is largely phenomenological; a comprehensive team can help advance work in fatigue and ductility.

The PRISMS proposal team has looked at appropriate mathematical descriptions to build a hierarchical understanding of computational efficiency. This is shared in an open source integrated platform. Dr. Vikram Gavini is working on real-space formulation of density functional theory as a basis for large-scale electron-structure calculations. A quasi-continuum technique and a linear scaling method allows for looking at multiple millions of atoms. Dr.

⁶ http://science.energy.gov/~/media/bes/besac/powerpoint/20120726/Allison.pptx Basic Energy Sciences Advisory Committee July 26 – 27, 2012 – Meeting Minutes

Anton Van der Ven uses traditional cluster approximations to work on free energies, mobilities and constitutive law in CASM and chemical constitutive law. Dr. Katsuyo Thornton is using phase field methods to study recrystallization and grain growth, and phase field crystals at an atomistic level and diffusive time scaleOne research challenge is to figure out how to deal with new methods as they emerge. Dr. Veera Sundararaghavan is working on grain level resolution of plasticity models. This will be fed by model parameters from first principles computations. Dr. Krishna Garikipati is working on a variational multiscale method for shear bands and cracking.

Experimentation is key and PRISMS tightly couples experiments and models. Experiments will help understand mechanisms, fill gaps in theory, and validate models.

Dr. Emmanuelle Marquis is working with Professor Allison on three-dimensional microstructural characterization for developing and validating microstructural models. Professor Sam Daly is doing full-field mapping at the microstructural length scale as experimental input and validation for computational efforts. Dr. J. Wayne Jones is researching ultrasonic fatigue at microstructural extremes with more quantitative data than is used with ordinary techniques.

PRISMS also has a goal in the Materials Commons. Dr. H.V. Jagadish and Associate Dean Margaret Hedstrom are working to develop an open source knowledge repository and virtual collaboration platform. Workflow processes are important and more streamlined processes are needed to get data in the right places and to establish standards for sharing practices and policies. The platform will be used for the Open Source PRISMS Community and viewed as a community resource.

In conculsion, we are at a tipping point. The DOE Software Innovation Center for Integrated Multi-Scale Modeling of Structural Metals has been designed to provide a suite of professional, open-source computational tools. Models are closely-coupled with unique experimental capabilities for model development, input, and validation.

Discussion

The PRISMS Center will focus on interesting model materials in the coming five years and seeks to develop the capability rather than new materials. However, there is poor understanding of magnesium alloys and why these have such high strength. Research will consider alloys with a small number of elements (4 or 5) to achieve a similar response.

In exploring the potential for a new computational capability that could be available others, Professor Allison sees the solution in discussions of open source policy. The community needs a trusted collaborator model with full access to code for continued development. His goal is for industry and academia to be able to use the new capabilties. Professor Allison was asked about executable software and if his group would provide support or if people would operate on their own and learn as they go. His group has discussed the need for continuing education and clear documentation. Spin-offs could be developed from this project and leverage the open space environment which would allow continuance of this work even if a center or project lapses. Dr. Hemminger sees the benefit of this concept and being able to generate usable code that can continue to be supported. He believes that BESAC understands this goal and responsibility.

Continuing the discussion of open source capabilities, Dr. French asked about putting this on Open Forge and continuing it there or hosting this at the University of Michigan. Professor Allison's project does not have any preconceived notions but sees a good model in the health community. Setting up standard practices and the type of site that is needed is important.

Presentation: Mesoscale Subcommittee Update

Dr. George Crabtree and Dr. John Sarrao shared an update on the subcommittee's work.⁷ The charge for this initiative was given in February 2011 and a report is expected in Fall 2012. In the interim, the subcommittee has presented a draft publication entitled "From Quanta to the Continuum: Opportunities for Mesoscale Science."

"Meso" is now more clearly defined due to town hall meetings and the collection of inputs at http://www.meso2012.com from more than 1,000 people. This has led to the production of more than 100 quad charts that describe the opportunity, approach, challenge, and impact, and helped distill overall thinking about this area of research.

Meso supports the need for continued innovation, the creation of new insights and tools. It does not replace other sciences such as nanoscience. Meso works beyond atomic, molecular and nano levels. It exists within the evolution from quantum to classical, from isolated to interacting collectives, and from simpler and perfect homogeneity to complexity. Within the mesoscale, dynamism and functionality are very important. Meso rests where structures come together and where functionality occurs.

