BASIC ENERGY SCIENCES ADVISORY COMMITTEE

MEETING MINUTES

Bethesda North Marriott Hotel & Conference Center

5701 Marinelli Road, North Bethesda, MD 20852

February 23 - 24, 2012

PARTICIPANTS

BESAC members present:
Simon Bare
William Barletta
Nora Berrah
Gordon Brown
Sylvia Ceyer
Ye-Ming Chiang
George Crabtree
Peter Cummings
Beatriz Roldan Cuenya
Frank DiSalvo
Roger French
Bruce Gates
Laura Greene
Ernie Hall
Sharon Hammes-Schiffer
John Hemminger, Chair
Bruce Kay
Max Lagally
William McCurdy, Jr.
Mark Ratner
John Richards
John Spence
Douglas Tobias
John Tranquada

BESAC members not present:
Allen Goldman
Kate Kirby

Also participating:
William Brinkman, Director, Office of Science
Wayne Gordon, DOE Office of General Counsel
Linda Horton, Director, Division for Material Sciences
Harriet Kung, Director, Office of Science, Office of Basic Energy Sciences
Arun Majumdar, Acting Under Secretary of Energy
Katie Perine, Office of Science, Basic Energy Sciences, Committee Manager
John Sarrao, Lawrence Livermore National Laboratory
Mike Simonson, Oak Ridge National Laboratory
Marc Kastner, Massachusetts Institute of Technology
Gary Rubloff, University of Maryland

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

MEETING MINUTES

Thursday, February 23, 2012

Prior to the full Basic Energy Sciences Advisory Committee (BESAC) Meeting, a closed session was held from 8:30 a.m. to 8:45 a.m. and conducted by **Wayne Gordon** of the U.S. Department of Energy (DOE) Office of General Counsel.

The public meeting was called to order by BESAC Chair **Dr. John Hemminger** at 8:49 a.m. Dr. Hemminger reviewed the agenda and welcomed **Dr. William Brinkman**, Director, DOE Office of Science (SC).

Presentation: News from the DOE Office of Science

Dr. Brinkman gave an update on recent progress and budget developments.[1] In opening, he noted that SC achievements are reflected by the more than 100 Nobel Prizes given to SC-supported researchers over the past 60 years. SC also provides 45 percent of all Federal support for physical and energy-related sciences and key research in biology and computing. SC supports more than 25,000 Ph.D. scientists, students, and support staff at more than 300 institutions. SC's portfolio of science user facilities is the largest in the world and supports 26,500 users.

DOE and SC efforts to support research lead to innovation and economic growth, and reflect the Administration's interest in science and technology. There is a continuing need to advance basic science and develop a highly-trained workforce as foundations for economic growth and to manage emerging concerns such as energy problems and diminishing state-based support for research institutions.

SC's capabilities are well-organized and address critical national needs. The role of the Energy Frontier Research Centers (EFRCs) will continue to expand. The Combustion Research Facility at Sandia National Laboratories is advancing, as is the Joint Genome Institute in Walnut Creek, CA, which will move to a second Lawrence Berkeley National Laboratory campus aimed at bringing together all biosciences activities in one place. SC's portfolio is rounded out by Bioenergy Research Centers, the five Nanoscience Centers, and the new Energy Innovation Hubs.

Three themes drive the SC FY 2013 budget request: 1) Materials and chemical processes by design, including the synthesis of materials and role of materials, 2) Biosystems by design, including work to find new microbes and analysis of genomic datasets, and 3) Modeling and simulation. Materials and chemistry by design was highlighted by Dr. Brinkman, in particular efforts to identify new functional materials through theory and then validate the theoretical work through materials synthesis. This could eventually lead to online software available for community use. He also emphasized work being done in Biosystems by Design.

[1] http://science.energy.gov/~/media/bes/besac/pdf/20120224/Brinkman.pdf

SC's overall FY 2013 budget request to Congress of $4,992,052K is 2.4 percent higher than the FY 2012 appropriation of $4,873,634K. Dr. Brinkman noted the 3.3 percent increase for Advanced Scientific Computing Research (ASCR) and 3.6 percent increase for Biological and Environmental Research (BER). Dr. Brinkman hopes that BESAC members and supporters will share their stories with members on the Hill, and he will continue to talk with elected officials.

Dr. Brinkman shared the DOE and SC organizational chart, expressing a desire to expand the workforce development program, which includes the SC graduate fellowship program, to train future leaders in science and technology.

Within SC, ASCR seeks to construct and manage next generation computers and supports a movement to exascale computing. Petaflop machines are currently in use, such as new 10 petaflop machines at the Argonne and Oak Ridge National Laboratories. The movement to exascale is challenged by the need for a roadmap and managing issues such as power use. An exascale computing system needs to use less power by a factor of 10 while also limiting statistical errors. A selling point for SC in Congress is the demonstration of DOE facility use by industry and the DOE's development of software for the marketplace.

The Basic Energy Sciences (BES) office of SC is meeting clean energy challenges with research in batteries, solar cells, and other areas. BES needs to upgrade and enhance facilities, such as the LCLS (Linac Coherent Light Source), the NSLS (National Synchrotron Light Source), and the APS (Advanced Photon Source).

The 46 Energy Frontier Research Centers are part of the BES portfolio. The Centers are being reviewed and 50 percent have been evaluated at this time. Congress wants know how the Centers are doing.

The Materials by Design component is advancing work in areas such as light absorption in wire arrays where Al_2O_3 nanoparticles are incorporated in a polymer surrounding light absorbing nanowires. The nanoparticles scatter light towards the nanowires resulting in more efficient light absorption.

Two other areas emphasized by Dr. Brinkman were the Fuels from Sunlight hub, and the increasing use of BES scientific facilities by industry. In the latter, the Eli Lilly Corporation, as one example, leverages facilities everyday to advance drug development.

The Office of Biological and Environmental Research (BER) has finished the review of three bioenergy research centers. They look very strong, and each has found its niche. The BioEnergy Science Center (BESC) is working on lignin synthesis in switchgrass. The Joint BioEnergy Institute (JBEI) is focused on using synthetic biology to create microbes that produce fuels. The Great Lakes Bioenergy Research Center (GLBRC) is examining plants and soils for the production of biofuels to inform land management strategies.

BER's Joint Genome Institute (JGI) is advancing metagenomics to manage challenges in culturing microbes and the complicated interactions among communities of microbes. BER is also supporting work on aerosols and how they interact, and examining water condensation on aerosols. DOE is making important contributions to a community earth model with work being done at Lawrence Livermore National Laboratories (LLNL) among other places. This impacts the work of the Intergovernmental Panel on Climate Change (IPCC). DOE also works with the U.S. Global Change Research Program (GCRP) to coordinate inter-agency climate research.

