Minutes of the
Basic Energy Sciences Advisory Committee Meeting
August 3-4, 2011
Bethesda North Marriott Hotel and Conference Center
North Bethesda, Maryland

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
Kate Kirby
Max Lagally
William McCurdy, Jr.
Mark Ratner
John Richards
John Spence
Douglas Tobias
John Tranquada

BESAC member absent:

Allen Goldman

Also participating:

Laura Biven, DOE Office of Science (SC),
William Brinkman, Director, SC
Patricia Dehmer, Deputy Director for Science Programs, SC
Dan Hitchcock, Director, Advanced Scientific Computing Research (ASCR), SC
Linda Horton, DOE Office of Basic Energy Sciences,
Henry Kelly, Acting Assistant Secretary, DOE Office of Energy Efficiency and Renewable Energy,
Tom Kalil, Office of Science and Technology Policy, the White House
Chi-Chang Kao, Associate Laboratory Director, Stanford Synchrotron Radiation Lightsource,
Harriet Kung, Associate Director of Science for Basic Energy Sciences, Federal Designated Officer,
Katie Perine, BESAC Committee Manager, DOE Office of Basic Energy Sciences
Joye Purser, Technical Writer and Recording Secretary,
Eric Rohlfing, Director, Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, USDOE,
Marvin Singer, Senior Advisor, Office of Basic Energy Sciences,
Rachel Smith, Oak Ridge Institute for Science and Education (ORISE).

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

Wednesday, August 3, 2011
Morning Session

Chairman John Hemminger convened the morning session at 8:43 a.m. He welcomed the new people on the committee and commented that this was among the best attended sessions he had seen. Rachel Smith provided safety and logistical announcements. Members of the BESAC then introduced themselves.

Next, **Dr. William Brinkman** of the DOE Office of Science provided a status update on the office. The debt limit bill recently passed by Congress included a 10 percent cut in discretionary spending which was substantial. More details will emerge as the budget for fiscal year 2012 (FY12) is developed this fall.

The BESAC's inputs regarding transparency in literature and research data were of great value to SC. Each of the DOE advisory committees' reports to SC will be helpful in supporting SC's ability to engage with the broader federal research community on this subject.

Dr. Brinkman provided a DOE budget update. BES comprises almost 34 percent of the SC budget. SC leadership is pleased with the Energy Frontier Research Centers (EFRCs). The first research "hub" is working well and is intended to aggressively pursue technologies for producing energy from sunlight. SC is working hard to get a second hub, the battery hub.

While DOE has made a lot of progress towards green energy, the current funding climate is difficult. It has been fiscally challenging to maintain user facilities. We need to expand some SC user facilities. The Advanced Photon Source (APS) upgrade is needed at Argonne National Laboratory. The Next Generation Light Source at Brookhaven National Laboratory is also a funding priority but the way forward is unclear.

The FY11 appropriation represents a one percent decrease. Some have said that compared to cuts in other federally funded research areas, SC is relatively "unscathed." But Dr. Brinkman was concerned with the current fiscal climate. He noted that SC relies on the BESAC to help determine how to spend the money wisely.

Dr. Brinkman then offered to answer questions.

Question: Can you clarify how the 10 percent cut in discretionary spending will be applied?
Answer: The cut will be implemented across the board on federal discretionary expending with the exception of the Department of Defense. DOD stands to take half the cut.

Comment: It is important for the federally supported scientific research community to articulate the priority areas to fund in this restricted fiscal environment.

Question: What is your view of the open literature issue?
Answer: Dr. Brinkman said he didn't think the NIH choice on open literature had a big impact.

Comment: But medical literature is different from chemistry and physics. So it may be difficult to apply the NIH model. Also, the NIH policy will cost NIH millions of dollars per year so the cost of that model is a serious consideration. SC should make sure it can promote data transparency without incurring costly bills expected at NIH.
Dr. Brinkman concurred, noting that there are many options on the table, and there are different ways the interagency committee could go.

Next, **Dr. Harriet Kung**[1], Associate Director of Science for BES, provided an update of news from the Office of Basic Energy Sciences. Her talk included a budget update, program highlights, research highlights, and information about new hires and staffing.