Meso is a space where multiple degrees of freedom interact as seen in biological complexity with inorganic materials. Consilience is a term that defines this. It is not a question of a single spatial, temporal energy scale but multiple scales that aid understanding and the exploitation of other challenges. In this scale, there is a natural challenge to think about things from a top-down and bottom-up way, and meso is an opportunity to think about it both ways.

The interacting degrees of freedom between light and matter are an example that can be exploited. Photonic behavior can be controlled to inspire new technologies. This gives a broad space for the science and impact and asks how interactions come together at varying scales.

Functionality at the mesoscale is characterized by defects and interfaces which can be exploited. This is only first obvious at the mesoscale and seen in catalytic reactive surfaces, superconductors, and in functional mesospores.

Previous work has been done at the mesoscale. What is exciting is shifting from a reductionist perspective to a constructionist view and the opportunities that then arise.

This emerging definition is a large part of what the subcommittee is addressing and has distilled into priority research directions in its draft report.

⁷ http://science.energy.gov/~/media/bes/besac/powerpoint/20120726/Sarrao_Crabtree-7_26.pptx Basic Energy Sciences Advisory Committee July 26 – 27, 2012 – Meeting Minutes

The first priority research direction is focused on mastering defect mesostructure and its evolution. We have a reasonable understanding of lattice deformation and understand how crack initiation and propogation happens. So now, how do we control it?

The second priority research direction on coupled reactions and pathway-dependent chemical processes relates to, for example, reactive surfaces, sequestration, and surfaces in batteries. Research on accelerating or inhibiting specific reactions can advance energy solutions.

The third priority research direction is on optimizing transport and response through design and control of mesoscale structure. Multiplicity of scale is central and a systems view is another piece. This is not just about controlling one degree of freedom but optimizing them all simultaneously to understand how they occur, recognize the possibilities in this space, and exploit the functionality.

Another priority research direction at the mesoscale is the elucidation of non-equilibrium and many bodied physics of electrons. At question is how to make contact with a variety of these electrons in systems that are intrinsically heterogeneous.

A fifth priority research direction is harnessing the fluctuations, dynamics and degradation for the control of metastable mesoscale systems. The significance is that for a particular intermediate length scale, dynamics are at many scales. In meso, you can elicit control as is shown in nature. At question is how to organize this to move beyond what biology does well.

A final priority research direction is the directed assembly of hierarchical functional materials. At the mesoscale, top-down and bottom-up are integrated. A set of architectures brought together can allow the harnessing of multiple degrees of freedom to give desired performance.

These research areas frame scientific challenges and demonstrate potential outcomes. Integration of synthesis, characterization and theory simulation can present new opportunities at the boundaries that have not been previously emphasized. Success is driven by the challenge of working together and using emerging tools to make progress.

There is opportunity for mesoscale tools and instruments. In synthesis by design, the development of meso structures from both top and bottom with function is a challenge. This can drive computational tools based on the need to observe the processes and expand understanding. Characterization is similar as it necessitates new understanding to advance functionality. We need to be able to observe an operating system. This requires multi-modal measurements that occur simultaneously. Part of the curse of opportunity is that the data produced is so massive that it needs to be mined effectively.

Theory and simulation tools are needed that work across scales in a robust and reliable way in order to exploit architecture for materials by design.

A community of mesoscale scientists is needed to address these opportunities. This is a modality of research that was foreshadowed in other discussions. New interdisciplinary research necessitates bringing people together to work across boundaries and interfaces.

Meso is an opportunity space that can have a transformational impact. Manufacturing practices can be transformed through advanced mesoscale understanding. It holds the promise to move from top-down to bottom-up design, producing next-generation technological innovation.

Discussion

BESAC discussed the appeal of the draft report to audiences with limited understanding or scientific knowledge. Drafting this as a teaching document with the help of a science writer and illustrations in the executive summary and introduction were suggestions offered to enable understanding of mesoscale science by Congressional staffers and other public stakeholders. A short pamphlet of about 10 pages with illustrations was suggested for staffers. The document could show how basic mesoscale research is fundamental to better batteries and other examples.

Industry partners could be powerful allies. Manufacturing and chief technology officers have a technology stake in mesoscale science and getting their input on the report could be useful. Industry needs to see this as the next frontier to be addressed.