Fusion Energy Sciences (FES) within SC is advancing several fusion approaches including inertial and magnetic confinement. ITER construction is advancing. The project budget is around $25B. The European Union will provide 1B Euros this year and next. The U.S. has requested $150M in FY 2013 and will deliver in-kind pieces such as the water cooling system and central solenoid. The U.S. is sending little money overseas. Around 80 percent of U.S. funds for ITER are being spent in the U.S. The FES portfolio also includes an upgrade to the National Spherical Torus Experiment (NSTX) fusion reactor at Princeton.

The FY 2013 request for SC's Nuclear Physics program includes ongoing support for the upgrade at the Thomas Jefferson National Accelerator Facility (TJNAF). The 12GeV upgrade at TJNAF is 60 percent complete and is expected to be complete in about one year. Another project in the Nuclear Physics portfolio is the Facility for Rare Isotope Beams (FRIB) at Michigan State University. It is designed to create rare isotopes and particular isotopes with high numbers of neutrons in the nucleus. SC and Nuclear Physics are also taking responsibility for supply of certain key isotopes not available commercially. SC is working to synchronize those who need isotopes and supply. Helium-3 became in short supply when DHS decided to use Helium-3-based detectors. Due to the short supply, DHS had to revamp and build detectors using different materials.

SC's High Energy Physics is undergoing changes. The Energy Frontier has shifted to CERN with the closure of the Tevatron. In the Intensity Frontier, work continues to quantify neutrino mixing and measure the neutrino masses. SC celebrated Saul Perlmutter, the 2011 Nobel Prize recipient in physics, for his work on dark energy and the expanding universe. High Energy Physics is also developing an experiment called LUX (Liquid Underground Xenon) at the Homestake Mine in South Dakota.

Dr. Brinkman concluded by expressing his appreciation for the service of BESAC members and its orchestration of input and recommendations for the basic energy research, noting specifically that SC activities have done many things based on reports from BESAC.

Discussion

Dr. Brinkman was asked about the inability of fellowship programs to gain traction. He noted that the National Science Foundation and the Department of Education are often seen as the ones to offer graduate fellowships due to their education missions. However, DOE has an interest in developing the future workforce in fields relevant to the Department's missions.

Dr. Brinkman was asked if the Hill recognizes the changing role of industry and government with regard to supporting and conducting research and the perception that both should be supporting and conducting research. He noted that he does not know the answer but that he believes that DOE has unique facilities and capabilities that industry will not build. DOE needs to think about how industry might take greater advantage of them.

Insight was sought on how to deal with increasing data and the costs associated with its management. Dr. Brinkman pointed out that there has been a lot of discussion but is has not been very conclusive. There is a huge spectrum of views on keeping data that is no longer used once it is published. Open literature is also a facet of this discussion.

It was pointed out that climate research is seen favorably on the Hill. Dr. Brinkman was asked if this hurts other aspects of DOE such as BES. He responded that the Hill has been inconsistent on this subject, reflected previously in cuts to fusion research. He noted that there are still those on the Hill who are skeptical of climate change.

Dr. Brinkman was asked if he had any feedback on the Materials for Energy Workshop held at Lawrence Berkeley National Laboratory earlier in the year. He was pleased with the workshop and talks but did not see any specific ideas on what to do next. Another workshop on computing is coming up in a few weeks in Austin, TX.

Presentation: News from the Office of Basic Energy Sciences

BES Director **Dr. Harriet Kung** provided an update.[2] BES' FY 2012 appropriation totaled $1,688M which is a $10M increase over FY 2011. The FY 2012 request for BES included a substantial increases to support new instrumentation, facility upgrades and expansion, and new research activities such as science for energy. Dr. Kung explained that the final FY 2012 has appropriation was substantially below the request and forced BES to make difficult decisions. BES started new activities such as NSLS-II Experimental Tools (NEXT), the LCLS-II upgrade, and continued NSLS-II construction. However, this accounts for the total FY 2012 increase; current facilities will not operate at optimal levels and core research was reduced.

BES is pleased to initiate the Batteries and Energy Storage Energy Innovation Hubs in FY 2012 at $20M with a $25M request for FY 2013. The Funding Opportunity Announcement (FOA) was published on February 1st with the award expected by the end of FY 2012. Core research will decrease by about $25M in FY 2012. However, an expression of interest was posted in Materials and Chemistry by Design, an area that BESAC has helped guide. The goal is to integrate predictive modeling with experimental work to transform the ability to design new materials and chemical processes. This is part of the President's Material Genome Initiative in collaboration with other agencies. BES is looking at three types of awards: single-investigator/small group, glue funding, and software innovation centers.

The EFRCs are progressing well. They have produced more than 1,000 peer-review publications, 40 patents, and at least three start-up companies. Science reviews are running from January through April 2012. Reviews will be used by BES for making future funding decisions.

[2] http://science.energy.gov/~/media/bes/besac/powerpoint/20120224/Kung-1.pptx

The Fuels from Sunlight Hub is operating at the Joint Center for Artificial Photosynthesis (JCAP). An onsite science review will be conducted in the spring of 2012. In its first year, JCAP has served as a hub to coordinate with the broader community in artificial photosynthesis and related activities.

Charts were developed to show the impacts of long-term research investments on manufacturing and commercialization sectors. Dr. Kung shared an example from Northwestern University that lead to a new aluminum alloy and consequent interest from Boeing and the Ford Motor Company. Another example is work in the co-location of catalysts and substrates leading to new mixed metal oxide materials and consequently new catalysts for biodiesel production from broader spectrum feedstocks. This technology has lead to the formation of Catilin, Inc., and a pilot-plant was built utilizing this technology. Catilin has since been bought by Albemarle and the commercial catalyst is now available.

In FY 2011, BES user facilities served more than 14,000 users, many of whom were graduate and post-doctoral students. The facilities are a training ground for the next generation of users and have supported more than 300 companies including 30 from among the Fortune 500. Facility use has created new small companies, indicating the facilities' usefulness in serving user communities and smaller companies.

BES has been working on strengthening communications with public officials, scientists, and the public. Three publications resulted. One product is the BES 2011 Summary Report.[3] It summarizes how BES does business and describes the divisions, EFRCS, and Hubs. Another product is the FY 2011 Research Summaries.[4] This includes summaries of more than 1,300 projects across the three BES divisions. These reports are on the BES website and will be updated annually. Coming next is the "Science Serving the Nation" brochure for the public.

Dr. Kung presented the FY 2013 budget request of $1,799.6M representing a $111M increase over the FY 2012 budget. The request shows the alignment of BES contributions to Administration priorities. Dr. Kung thanked BESAC for generating community-wide support through workshops, strategic planning for facilities, and especially the ongoing mesoscale activities.