Regarding federal funding, FY11 was an unusual year, with a 196 day continuing resolution and thus a delay in final FY11 appropriations until halfway into the fiscal year. The delay is further compounded by the significant cuts in the House-passed H.R. 1 mark. The two factors have hampered agency efforts to execute the budget according to plan. As a result, BES has held back most new and renewal grant support. There have been impacts on graduate students and postdoctoral fellows. And because of the compressed funding schedule, the full FY 2011 year's program execution will occur in 2.5 months.
SC staff has worked very hard to get plans executed.

The FY11 BES appropriation is about $1.678 billion, a $42 million increase from FY10 appropriations. Core research includes $100 million for Energy Frontier Research Centers (EFRCs). Overall, core research support was flat relative to FY10 funding. The Experimental Program to Stimulate Competitive Research (EPSCoR) will be funded at the $8.5 million budget request. Scientific user facilities operations will see a modest increase in funding, especially the synchrotron light sources, neutron scattering facilities, and nanoscale science research centers.

On May 25-27, 2011, the EFRC Summit and Forum, ***Science for Our Nation's Energy Future,*** was held, in Washington, D.C. The summit spotlighted research opportunities and explored our nation's most pressing energy research problems. It highlighted the early successes of the SC EFRCs and was intended to promote collaborations across the national energy enterprise. Over 35 plenary speakers attended, including DOE Secretary Chu, Senator Jeff Bingaman, Congressman Daniel Lipinski, and Congresswoman Zoe Lofgren. The event showcased the winners of the *Life at the Frontiers of Energy Research* video contest. The summit poster reception featured work done at the 46 Energy Frontier Research Centers. There were nine parallel technical sessions (46 hours of talks), three topical lunch discussions, two poster sessions on EFRC research (300 posters), and one networking poster reception with other DOE offices. SC's Advanced Scientific Computing Research (ASCR) division, the DOE Office of Energy Efficiency

[1] Dr. Kung's presentation is available at: http://science.energy.gov/bes/besac/meetings/#0928

and Renewable Energy (EERE), and the Advanced Research Projects Agency-Energy (ARPA-E) were invited to these poster sessions as well.

The first day of the summit began with a discussion of university/ industry/ national laboratory perspectives on energy research and development (R&D). In the afternoon, there were three panel discussions. International speakers from Japan, the United Kingdom, and other European nations provided a broad context of collaborative opportunities. Early research success stories were also shared by representatives from each EFRC.

Dr. Kung discussed some public affairs and outreach efforts by the EFRCs, beginning with the *Live at the Frontiers of Energy Research* video contest. Twenty-six EFRCs created short, engaging films to educate, inspire, and entertain an intelligent but not expert audience about the extraordinary science, innovation and people in their centers. Five winners were selected by judges, and there were over 8,000 votes for the People's Choice Award.

The EFRC Brochure is now complete and available in print and on-line. It contains an overview of the EFRC program and a one page summary with early achievements for each research center. The EFRC program website address is www.energyfrontier.us.

Slides and videos of plenary talks including Secretary Chu's and Pat Dehmer's presentations (www.energyfrontier.us/content/agenda) are available. Pat Dehmer's talk is widely used by the EFRCs for education and outreach activities. There also is a photo gallery, full schedule, and electronic abstract book from the conference. In addition, the website features *Life at the Frontiers of Energy Research* videos (www.energyfrontier.us/video-contest). ScienceCinema, the DOE OSTI multimedia search tool, will archive the videos.

Dr. Kung discussed the FY12 EFRC Science Reviews. She said all 46 would be entering the third year of the five year award period. The review will occur between January and April of 2012. A few regional cities were selected to conserve travel costs. Thought has been given on the types of documents that will be required of the EFRCs for the reviews. The review outcomes will inform funding and portfolio management decisions.

The Fuels from Sunlight Hub has no major issues. Its research program is proceeding on schedule. The Joint Center for Artificial Photosynthesis (JCAP) North, near Lawrence Berkeley National Laboratory (LBNL), occupies 14,000 square feet of leased space. JCAP South, at Cal Tech, is occupying temporary space. Renovation of the permanent space is expected to be complete by March 2012. There will be a BES management and operations review of JCAP in April 2012. Staffing is proceeding well at all levels, including senior staff, postdocs, and students. Two scientific publications and three invention disclosures have been submitted. The JCAP internal intellectual property (IP) plan has been finalized. JCAP will host an *Artificial Photosynthesis Futures Meeting* at LBNL on September 15-16, 2011, with approximately 40 EFRC participants.