Cross-cutting themes were seen as missing from the current draft. It explores priority research directions, but what are the commonalities, tools, theories and capabilities that are needed. Dr. Crabtree explained that this part of the report could feature more cross-cutting themes and describe possible impacts.

Other missing pieces are societal connections and impacts, and connections to the biological world. It was suggested that additional input from a biologist could be helpful. It was suggested that research areas five and six may not fit as separate and important research directions.

It was suggested that the scope of the report may be too broad. It may be promising or demonstrating that meso is all important and thus not really anything. Dr. Rubloff responded that the societal impacts and values must be clear. There are a lot of themes in the report, but there are others that can be developed that are specific to the mesoscale problem.

While communicating to Congress is important, Dr. Hemminger reminded BESAC of Dr. Brinkman's concern about over-emphasizing applied science. Scientifically-minded readers can see that there are fundamental scientific issues to which we lack answers. BES is about basic science and there is a lot of fundamental science to be done in this area before achieving a societal impact.

Presentation: Linac Coherent Light Source Update

The Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory is an Office of Science User Facility. It houses an x-ray free electron laser.

An x-ray free electron laser (XFEL) is based on free electrons and not atomic or bound electrons. Electrons are bunched and the bunches are amplified either by their own radiation or imposed radiation. The electrons fall into order and march simultaneously to generate significant intensity.

The LCLS is one of two free electron lasers in the world and is the most powerful. Currently it only uses one kilometer of the linac. It is precisely aligned, with variance less than the width of a human hair over 100 meters. The x-ray tunnel is 200 meters long.

There have been 703 proposals received with about 15 scientists per proposal from all over the world. Only about one in five proposals are accepted. This is based on scientific merit and beam delivery is up to 95 percent of the beam time. There have been many publications. Most take about 18 months and appear in high-impact journals.

Dr. Stohr explained the properties of the x-ray laser. In a storage ring, the electrons are independent and independently radiate. The pulse width is about 100 ps. The pulse effect causes electrons to move in two and result in the number of electrons squared at a rate of 10 to the 10. Comparitively at 1 eV, the numbers of XFEL photons per pulse approximately equals the number of storage ring photons in one second. The photons from the XFEL are coherent and indistinguishable.

The size and speed of things are relative, with the notion that smaller equates to faster. We can currently study things on timescales of nanoseconds. If we can study things on timescales of femtoseconds, we can get five orders of magnitude in efficiency

Optical lasers are blind to the nanoworld due to diffraction. Synchrotron sources, however, can see the nanoworld but lack the ability to study the ultrafast. X-ray lasers can achieve all that is needed. Fundamental to this is knowing how fast things move. Small things will always be faster. Light is a fundamental aspect to this.

Dr. Stohr shared three examples of work coming out of LCLS that can impact society. Within biological structure and function, drug design and health are being impacted. Biological studies are conducted on very large structures. The central challenge is that high radiation dose causes changes in molecular structure or damage. LCLS has learned the tolerable dosage limits in cryogenically-cooled crystals. Large crystals are not a problem, but small ones can suffer damage due to lengthy exposure. The new paradigm being explored is nanocrystal diffraction.

A second example is in chemistry looking at photosynthetic reaction centers. Photosystem II underlies photosynthesis and work is being done on magnesium clusters. This cluster is not well understood since x-ray damage has prevented conclusive structure determination. LCLS used ultra-fast pulses for x-ray diffraction to elucidate the atomic structure. People are also looking at electron bonds, but the techniques are sensitive. Future studies will look at reaction dynamics.

The third example is in materials science and resembles the meso discussion. It addresses data storage challenges and the need for incredible amounts of storage. The magnetic bits of data must be stable for years but you must be able to flip the magnetic spin very fast when writing

data. The technology roadmap calls for lasers in hard drives with the ability to zap bits to bring about switching. A laser can focus in a small area and studies have shown that magnetic materials can be used with lasers. An experiment was conducted on a GdFeCo alloy where optical pulses triggered a switch in magnetization. The LCLS beam went through the same spot and generated a diffraction pattern. Magnetization was studied as a function of time and as a function of location to understand what happens on the atomic scale. Nanoscale order was found in this "amorphous" material. The magnetization of the nano regions switches first to drive the macroscopic switching.

LCLS-II is expanding the capability and capacity of LCLS. There is competition from Japan, Korea, Switzerland and Germany that is pushing the U.S. to stay competitive.

Dr. Stohr believes that x-ray lasers are the latest step in the light revolution, starting with the light bulb in 1879. The x-ray free electron laser in 2010 marks the next step when lasers entered the scene.