The Energy Innovation Hubs, the EFRCs, and two pieces of core research – the Materials and Chemistry by Design and Science for Clean Energy – all have increases in the FY 2013 request. In addition, an increase of $42M for user facility operations will bring BES to near optimal operations. The request allows continuation of the NSLS-II construction and supports upgrades and new instrumentation at other facilities.

The Science for Energy research area is built around mesoscale research that BESAC is currently reviewing. It recognizes that science has advanced in the past decade due to research in nanotechnology. Dr. Kung highlighted the impact of mesoscale behaviors and impacts on MRIs and other commercial applications.

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[3] http://science.energy.gov/~/media/bes/pdf/reports/files/BES2011SR_rpt.pdf
[4] http://science.energy.gov/~/media/bes/pdf/reports/files/bes_fy2011_research_summaries.pdf

The FY 2013 request included R&D for clean energy, jointly funded by SC and the Office of Energy Efficiency and Renewable Energy (EERE). If funded, the activity will look at translation opportunities knowing that sometimes it can be difficult to cross from basic to applied research. Each DOE office will contribute $35M and the supplemental funding will be competed.

In FY 2013, SC's work in Materials and Chemistry by Design will expand especially with regard to software tools. Software development has not been as organized as in other communities, yet there are significant potential gains possible by owning and developing software and making it widely accessible. These tools coupled with modeling will strengthen and accelerate the innovation cycle. The emphasis of the request of $20M is on software tools and data standards and will allow for better use of high performance computing tools.

On the facilities side, SC needs to continue to maintain its global leadership in light sources. Progress has been made on the NSLS-II Ring Building due in part to additional funding from the Recovery Act. Two laboratory office building shells have been added to the project scope using contingency funding. Work on the accelerator system has progressed despite challenges with magnet procurement. The project has a strong management team.

The LCLS-II is proceeding as planned. The project is moving to a two-tunnel option to allow space for four more experimental stations. The total project budget is slightly more than $400M and well within the estimate.

The APS-Upgrade (APS-U) has been one of the more productive light sources based on the number of users, publications, and impact. To maintain leadership, APS-U will provide an unprecedented combination of high-energy, high-average-brilliance, and short-pulse x-rays together with state of the art x-ray beamline instrumentation.

In comparing budget requests with appropriations, Dr. Kung pointed out that appropriations have exceeded the request just once between FY 1996 and FY 2012. In particularly tough year, this resulted in the termination of facilities and declination of proposals. BES has been better prepared in the past two years to manage discrepancies between the request and final appropriation. Dr. Kung noted that there are tremendous opportunities in FY 2013 to advance science and stands ready to work with BESAC and the community to give a strong justification to support the President's request.

Dr. Kung shared the BES staffing chart and pointed out several new staff members. She also highlighted planned reports in mesoscale science and a detector R&D workshop. BES hopes to leverage the community broadly for expertise to help shape R&D research.

Discussion

Dr. Kung was asked if there are barriers that inhibit industry users from accessing facilities and how proprietary information is handled, particularly in light of the growth of the facilities and potential for accommodating more users. BES is working with facility directors to identify limitations to access and to address intellectual property issues. Various SC facilities are organizing a workshop to engage industry and understand ways to lower barriers. The goal is to understand best practices for resource use and how to contribute to industry success.

A clarification was offered with regard to the origins of the Materials Genome Initiative. Several agencies and program managers conducted studies and workshops that lead to the creation of an ad-hoc OSTP (White House Office of Science and Technology Policy) committee on materials and chemistry by design. The initiative evolved over a long period of time. It originated within the scientific community and was worked through OSTP.

Dr. Kung was asked if instrumentation for NSLS-II was being developed in parallel to the construction project to allow immediate usability when the construction project is complete. Dr. Kung replied that 6 instruments are being developed within the NSLS-II project and NSLS-II Experimental Tools (NEXT) is ongoing. Discussion continues and user input is needed on the specific instruments needed. She sees this as a natural progression and community input can drive this parallel to the construction timeline. Dr. Kung foresees an exploratory workshop being planned for this.

Dr. Kung was asked how the Materials and Chemistry by Design initiative links to the Materials Genome Initiative, and how BES is contributing. She clarified that BES is one of the agencies contributing to an OSTP-chaired inter-agency group. Regular meetings are conducted in coordination with NSF as NSF is moving forward with its solicitation for proposals. Dr. Kung sees Materials and Chemistry by Design as part of the core science efforts in BES.

It was noted that the EFRC reviews have been thorough and very good. Dr. Kung was asked about post-review actions and the possibility of another call for EFRCs or renewal of current EFRCs. She explained that the reviews will inform the plan and that the results will be taken into balance in the context of overall research activities. All options are being considered at this time, including the development of a new solicitation based on broad community participation.

It was noted that there is an increasing gap between budget requests and appropriations, and that there seems to be greater industry involvement than before. Similarly, there is also more evidence of a link from fundamental research to a final product used by industry. It seems that there is a path for BES to focus on industry, yet this message is not reaching the Congressional level. Dr. Kung was asked if other committees and advisory groups are having similar discussions about linkages and what is needed to link industry with BES. As demonstrated by the research impact charts, DOE research can benefit industry. The importance of a feedback loop from industry was pointed out to Dr. Kung to help gain input on BES' scientific challenges. She noted that the basic needs workshop identified some of those challenges.

Presentation: News from DOE Technology Programs

Dr. Arun Majumdar, Director of the Advanced Research Projects Agency - Energy (ARPA-E), discussed the DOE applied programs and how they complement the work of BES.

As a technology matures, it follows a learning curve. Cost over performance resides on the vertical scale, size and volume on the horizontal scale. As cost comes down, scale goes up. Dr.

Majumdar explained that many applied programs such as EERE or the lithium-ion battery are advancing along these learning curves and trying to do research to reduce costs of existing technologies and develop better materials. Scientific understanding is needed for this process to occur.

Dr. Majumdar explained that R&D creates an entirely new learning curve. By its own nature, R&D is risky, but positive disruption is possible when new learning curve achieves higher performance at a lower cost. Some experiments fail, some are successful, and both provide lessons learned. ARPA-E is working to remain competitive and requires basic science to do so.

The SunShot Initiative was described to BESAC. It seeks to optimize the use of solar energy to achieve goals of $0.05 to $0.06 per kilowatt hour. This requires addressing balance of systems issues along with technical issues. The Sunshot Initiative may ensure U.S. competitiveness and presents a coordination opportunity for solar activities across the Department. DOE needs to galvanize the research and use resources effectively to get to the SunShot goal.

This coordination approach is being implemented across DOE within different business lines. Examples are batteries, biofuels, grid technologies, and carbon capture utilization and storage. DOE is thinking of other areas where cross-DOE integration can be effective.