The Linac Coherent Light Source (LCLS) at SLAC, the Stanford National Accelerator Laboratory, has seen early success, driving rapid user growth. There have been 427 use proposals submitted to date, representing more than 1,297 scientists from 28 different counties between September 2008 and January 2011. Each research team contains about 15 collaborators on average. The largest collaboration team contains 60 people. Exciting results in the biological science field, including the capability to probe a sample before destroying it, has opened new fields in materials and chemical science. The equipment's probing electronic functions have been revolutionary. Currently, the acceptance rate for research proposals is 28 percent; proposals must be very competitive to get beam time at the LCLS. There is a need to expand and support the LCLS 2 proposal.

Light sources produce fruitful collaborations with industry as well. A group from General Electric has used the LCLS to characterize commercial scale batteries to replace lead acid batteries. In situ studies were performed on prototypes of batteries designed by GE for hybrid diesel locomotives. Energy dispersive X-ray diffraction (EDXRD) measurements revealed local electrochemical kinetics in unprecedented levels of detail deep inside of commercial-size batteries. GE has recently announced that it will build a $100 million manufacturing facility in upstate New York to produce a sodium metal halide battery and will use EDXRD at the NSLS to improve their performance.

In biosciences, x-ray crystallography at ALS, SSRL, and APS has enabled Plexxikon, Inc., to develop new drug against malignant melanoma. The company targeted a mutant protein found in half of all melanoma patients. They examined over 500 crystallized protein samples at the three DOE facilities to find a drug molecule that blocks the runaway cell growth triggered by the mutation. For patients in recent Phase III clinical trials who had late-stage malignant melanoma and the gene mutation, and received the drug Vemurafenib, the risk of dying was 63 percent less than for those who received conventional treatment – a dramatic improvement. The results represent a clear victory for the targeted drug development process.

The National Synchrotron Light Source-II (NSLS-II) project, at Brookhaven National Laboratory, is 56% complete. The facility is now fully enclosed and the laboratory-office building is under construction.

For FY12, the BES budget request is $1.985 billion. Areas of focus include:

- Research programs
    - Energy Innovation Hubs
    - Energy Frontier Research Centers
    - Core Research: increases in basic research for energy; materials by design; nanoelectronics; methane hydrates
- Scientific user facilities operations
    - Synchrotron light sources
    - Neutron scattering facilities
    - Nanoscale Science Research Centers
    - Instrumentation for clean energy

- Construction and instrumentation
    - National Synchrotron Light Source-II and instrumentation (NEXT)
    - Spallation Neutron Source instruments & power upgrade
    - Advanced Photon Source upgrade
    - Linac Coherent Light Source-II
    - TEAM-II

Funding increases are planned for core research in Materials by Design, nanoelectronics, and methane hydrates. The appropriations bill passed at the House committee level reflects a $300 million decrease relative to the FY12 budget request. Decreased funding within the construction and instrumentation budget would be problematic, especially for the LCLS-II. Further, any funding reductions relative to budget could threaten the status of the construction projects. The research programs account essentially increased by only $20 million.

The House mark also contains specific language stipulating reporting requirements and expenditures. The House Energy and Water Development Appropriations Committee recommends $1,688,145,000 for Basic Energy Sciences, $9,950,000 above fiscal year 2011 and $296,855,000 below the request. Within available funds, the recommendation includes $20,000,000 to establish an Energy Innovation Hub for Batteries and Energy Storage. The House bill language states that DOE should not assume that all, or even most, Energy Frontier Research Centers will be continued beyond their fifth year in fiscal year 2013. Further, the department is directed to provide to the appropriations committee, not later than March 1, 2012, a report including the five-year research goals for each EFRC, each center's current status towards reaching those goals, and the department's latest rating of each EFRC's performance as they pass their half-way point and the Committee considers funding for the last year of the initial five-year awards. The recommendation, at $8.52 million below the request, provides no funds for the Experimental Program to Stimulate Competitive Research (EPSCoR).