Discussion

Dr. Ratner asked about the ability to study the dynamic structure of the photosystem II example. Dr. Stohr explained beam time is the limiting factor. The time scale is quite long and LCLS can hone in on a specific piece of that cycle. Nanoseconds are too slow so work must be done in femtoseconds. Dr. Ratner suggested working in picoseconds. Dr. Stohr commented that working in that time scale requires taking pictures to create a movie. The pictures themselves are in femtoseconds to avoid radiation damage.

Discussion: Mesoscale Discussion

Dr. Crabtree thanked BESAC for prior comments on the report and thoughts on outreach to the scientific community, Congressional staffers, and the public. The report will be revised accordingly.

Dr. McCurdy commented that the subcommittee was asked to define meso and the space in which it operates. It has been given an intellectual problem but little direction on how to solve it. The examples in the report are good but are somewhat disparate.

BESAC took up the discussion of developing a front-end portion of the report to inform nonscientific audiences. Several members noted that a definition of mesoscale science is still lacking. Dr. Chiang pointed out that there are multiple definitions being discussed.

Several members highlighted the need for a clearly-worded summary. Suggested approaches included a six to ten-page executive summary that could be used to develop an elevator speech. Elevator speeches should be tailored for specific audiences. There are a number of suitable examples available with interesting functions that do not exist in isolated systems. Dr. Hemminger urged that that connection be made and emphasized to show what is important about mesoscale interactions. "Interactions" is a key word.

Dr. Hemminger reminded BESAC that push-back from Congress came from a staff member who asked for a plan of action. This was at a time when BES did not yet know what to do about meso.

Dr. Tobias suggested putting more emphasis on the need for organizing principles and new laws of physics that inform how function emerges from smaller building blocks. This gets back to questions about laws of nature that are not understood. Dr. Crabtree noted that there are intereresting questions for the community such as: What directs self assembly? What determines a dynamic steady state? What unifies top down and bottom up? Dr. Greene suggested that explanations of the area between the quantum and continuum, electronic self-organization, and building a functional superconductor are needed and could be part of the elevator speech. Dr. Hemminger commented on the apparent need for an intermediate length document that could evolve from a solid executive summary and be something that people are interested in taking to industrial contacts for input.

An elevator speech for the scientifically-educated person is needed, said Dr. Ceyer. The microscopic and quantum properties of atoms and molecules are known, but we don't know how to build statistical mechanics for interacting particles or non-equilibrium systems.

Dr. Barletta suggested care in describing the societal impact of meso. Something that provides a short-term benefit is not useful. The enumeration of big problems that require deep science is needed where mesoscience will enable us to overcome roadblocks. Giant magnetoresistance is one example of a mesoscopic phenomenon, said Dr. Hemminger. One could argue that this phenomena is responsible for revolutionizing memory storage. It is important to talk about potential impacts we can have in areas the lay person is interested in.

Dr. Berrah pointed out that the second charge to the subcommittee talked about how current and future facilities can advance mesoscale science. The draft report illustrates the current role but not a future one.

The issue of training is one that could be emphasized in the document. There could be many models and ways to think about the future workforce at facilities, and how to generate more scientists and students. In the context of workforce development, Dr. Hemminger would like thoughts from BES on audiences for this report. He wonders if it is acceptable to state that DOE should make fellowship investments and support student and postdoctoral interactions, as well as position people at BES facilities with facility staff who could serve as mentors. Dr. Kung commented that prior successful reports have remained at a higher level and left execution to the DOE offices. The Grand Challenges report is an example that offers balance in terms of the type of recommendations offered. She noted that workforce development is supported as part of research investments. SC is not in the mainline business of training or education yet this is recognized as an integral output of SC's investments. Dr. Crabtree suggested that training should be described in the report as a component of research. Combining students with mentor teams and national laboratories can provide broader exposure for students. Dr. Hemminger urged the subcommittee to not be overly prescriptive but to take care in discussing the integration of characterization, sythesis, and theory and how students and postdocs can be trained to be conversant across them. Dr. Barletta suggested finding the right words to describe how students

can enter society and tackle hard problems, but need new capabilities and tools for these challenges.

Dr. Hemminger asked the subcommittee to prepare a response to the day's discussions for the start of day two, especially consideration of multiple audiences and a well-written executive summary and introduction.