Dr. Majumdar is also interested in the mesoscale, particularly as it pertains to interacting degrees of freedom and the lithium-ion battery. DOE needs to understand meso on a fundamental level, but also look at how to use computation and other aspects in real-time to understand lithium-ion and other batteries. Dr. Majumdar described this as a good example where fundamental understanding of science can influence cost and scalability.

He also pointed to the self-assembly of inorganic particles and the need to look at rare-earth-free magnetic materials for motors and generators. DOE is working to develop materials with iron and nitrogen, and work by a group from the University of Minnesota, Oak Ridge National Laboratory, and Case Western University have shown this in thin layers. The next step is moving this to bulk magnets and scaling up from nanoscale particles.

Power electronics is another area of interest and is a huge issue for power grids. The current grid is aging and hosts about $1 trillion in assets. The average age of these assets is 42 years old; this is two years beyond their predicted lifetime and significant funding will be needed to replace these assets. Dr. Majumdar used the example of an 8,000 pound distribution transformer. A crane is needed to install the transformer, it is usually purchased from an overseas vendor, and the technology is not that different from what Tesla developed. Dr. Majumdar proposed developing the same level of design and integration through a scientific and integrated approach to produce a single 100 pound transformer. It would require soft magnets and be made out of materials that have low losses and run at high-frequencies. He emphasized that there is a lot of interest in bridging what happens at a small scale to a larger scale for application.

Dr. Majumdar presented two additional scenarios focused on fast magnetics for fast switches, and issues with metrics and air conditioners and the extraction of humidity to lower emissions.

He closed by informing BESAC that there are currently three Energy Innovation Hubs. Two new Hubs will be awarded in FY 2012 on batteries and energy story and critical materials, and in FY 2013 an electricity systems Hub is proposed with involvement of local regions and stakeholders.

Discussion

Dr. Majumdar was asked to discuss phenomena that need to be understood at a fundamental level that emerge at a 100 nanometer scale, especially since the examples he referred to reflect integration of coupled components. He suggested there is room for research to be able to change magnetic properties with an electric field and use that in a device. These ideas are being explored and the potential for applications in the energy area is high. To achieve this, scientists and engineers need to work together.

It was noted that Dr. Majumdar's presentation was similar to the BES report *Science for Energy Technology: Strengthening the Link between Basic Research and Industry*, and the potential for better integration of fundamental science and applied research. Choosing a common goal is important, the process of which requires getting university researchers and industry in the same room. Dr. Majumdar agreed, explaining that the SunShot Initiative relied on this type of process. There was agreement on needing common goals that focus DOE efforts and brings science and technology areas together.

Dr. Majumdar was asked for input on thermoelectrics, which can be seen as a meso problem, and to identify critical needs. He responded that on the phonon side, we understand why nanostructuring helps. On the electronics side, we need high effective mass materials and sometimes nanostructuring to manipulate the band structure. The integration of each side into a single material has not happened. He urged that new physics is needed and work in his lab is pushing toward this. He also added that there are a lot of system and device level issues.

It was noted that Dr. Majumdar's talk implied that the grid is far away from basic science. It was suggested that more thought be given to fundamental processes. Dr. Majumdar made clear that the grid is not far from basic science but he believes that it lacks common goals. He pointed to electrical routers as an example; there are no routers on the grid. Routers could reduce congestion and optimize power flow in real time. There are important computational issues which is why ASCR is involved in the grid team. He also noted that there are materials issues in power systems.

Dr. Majumdar described how cross-DOE teams from basic and applied are collaborating and the potential for cross-agency working groups on these topics. Team formation depends on common goals and how teams gel and integrate. It takes time. The batteries team has drawn on expertise from across DOE and generated the Hub funding announcement. Some teams are just forming now. The Department is looking at cross-agency communication in manufacturing.

Dr. Majumdar was asked how DOE will apply materials by design approaches to other complex systems. Success depends on the problem to be solved and effectively defining that problem. There are avenues of known physics that help, but there are unknowns too where an approach is not yet understood. Dr. Hemminger commented that BES could address areas where not enough is known about nature with the notion that BES could give input on the most important problems and couple with other offices. Dr. Majumdar applauded this type of approach, as this is what SC funded him to do before he came to the DOE.

Dr. Majumdar was asked how DOE will change in the coming years and decades. He expressed that there a few things that the Department is trying to institutionalize to live beyond the current Administration. The goal is to make the U.S. competitive.

Dr. Majumdar expanded on what has to happen for ARPA-E to be a convincing change in how DOE does business and in a way that does not muddy the way that other offices work. Some definition of success is needed, but the impact will be in 10-15 years (e.g., marketshare, greenhouse gas emission reductions, reducing imports of rare earths, etc). There is difficulty in defining success in the 5-year timeframe. The only thing one can do is to determine the vectors and metrics to show that there is potential for success in 10 to 15 years. One can ask questions such as: Does DOE have the best minds working on energy issues? Do we have the world record in technology areas? How much intellectual property has been created and licensed? Has this lead to private sector investing in and leveraging DOE technologies? Answers to these questions do not by themselves indicate success, but together can point to success.

Presentation: Update on the BESAC Mesoscale Science Subcommittee

Dr. Hemminger pointed out that the term "meso" appears frequently in the FY 2013 budget request indicating rapid adoption of this concept and the need to inform others about mesoscale science.

Dr. John Sarrao and **Dr. George Crabtree**, co-chairs of the BESAC Mesoscale Science Subcommittee, gave an update on the subcommittee progress..BESAC reviewed the charge from Dr. Brinkman issued on February 14, 2011.[5] A report is due to Dr. Brinkman by fall 2012. Included in the meeting materials was an interim report, "Quantum to the Continuum: Opportunities for Mesoscale Science"[6] and a presentation describing outreach activities.[7]

The background for the study includes three recent DOE reports.[8] Additional help is sought from BESAC to define this very rich field. Community outreach (www.meso2012.com) has also supported the subcommittee's recent work. The subcommittee has sought to define what meso is, why it is important, and why it is important now.

Meso refers to in-between, intermediate and middle. It is in between quantum and classical, in between an isolated particle and bulk material, and in between simple atoms and complex systems. For example, a system of interacting particles can exhibit different behaviors than an isolated particle. Structure, dynamics and function are all important in mesoscale science.

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[5] http://science.energy.gov/~/media/bes/besac/pdf/Charge_2011.pdf
[6] http://science.energy.gov/~/media/bes/besac/powerpoint/20120224/Quantum_Crabtree.pptx
[7] http://science.energy.gov/~/media/bes/besac/powerpoint/20120224/Outreach_Sarrao.pptx
[8] 1) Science for Energy Technology: Strengthening the Link between Basic Research and Industry, 2) New Science for a Secure and Sustainable Energy Future, and 3) The Grand Science Challenges Report: Directing Matter and Energy: Five Challenges for Science and the Imagination

A lithium-ion battery is an example, wherein there are multiple interacting parts. The phenomena involved in the battery include ionization, ion insertion/extraction, electronic/ion conduction, and volume expansion/contraction. High functionality results from all these phenomena.

Another example is in light and matter interactions including photonic crystals, metamaterials, and surface plasmons. The mesocale has potential for these areas akin to revolutions in laser technology.

Mesoscale also refers to intermediate time scales from attoseconds to eras. The specific timescale depends on the problem being studied. For example, a solar water splitting device includes timescales from attoseconds (electronic excitation) to seconds or decades (crack nucleation and propagation in the device). Mesoscale can also cover timescales of millennia or eras for geologic phenomena.

Meso is an opportunity space where multiple degrees of freedom interact constructively. Biology is an example of this; the cell is a very dynamic and multi-functional meso unit and is able to achieve this due to its complexity. Biological complexity with inorganic materials is one goal.

New organizing principles are needed at the meso scale. One question is what laws govern self-assembly?

Five representative areas have been identified by the subcommittee for continued work:

- Damage accumulation and materials lifetime
- Functional mesocale systems
- Self, guided and deterministic assembly inspired by biology
- Reactive transport through mesoporous media
- The role of fluctuations in driving mesoscale dynamics

The subcommittee is seeking input and examples from the community and BESAC, and has received around 30 examples so far. An example was shown on the self-assembly of inorganic nanoparticles.

Tools and instruments for advancing mesoscale science were described in the areas of synthesis and assembly, characterization, and theory/simulation. An example of advances needed in characterization is multi-modal experiments. In addition, there are cross-cutting challenges such as the co-design/co-location of synthesis, characterization, and theory/simulation.

If the meso initiative is successful, it could lead to biologically-inspired complexity and functions with inorganic earth-abundant materials that cannot be achieved in biology now. We could move from top-down design to bottom-up design with atomic, molecular, and nano functional units. We could discover and exploit mesoscale organizing principles. We could end up manufacturing at the mesocale resulting in products that are faster, cheaper, highly efficient, and longer lasting.

The subcommittee will continue to collect community input. Town hall meetings are scheduled for:

- February 29, 2012 at the American Physical Society meeting in Boston, MA
- April 9, 2012 at the Materials Research Society meeting in San Francisco, CA
- April 12, 2012 online webinar through the American Chemical Society
- Mid-May, 2012 in Chicago, IL

Discussion

Mesoscale science can now leverage the capabilities that nanoscience research developed in areas such as self-assembly and top-down manipulation. The nano revolution was driven by the ability to do things experimentally that were not previously possible; the expansion of the "why now" question is thinking about the tools and knowledge base that makes mesoscale science an imperative. Advanced computing capabilities will emerge over the next decade as technology passes the exaflop regime to help solve mesoscale problems.

The group discussed how to communicate mesoscale science. There is a tendency to point out what is not understood; the statement should be reversed to what would be possible if we understood "x". These statements need to be written clearly. The societal impact of this work and informing the public are important, using examples such as self-repairing or self-healing materials. One could also speak to things such as lower cost efficiencies, advanced manufacturing partnership opportunities, making qubits and complex computing, better batteries, advanced sensing capabilities, protein design, and catalysis. Another example is the opportunity made possible by analyzing large bodies of data and using diverse approaches to studying what is around us. Communication lessons may be borrowed from the early days of nano, especially as nano has lead to meso.

Interest may also be generated by looking at multi-modal experiments and four-dimensional materials science. Mesoscale science may influence the advancement of tools and instruments. A remaining question is how to capture complexity when most instruments look at one process. A meso challenge may be having characterization tools that embrace complexity.

It was suggested that Dr. Sarrao's presentation prompts BESAC to not just restack reductionist elements but to think altogether differently to discover new organizing principles which could help us advance without the reductionist step. Dr. Sarrao noted that that is what biology does—it works from the bottom-up.

However, the organizing principles for meso are not yet clear. For example, as systems become more complex they become increasingly functional; exploring how that functionality arises means putting pieces together in a bottoms-up way and studying them. Quantum mechanics helps for very small things and classical mechanics for very large things, maybe there is something different for understanding in between, in the mesoscale. At the mesoscale, we can control quantum mechanics with macroscopic tools and mesoscopic structures. This is where we go from discovery science to control science, resulting in deterministic control of long rage interactions.

Biology tells us that creating things from the bottom-up, atom by atom can be raised to an industrial scale. It was asked if biological scientists see this as a challenge, and Dr. Sarrao responded that perhaps this could be done at a small scale; synthetic biology is an example. It was proposed that the biological aspects could be part of the ACS webinar and a question could be proposed to the biology community.

Dr. Hemminger expressed concern about the need to generate a report amidst all of the interesting examples and possibilities that were mentioned. He noted that organization, structure and chapter headings are not yet visible. He asked that BESAC members think about organizational aspects of the report and chapters.

Presentation: Update on BESAC Mesoscale Science Subcommittee Outreach Efforts

Following a break, **Dr. John Sarrao** presented outreach efforts and summarized input from the community received to date. These inputs helped form the following six key themes:

Damage accumulation and materials lifetime
Issues around damage and cracks have a long history. Research needs to move from a microscopic to mesoscale arena. The "why now" is the potential to expand the lifetime for established and new materials, to identify and understand defects in mesosystems, to focus on the defects-process-structure-properties paradigm, and to create new and improved materials for transportation, energy, and medical applications.

Functional mesoscale systems
Mesoscale systems can be self-organized and designed to provide scientific and applications value if they are understood and controlled. This can take a common understanding through a meso frontier and lead to the next generation of high performance materials and systems for energy applications and new approaches for computation, synthesis and measurement. Other examples submitted by the community include "upscaling" nanoscale thermoelectric and measuring quantum effects in nanostructures.

Catalysis at the mesocaslce
Catalysis is achieved with many different kinds of materials. At the mesoscale, catalysis in pore structures is important and needs to be studied at long and short time scales.

Reactive transport through mesoporous media
The ability to do multiscale, multiphase modeling of sequestration sites for capacity, injectivity, and containment would provide the basis for understanding how to successfully sequester CO_2. Successful physical and/or chemical trapping of CO_2 will help solve one of the major environmental problems facing mankind.

Self- and guided-assembly in biology
This gives a way to understand how to develop inorganic systems to do what nature does very well in organic systems. Impacts include the development of new biomimetic materials, biosynthetic materials, and the sequestration/transformation of environmental contaminants such

as arsenic and radionuclides. Another example presented focused on multi-valent interactions in polyelectrolytes.