Public comment

Miguel Salmeron of Lawrence Berkeley National Laboratory commented that the choice of the word mesoscale is important. "Nanometer" is a term that is immediately understood. Mesoscale needs to mean something and convey the potential of this science. The function that results from complexity should be described and translated for anyone to understand.

Sean Smith of Oak Ridge National Laboratory suggested that the subcommittee consider a tiered-approach of explanations, based on comments from the Senate and House and helping them understand the scientific examples that explain where mesoscale fits. An example is developing a break-through material that can impact society. A tiered-approach with examples at a higher level could lead down to the fundamental science that is needed.

Charles Barbour from Sandia National Laboratory expressed concern about how meso will go beyond nano. This discussion ties back to a prior workshop on complex coupled phenomena. The subcommittee might look at the scientific questions that were addressed then since a huge part of the mesoscale discussion is the behavior emerging from complex systems.

Board business

The meeting was adjourned at 4:58 p.m.

Friday, July 27, 2012

Dr. John Hemminger, BESAC Chair, began the BESAC meeting began at 9:00 a.m. He reiterated the desire to wrap-up the mesoscale discussion. Each year, BESAC organizes a COV for one of the divisions. Dr. Hemminger reminded BESAC that the Facilities Division COV will occur this year and there will be a COV for the EFRCs and the Fuels from Sunlight Hub solicitation. In addition, Pat Dehmer has asked for a COV for the SC WDTS (Workforce Development for Teachers and Scientists) program. These COVs will entail greater BESAC involvement than prior years.

The next BESAC meeting will occur on February 28 – March 1, 2013.

Presentation: Science Serving the Nation

Dr. Linda Horton, Director, Materials Sciences and Engineering Division, Office of Basic Energy Sciences, described recent BES publications for improved communications. Three

reports have been completed over the past year. Dr. Horton described the "Science Serving the Nation" brochure.⁸

The original document was published in 1996 and featured specific relationships, products, and a demonstration of BES research impacts. The new document was developed from success stories from laboratories and grants featured on the SC website, the BESAC workshop "Science for Energy Technology: Strengthening the Link between Basic Research and Industry," and the Basic Research Needs workshops. Content was gathered from principal investigators (PIs) and a working group selected highlights and consolidated inputs.

The brochure captured content from three-panel charts that highlighted BES-supported science, applied research funded by others, and commercial applications. This lead to vignettes sorted into four themes. Dr. Horton shared three vignettes demonstrating one of the themes in the brochure: "Better Ways to Tap the Sun's Energy." The brochure features scientific impacts including Nobel Prize recipients, BES PIs who are members of the National Academies, and BES user facilities.

BES' next step is to more detailed information on the SC website to accompany the brochure. The format is similar to the SC "Discovery and Innovation Stories." Photographs, taglines and teasers compel users to read more and follow links to more information.

The BES website will soon include a "BES Highlights" page that will be a repository for stories featured in the brochure and new ones going forward. A link to each highlight will allow for more in-depth information on the science, the impact, company names, and details including the lead researcher or point-of-contact, funding details, publications, and related links. Company names are not found in the brochure.

A final step is revising the "Benefits of BES" webpage. The revised page will feature excellence in science, such as Nobel prizes; user facilities; and short summary text on the impact on energy technologies within each theme of the brochure. One change from the brochure will be changing the title of the theme "Innovative Seeds for Clean Energy Technology" to "Science Driving Transportation Innovations."

New examples will be added on a frequent basis and the newest vignettes will appear at the top of the web page. The format on the web will be standardized and is nearing completion. The web resource will serve as a living document and continue to be refreshed while the brochure will not be republished.

Discussion

Dr. Ratner expressed appreciation for the ability to easily find this information on the website.

Presentation: COV for the Materials Sciences and Engineering Division

⁸ http://science.energy.gov/~/media/bes/pdf/brochures/files/BES_SSN.pdf Basic Energy Sciences Advisory Committee July 26 – 27, 2012 – Meeting Minutes

Dr. Matthew Tirrell, University of Chicago, provided a review of the COV for the Materials Sciences and Engineering Division. A lot of work was done beforehand with Dr. Hemminger and Dr. Horton to plan the COV and compose the participant list. It consisted of a mix of researchers who currently receive funding from BES and those that do not; academic, national laboratory, and industrial researchers; those who have previously served on a COV and those who have not; and representatives from EPSCoR states. The final work was done in collaboration with panel leaders Margaret Murnane, Juan de Pablo, Max Lagally, and John Sarrao. The COV consisted of presentations by Dr. Kung and others.