Role of fluctuations in formulating organizing principles in mesoscale systems
The motivation in this theme is to stimulate thinking.

Dr. Sarrao emphasized that answers to the “why now?” and “why not yesterday?” questions are to think about the tool set needed for science. There have been significant advances in the tools and instruments for science that allow new questions to be asked. People are doing things that span various domains and tools can begin to shape the understanding of materials at a mesoscale.

He pointed out that examples provided are not a complete set but a positive start. Next steps are leveraging available tools to understand how they can impact mesoscale sciences, moving beyond quantum space. Dr. Sarrao noted that the mesoscale website received 25 contributions as of February 20, 2012 and is intended to motivate a broader discussion.

Discussion

IUPAC defined meso from two nanometers (below that is micro) to 50 nanometers (above which is macro). It was pointed out that catalysts in fuel cells operate in dynamic conditions. The surfaces are continuously changing and it may be that the dynamic surfaces in catalysis are important. Ultimately, surface dynamics and understanding may be important for mesoscale.

Concern was expressed that mesoscale is already being worked on. Reports such as the one on catalysis show this. Calling this area of research meso may not be the answer. What would be a new program that doesn’t already exist? The strongest examples may be phenomena that don’t exist in a few atom systems. We’ll need to find the things that are fundamentally new.

The challenge is in identifying what’s new and identifying new ways of thinking, while avoiding strong overlap with other reports and prior work. We also need to articulate this complexity to Congress and focus on the BES mission.

It is important to galvanize the community-at-large and gain their involvement. This could point to distinctly useful examples, particularly those around phenomena that do not exist and examples that are new.

It was noted that movement beyond reductionist thinking may occur through scenarios such as attempts in biology to understand complex concepts in the energy landscape. This can lead to new understanding that invokes a very novel concept. This may show up more frequently through thinking about meso and moving beyond reductionist thinking. Protein-folding was mentioned as an example where a new concept emerged from studying the problem. It was expressed that it may not be a useful example as it is sometimes in the meso realm but more intermediate examples that highlight complexity and are biological should be sought.

The subcommittee was urged to consider instrumentation as well, since studying materials in whole and at many time scales requires multiple probes.

It was suggested that a systems approach to materials science versus a reductionist approach may be a new way of thinking. People working on complex systems such as in systems biology have very useful tools for managing complexity in real systems that could be applied to mesoscale science. Consideration of complex systems is useful for getting to a scale with real impact.

A committee member asked about mapping to the Materials Genome Initiative. This is not mandatory; the initiative will move forward regardless. To the extent possible, it may be smart to take advantage of that, especially the computational aspects of the initiative. Some of the questions about meso are captured in the initiative so there could be some synergy.

At the request of Dr. Hemminger, the subcommittee was asked to meet after day one to develop some examples and chapter headings to be presented to BESAC on day two. It was suggested that a discussion of the range of length, time, and energy scales could support developing a reasonable definition. However, it was resolved that examples be considered first that are uniquely different from ongoing research.

Presentation: Basic Research Directions Workshop on User Science at the National Ignition Facility

Dr. John Sarrao reported on the "Basic Research Directions Workshop on User Science at the National Ignition Facility" held in May 2011.[9] A report from the workshop is available online.[10]

One basic research need is understanding materials in extreme energy environments. Several years ago, a talk was delivered at a BESAC meeting on thermo-mechanical challenges. It described the need for a suite of measurements, what chemistry looks like in these environments, the domain of high pressure responses, and how to conceive environments that have not previously been used.

Dr. Sarrao offered as an example the changes that can occur to a solid exposed to high pressure and the resulting charge structures. A whole new domain of materials chemistry can be done, particularly if thinking about studies at atomic pressures.

The National Ignition Facility (NIF) hosts a high-powered, 192-beam laser to create previously unseen extreme environments. These capabilities and the opportunity to merge the programmatic sides of DOE and SC with the National Nuclear Science Administration (NNSA) were a basis for holding the workshop.

Nearly 100 attendees from 49 institutions and six countries summarized the current state of scientific research and understanding in key fields, and defined grand science challenges. The workshop also considered research directions at user facilities and how NIF could support these activities. Discussions were held on facility governance including individual responsibilities,

[9] http://science.energy.gov/~/media/bes/besac/powerpoint/20120224/NIF_Sarrao.pptx
[10] http://science.energy.gov/~/media/sc-2/pdf/reports/SC-NNSA_BRD_Report_on_NIF_User_Science.pdf

user access and the allocation of facility time and resources, and other policies and procedures relevant to users.

The workshop produced sixteen priority research directions from the panel deliberations. In his presentation, Dr. Sarrao addressed the five priority research directions identified by the materials at extremes and planetary physics panel:
1 – Novel quantum matter to star matter
2 – Elements at atomic pressures
3 – Kilovolt chemistry
4 – Pathways to extreme states
5 – Exploring exoplanets at NIF

Dr. Sarrao elaborated on the fifth priority research direction, explaining large exoplanets are being discovered and that little is known about their interior composition. At NIF, one measure tailored high-precision compression paths to achieve interior conditions of gas and ice giants and super-earths.

The NIF user program has eight teams. One is accessing pressures at remarkable extremes and demonstrating what is possible. The rate at which experiments are done is not the same as at a photon source as the experiments require a lot of background work.

The workshop concluded with three principles that underlie the recommendations:
1 – Make science at NIF successful on long-term timescales
2 – Build a sense of scientific community among NIF users
3 – Use best practices and lessons learned from relevant facilities at NIF

Dr. Sarrao presented recommendations spanning three areas:
Policy and governance, facility operations, and outreach and education

One week prior to the BESAC meeting, NIF held a user meeting to explore these domains. Discussions around policy and governance pointed toward the need to be open and transparent. Facility operations were addressed by looking at the best ways to balance machine availability for multiple teams. Outreach and education discussions examined how to be successful in building a community of scientists and involving them in intellectual centers. The meeting concluded that there is an opportunity for the community to shape the facility and to drive research and development.

A phrase that emerged is “NIF Science 2020” in recognition that the science opportunities go beyond high energy density science. The time to seize the opportunity is now, and partnering between SC and NNSA is essential to realize the full science potential of NIF.

Discussion

Kilovolt chemistry is one new potential dimension for the study of materials. Dr. Sarrao was asked if this is simply about the chemistry of stripped electrons. He responded that NIF is not just a high-pressure regime but a variety of extremes including high voltage.

NIF can produce x-ray beams with a flux of exceedingly shorter lengths. This allows for work in strong field electrodynamics. In looking at beam and plasma physics, NIF has 192 beams yet one could do this with 50 beams; NIF could do other things with simultaneous multiple probes. It was pointed out that a lot of science could be done with multispectral probes, especially at the mesoscale.

Dr. Hemminger reminded the BESAC of the town hall meeting on February 29, 2012, at the American Physical Society meeting in Boston, MA, and April 9, 2012, at the Materials Research Society meeting in San Francisco, CA. A town hall meeting will be run at the American Chemical Society meeting on March 27, 2012, and run by BESAC member Dr. Doug Tobias.

Public comment

None

Board business

The meeting was adjourned at 4:57 p.m.

Friday, February 24, 2012

Dr. Hemminger called the meeting to order at 9:04 a.m.

Presentation: Upcoming COV, Materials Sciences and Engineering Division

Dr. Linda Horton, Director, Materials Sciences and Engineering Division, provided a briefing on the upcoming Committee of Visitors (COV) Review of the BES Materials Sciences and Engineering Division.[11]

The first SC-BES COV was in 2002. The process is similar to that of the NSF. Prior reviews are posted at http://science.energy.gov/bes/besac/bes-cov. Recommendations are taken seriously and have resulted in substantive changes.

The COV charge is to assess the efficacy and quality of the processes used to (a) solicit, review, recommend, and document proposal actions and (b) monitor active projects and programs. The COV will also look at the breadth, depth, and quality of the portfolios.

The COV will cover FY 2009 – FY 2011 activities including the Single-Investigator and Small-Group Research (SISGR) programs. The COV will examine other solicitations including the Hydrogen Fuel Initiative (HFI), the DOE Experimental Program to Stimulate Competitive Research (EPSCoR) Program that is managed by this division, and the Computational Materials and Sciences Network (CMCSN/MCSN). The COV will not cover the EFRCs as they are subject

[11] http://science.energy.gov/~/media/bes/besac/powerpoint/20120224/Horton.ppt

to a COV next year. The SC Early Career Awards will be assessed as a whole later on, and the SC Graduate Fellowship Program and BES Equipment Supplement Program are other exceptions for this COV.

The Division consists of three research teams and the COV will look at the programs of each team in the division. There are cross-cutting themes among the teams.

The EPSCoR Program will be reviewed by the COV. It was established by Congress as a way to broaden the geographical distribution of federal funding for academic research. EPSCoR helps them be more competitive for future solicitations. More than half of all U.S. states are supported. Some have very large DOE laboratories, hence the effort to focus on laboratory and state partnerships. The annual budget for EPSCoR is $8.5M.

The COV in FY 2012 will be lead by Matthew Tirrell of the University of Chicago and Argonne National Laboratory and held on May 22- 24, 2012, at DOE's Germantown facility. Four panels of 33 participants will represent a diverse mix from academia, DOE labs, industry, and at least one other country. Participants are both recipients of BES funding and non-recipients. Three reviewers are on BESAC.

The COV Chair will visit the Division on March 16, 2012, then a conference call will be conducted with the Chair, panel leads, the Division Director, and team leads. The COV website will provide read ahead information for COV members.

Dr. Horton reviewed the agenda for the event.

Discussion

Dr. Horton confirmed that program managers will give the COV panels a brief overview.

When asked about international benchmarking, Dr. Horton responded that BES touches on international research investments at every workshop. Principal investigators also need to demonstrate awareness of international activity in their research proposals and it is considered during the peer review processes. Dr. Kung shared that there is no general guidance but that BES participates in bilateral and multi-lateral meetings from which to glean insights on competitors and global development. The DOE has previously sponsored studies to better understand this aspect.

It was noted that the demographics of the COV seem weighted toward academia. The COV is representative of the last COV balance. Dr. Hemminger added that the BES does not select the COV members. BESAC and BES work together to select the COV Chair. The BESAC and COV chairs select committee members with recommendations from BES staff.

It was suggested that COV participants should begin writing immediately.

The COV chair will report on the COV outcomes at the next BESAC meeting on July 26 – 27, 2012.

Presentation: ASCR / BES Data Workshop Report

Dr. Mike Simonson provided a summary of the ASCR/BES Workshop, "Data and Communications in Basic Energy Sciences: Creating a Pathway for Scientific Discovery" held on October 24 – 25, 2011, in Bethesda, MD.[12] Dr. Simonson and Dr. Peter Nugent were the workshop co-chairs.

The workshop charge was to review the status of current data and communication pathways for scientific discovery in basic energy sciences, to determine methods and tools to mitigate current and projected shortcomings, to understand the opportunities and challenges in data and communication with the combination of techniques in single experiments, to identify research areas in data and communications needed to underpin advances in the next ten years, and to create the foundation for information exchanges and collaborations among ASCR-BES research and facilities communities.

Four breakout sessions brought together ASCR and BES researchers to identify opportunities to link ASCR capabilities with BES needs. The breakout sessions focused on workflow management, theory and algorithms, visualization and analysis, and data processing and management. Areas examined included evaluating the status of facilities and their data management needs, data challenges as facilities and needs expand, sharing experiences and lessons learned, and future challenges for BES and ASCR.

There are many ongoing activities related to this topic. For example, there is an interagency working group on Big Data, data is a key part of the Materials Genome Initiative, and there is an SC working group on digital data. There are also challenges in mesoscale science that deal with the extraction of science from the experimental information.

Facilities can produce terabytes of data daily from single beam lines. Improved data handling is needed to extract the full value from experimental data. In addition, new techniques such as time resolved and tomographic studies are producing increased amounts of data. A new level of understanding is needed utilizing sophisticated applied mathematics and computer science techniques.

At the LCLS, femtosecond crystallography experiments generated high levels of data and large teams that self-assembled to address project challenges. The output was 18 terabytes of data in eight hours. This puts pressure on data analysis and data handling to serve users' needs.

Currently, the number of scans of reciprocal space data is large; with new detectors coming online, real-time analysis would produce data in the exaflop range especially to implement controls in real-time. Advances are needed in computing power, theory and algorithms, and local processing.

[12] http://science.energy.gov/~/media/bes/besac/powerpoint/20120224/Simonson.pptx

Another example is handling data from new neutron instruments. The size and complexity of systems and the capabilities for experimental control are increasing. High data rates and large data sets are generated. When the Spallation Neutron Source is in full operation, the data rate could move to 4 terabytes per second. The need for fast communication and raw processing power is very clear.

The workshop proposed areas for improving data analysis and enabling facility efficiency:

1 – Integrate theory and analysis into workflow – The utility of common data formats should be examined, capitalizing on investments made in data visualization and analysis tools.

2 – Move analysis closer to experimentation – Real-time (in-situ), streaming analysis at beamlines would help increase data quality, improve the efficiency of the experiment, and improve off-line analysis.

3 – Match data management access and capabilities – There is a need to remove bottlenecks and improve workflows through the entire system. For example, once could apply forefront mathematical techniques to more efficiently extract science from the experiment.