Information on the Division was shared on the morning of day one and the first panel read was completed by the end of the day. On the second day, the COV panel members switched for a second read. Each panel considered about 30 proposals presented in technical program areas, and initially selected by DOE staff. The proposals ranged from easy to difficult award decisions, both recommended awards and declinations. The COV worked well together and completed its work on time.

The COV resulted in many findings. Dr. Tirrell pointed out that the work supported by the Division is of a very high standard, nationally and internationally, and the work balances superb scientific quality with investment in high-risk and high-reward research. The caliber of staff work meets a high standard of professionalism. Proposal reviews are done with thoroughness and consistency, and program managers use the review process well. In the spectrum of agencies supporting materials research in the U.S., the Division plays a unique and valuable role, helping to maintain the U.S.'s position in this field. There is sufficient dynamism to support turnover of the work.

The research being supported is worthy of support but there are many untapped areas that are also worthy of support. An example is increased funding for small and intermediate scale instrumentation. There is no data available on the gender and demographics of research PIs and students. It was noted that the presentation of information to the COV for university grants and for laboratory programs was different. There was concern that this was leading to different degrees of attention paid to the programs in the reviews.

The COV discussed the use of white papers and how they could be leveraged. People might have unsuitable ideas that are discouraged. This form of declination is not accurately reflected in the statistics on proposal pressure. The COV wanted to understand better the stats on white papers. White papers might provide useful information on content and trends in the Division programs.

There is untapped potential with good ideas being left on the table. More research support would produce more good results. Program managers in all Division programs benefit from and are constricted in their ability to travel due to funding. They maintain contact with the scientific community as well as they can. A modest increase of support in this area would go a long way.

There is a need to maintain a balance between scientific funding of PIs and funding of facilities in order to take advantage of facilities. The Portfolio And Management System (PAMS) needs to be implemented as the current information management approach is inefficient.

The COV would like to see a database on the demographics of people supported by the Division. Also, although the time-to-decision statistics are improving in significant ways, the declination of proposals, even if given verbally, should be put in writing.

The COV likes the use of white papers but would like to see them tracked more clearly and with more documentation in the review process for the next COV and possibly to document the kinds of requests that come to the Division.

The use of rebuttals in the review process can help shape close decisions and provide feedback on the job that reviewers are doing. Program managers need to understand the style and substance of reviews that they are getting.

Future COVs should be provided a better perspective on the review process and oversight for laboratory programs to complete a proper evaluation. The COV bears some responsibility for not dealing perfectly with differing levels of documentation, especially with big laboratory projects versus smaller university grants. If there is any issue here, it is probably more on the side of how COV works versus how the Division works.

A review of EPSCoR was led by Dr. Sarrao. The renewal rate should be lower than the DMSE core program and current limitations can promote positive turnover and meet the program's aim to develop science and engineering capabilities in EPSCoR regions. It was recommended that longitudinal tracking of EPSCoR PIs using quantitative metrics would be valuable.

The last three fiscal years were very strong for DMSE. It supports a strong scientific portfolio, and overall decision-making and review processes are excellent.

Discussion

Dr. Barletta thought it striking that there were not enough funds for program managers to travel. He was unsure how the ARPA-E program managers have enough funds to go into the field twice per year.

Because all submissions are electronic and managed electronically, there was discussion on why the portfolio management system is not yet functioning. It was pointed out that and the system will be used not only to submit proposals, but for all aspects of proposal management. Under Dr. Dehmer's direction, SC has taken this on and has worked hard to make this effective. The system is SC-wide and has to take in all offices' policies and procedures and must interface with other IT systems, not only grants.gov. Long ago, every reviewer had their own list of proposals and information. Every COV has brought up this issue. The impression is that SC is getting closer to something more functional.

The recommendation on looking at the demographics of PIs and graduate students was well received. Dr. Kirby noted that it is hard to understand trends if you don't at least have a starting place to understand the community and make it more diverse. The COV thought this would be valuable and there are some political obstacles to be overcome. It was suggested that data can be collected voluntarily, as NSF does. When NSF gives that opportunity, people tend to provide that

information. In Linda Blevins' discussion of PAMS, she pointed out that SC is tackling this and they have to work through approvals, using enough firewalls in the database.