Dr. Simonson noted that any one of these topics could be the focus of a workshop to detail the research needs to achieve these goals. Overall, this workshop focused on the experimental side yet there needs to be a path from the inception of an experiment to the publication of results. The workshop report is in revision and expected in the very near future.

Discussion

The workshop did not address backing-up data or archiving, but suggested the need for storage capabilities to handle data at certain points in time and avoid the loss of data.

The workshop did consider the need for staffing that goes along with hardware advances. With increasing experimental complexity, users will have less ability to optimize their experiments so staff resources will be necessary.

Discussions did not delve into screening and hardware right at the detector or the elimination of routine data. These topics can be integrated with future discussions of next generation detectors. In many cases we may need the overall data set (for statistics), rather than a rare event.

The workshop examined advances in analysis and visualization of theoretical data sets and applying those advances to experimental data sets. LCLS has work ongoing already where they are streaming live data to a facility that can process in real time then stream back to the facility for adjustments to the experiment.

Data shipment can take weeks; hence there was focus on improving data transfer speeds. This is true for international exchanges or other DOE-sponsored facilities. Unless there are terabyte networks in place for every home institution, users may have to look at onsite analysis until data is transferred to their institutions.

It was noted that the recommendations seemed very general, and that if the ASCR and BES are to advance they must consider limitations such as the data they expect to keep and if networking is the best solution. A five-year or longer term projection of hardware, software and infrastructure bottlenecks is needed. At the workshop, this was highlighted in discussion of the volumes of data being produced, and in the generalities of what will be required. The charge was to get user facilities and computational facilities together. The workshop did not develop a roadmap to get to certain points.

In many cases there is a lack of awareness of existing capabilities, yet there were some discussed along with future needs such as algorithms for handling data. This workshop looked at common data needs and processes across user facilities. The recommendations will be taken seriously and dialogue initiated; the ASCR FY 2013 budget request includes funding for big data science.

Dr. Simonson responded to a question about working groups at each facility, noting that while it is less common to get together and discuss best practices and implementation, the NSRCs and photon sources do collaborate. He noted community concerns about the discussion of standards, but that there are ways to do things that are tailored for particular experiments and beam lines, and ways to bring things closer together and identify general solutions. Dr. Hemminger suggested that each facility director look at assembling working groups to comment on and share best practices and identify problems.

Presentation: Continued Discussion of the BESAC Mesoscale Science Subcommittee Activities

Dr. John Sarrao and **Dr. George Crabtree** resumed the BESAC discussion of the mesoscale charge. Members of the subcommittee presented discussions that occurred after day one.

The discussion from day one pointed out the need for clearly presenting the concept and then finalizing the report at the BESAC meeting in July. This will draw input from the town hall meetings and other mechanisms.

Dr. Sarrao believes that the focus should be on the uniqueness of meso to engage communities effectively in town halls. It should emphasize what is new and why now, and the discussion should feature specific examples. There are two main messages from the previous day's discussion:
1 – Quantum to the continuum is the key theme
2 – Mesoscale is a frontier for control science

BESAC has been working toward a mesoscale report with very clear rationale: there is a class of problems that lack sufficient breakthroughs and innovations. The "why" for mesoscale is driven by current tools and lessons being learned. It is also driven by specific basic science challenges for energy and matter that were somewhat captured in the Grand Challenges report.

The discussion of mesoscale could start with what is to be imagined but falls back to understanding the span from quantum to classical, from isolated to interacting effects, and from simple to complex. These define the domain of "what is meso." This is an opportunity space to span across degrees of freedom and across various time and length scales.

The following are key themes that have emerged to date on mesoscale science:

1. *Defect evolution and damage accumulation.* This examines the range from atomic scale deformation to bulk failure. There is no predictive model describing how this occurs.
2. *Functional mesoscale systems.* This area focuses on multiple functions working together to provide a system-level outcome. There are a suite of unknowns in this space that require an understanding of how these things work in real-time.
3. *Reactive transport in mesoporous media.* The reactive transport domain is captured in a surprisingly broad area of problems such as fuel cells or geological gas storage. There are multiple spatial scales and time scales at which reactions are played out that are central to current questions.
4. *Bio-inspired assembly and transduction.* This proposes understanding how to do things that nature does well. It also looks at the energy landscape in things such as protein-folding and how to harness diverse degrees of freedom for optimal performance.

The subcommittee discussed the attributes of synthesis, characterization, and theory. A central facet is how to integrate all three to create multi-component systems that can be scaled to address critical problems. There are multi-modal measures that are simultaneous, sequential, and predictive – currently there is no way to simulate these.

Discussion

The development of this report is more challenging than predecessor reports. We need to find a positive expression of what we don't know what to do, and we want to exclude the problems that have been solved in classical ways. It was suggested that the examples in the quad charts could be used to capture the uniqueness of mesoscale. Careful writing could explain this along with solved problems that show the impact of phenomena at these scales. Exciting and inspirational examples should be used as was done in the Grand Challenges Report.

Dr. Sarrao's description of the potential themes was appreciated yet it was asked if there is a slightly higher level of detail. This may emerge from workshops and feedback, and as the community considers examples.

It was pointed out that the quantum to the continuum platitude has been around. It might be better to lead off with the point that mesoscale is a frontier for control science and will lead to something useful. A member commented that it is okay to include some platitude and that there is value in including this to capture some peoples' imaginations.

The idea of control science is still fairly new, yet it was discussed in the Grand Challenge report. Hence this report needs to focus on using control to address applications, make things.

Concern was expressed about public acceptance of the term "control science;" one member responded that the town halls could be a time to test this term. Another noted that perhaps the report title should reflect control, offering the title "Challenges and Opportunities: Translating

Nanoscience into Control Science." Dr. Hemminger asked members to offer suggested titles on the mesoscale website.

In response to a question about BESAC members' participation at town hall meetings, Dr. Sarrao asked members to think about how to articulate things about which they are passionate in a quad chart framework and share them at a town hall. This would help shape an organic evolution versus forcing the concept onto attendees.

Dr. Hemminger asked how many BESAC members will be at the town hall meetings; around 10 members raised their hands. Dr. Sarrao asked members to urge colleagues to participate. It was suggested that people in other disciplines should attend to broaden the conversation.

Dr. Hemminger commented that an electronic flyer could be sent to BESAC members and provided to others. It was also suggested that someone check with the societies hosting the town hall meetings to see if attendees can participate without registering for the full conference. In addition, the subcommittee could gather after each town hall meeting to reflect on the discussion.

Dr. Hemminger pointed out that the two-day meeting in Chicago is one of most important meetings and has not yet been scheduled. He suggested that the second day of the meeting could be a working meeting of the subcommittee.

Public comment

None

Board business

Dr. Hemminger adjourned the meeting at 10:48 a.m.