Dr. Cuenya asked about the rate of renewals from different prgorams. This review was not a comparative review, but the belief is that people have a fair shot at acceptance regardless of program. Different program managers saw a reasonable number of new PIs in their program and things looked reasonable when comparing programs in the division.

There was a motion to formally accept the recommendations that will then be submitted to Dr. Brinkman. BESAC agreed to accept with no dissention. There was a reminder to ask the Division Director to address BESAC at its next meeting on response to the recommendations.

Presentation: Resumption of Mesoscale Discussion

Dr. Crabtree and **Dr. Sarrao** shared a response to the previous day's discussions. They presented a six-point plan for bringing closure to the mesoscale report.

Editorial issues and cleaning-up of content will be addressed by subcommittee members. Dr. Crabtree and Dr. Sarrao would welcome and input and notes from BESAC members and will follow-up after a review of these notes.

Comments on priority research areas have been gathered and will inform the revisions of these descriptions.

The subcommittee will enhance the issue of cross-cutting themes to show links to future capabilities and workforce development.

The executive summary and introduction will be enhanced with imagery and sidebar information, and the subcommittee will work with BESAC members to accomplish this.

A shorter document will be explored with an emphasis on reaching general audiences.

An outreach plan will be developed that considers an elevator speech to drive home the message of the report. An important facet is engagement with the industrial community. Industry input in the report needs to be balanced.

The subcommittee will work to complete the report by the end of August 2012 and deliver on the six directions that have been described.

The report will also transform the draft message from a scientific view of meso to a broader message that includes information on the potential outcomes of meso. It will elaborate on harnessing the ability to creates things at lower costs and faster rates with greater performance and lifetimes. The potential is to work like nature can in driving energy conversion, transmission and storage with earth abundant materials. And there is potential to create functional design in top-down and bottom-up ways to enable a new generation of technological innovation.

Discussion

It was urged that the message not be too overarching and overreaching. The subcommittee will discuss the engagement of a science writer to help edit the content. It will also discuss the creation and implementation of one well-arranged report or several different types of documents to address varied audiences, or just a layman-level abstract and then the subcommittee document. One could be for Congressional staff members and the public, and strive to make a compelling case for meso, tying it to national needs and applications. Another could speak to scientists and hope to generate new ideas. An executive summary might be accessible to all readers and should emphasize the possible outcomes and vision of success. Sidebars may also help to call out unsolved problems and potential solutions. A preface might also be a useful component that allows skipping to the main report.

The BESAC members discussed the content of the draft report and what might be missing.

A compelling title might speak to how a collection of smaller objects unite and how function emerges from this. An example could be "Building Blocks to Function." This could help get past words such as "quantum" and meso that are not clear to everyone. Dr. Crabtree commented on how this could be part of a subtitle.

Questions at the beginning can highlight problems that cannot be solved now. Describing the return on investment could convince a reader why they should care about meso. By the title alone, there is not a call of a great new thing. Mescoscale science relies on new instrumentation, and will capitalize on investments in current facilities, including the nanoscience centers.

The document could touch on seeing inside operating systems at the nanometer level. New ways of doing this are being developed. The report should focus not just on nano but also different length scales and time scales to convey the benefits to the public.

The report could also emphasize scalability, such as using the same instrument for nanometer and micron measurements, and the need for new instrumentation to achieve the goals in the report. Functionality and the potential outcomes are another needed piece in the explanation.

Specific topical areas should be sensitive to political implications and as straying beyond BES' mandate. For instance, an example that describes drug delivery might be perceived as encroaching upon work that NIH supports.

The report should use simple and easily-interpreted figures and captions that also show how things are related. Figures used in an executive report or in a preface could also be repeated later in the document.

In discussing the timeline for the report, Dr. Hemminger noted that the report needs to be completed by the end of August. Previously, there have been meetings to give feedback to subcommittees tasked with report development. For this is to be a BESAC report, a process for the subcommittee needs to be provided today.

Dr. Hemminger noted that many BESAC members have volunteered to support the report development and he encourage the subcommittee to reach out to BESAC members for help. He asked BESAC if enough feedback has been provide and if the process going forward can be approve. Dr. Lagally approved the motion, Dr. McCurdy seconded the motion, and all were in favor.

Public comment

None

Board business

Dr. Hemminger reminded the BESAC that the mesoscale science report will have to be done by mid-August. He also noted that members will be contacted about the upcoming COVs.

The meeting was adjourned at 10:33 a.m.