The House appropriations committee is also concerned that Basic Energy Sciences is not holding its research groups sufficiently accountable, and that it is not terminating underperforming grants. The House mark directs the department to create a performance ranking of all ongoing multi-year research projects across BES, including those at universities, national laboratories, Energy Frontier Research Centers, Energy Innovation Hubs and other recipients, by comparing current performance with original project goals. The department is directed to terminate the lowest-ranking awards within Basic Energy Sciences in the amount of $25 million and to report to the committee, not later than March 15, 2012, on the results of the ranking exercise and selected terminations. At this time, it was unclear whether this language would remain in the final appropriations bill passed by both the House and Senate, signed by the President, and enacted into law.

Planning activities are ongoing regarding mesoscale science and the Materials Genome Initiative. For mesoscale, Dr. Brinkman of SC, in his mesoscale charge letter, stated that,

"A central theme of these reports is the importance of atomic and molecular scale understanding of how nature works and how this relates to advancing the frontiers of science and innovation. I would now like BESAC to extend this work by addressing the research agenda for mesoscale science, the size regime of hundreds of nanometers where classical, microscale science and nanoscale science meet. I see two parts to this new study:

1. Identify mesoscale science directions that are most promising for advancing the department's energy mission.
2. Identify how current and future BES facilities can impact mesoscale science."

Regarding Materials by Design – the Materials Genome Initiative (MGI): we are at the threshold of a new era where predictive modeling will transform our ability to design new materials and chemical processes, enabling rational discovery strategies for systems that were not tractable a few years ago. A recent workshop helped to inform a white paper, "Computational Materials Science and Chemistry," and the MGI report published this June 2011. The white paper and report were prepared by the ad-hoc interagency Group on Advanced Materials and formally approved through the National Science and Technology Council, Committee on Technology.

The report discusses the improvements in computational power to shorten innovation cycles and accelerate collaborative science. The Materials Genome Initiative brings together SC, EERE, NIST (the National Institute of Standards and Technology), and DOD research agencies and is part of the American Advanced Manufacturing Partnership initiative.

Finally, Dr. Kung discussed recent staffing changes at BES. She then concluded her remarks and offered to answer questions.

Chairman Hemminger invited the BESAC to ask questions or provide comments.

Question: Were you as surprised as we were at the House appropriations committee language in the committee-passed bill regarding BES?
Answer: In the past BES has been regarded as a model for responsibly managing a research portfolio. So it was a surprise. We need to inform House staffers on how we are holding PIs accountable. At the root is communicating the overall strategy on accountability, in addition to showcasing the impact from our research portfolio.

Question: Regarding pending cuts to user facilities: how will those cuts be implemented? Light sources are important; that research should be highlighted. Those planned upgrades and construction projects are very important. How can the BESAC help in communicating with Congress? Visiting the Congress in the past seemed to make an impact. The BESAC should work to help educate members and staff on the importance of the science and how those cuts could be disastrous.

Answer: That is a very good point. Communication is the key. We should solicit better information on our research impacts. BES could use that to better communicate that impact to others.

Comment: We could go as a delegation to visit Congress.
Answer: We will leave it to Dr. Hemminger's discretion as chairman of the BESAC. It is a fine line. We are not a lobbying group, but certainly, talking to Congress is important.

Question: Since the EFRC showcase, has the tone been any different regarding understanding of the value of energy research? The EFRC itself should have been an effective communication tool.
Answer: The feedback from the community was positive. Also, the event helped form a sense of community and reinforced the idea that EFRC investment is a key part of a balanced BES portfolio.

Question: Will instrumentation needs at labs and universities be supported in the future.
Answer: There was no guidance on the FY11 budget until very late. There is concern about the overall funding support for instrumentation. It is hard to predict, and the funding projection is not as rosy as we thought.

Question: The SC requested a 20 percent plus-up for FY12. What rationale was provided to Congress for the budget increase?
Answer: Three priorities were communicated to Congress for SC: Materials By Design; Computing by Design, and energy efficiency. The overall budget is a factor in determining the final funding amount each program is given. Comparing BES within the overall SC funding, we didn't do too poorly. At same time, we are seeing a 15 percent cut from the request level. Overall budget constraints and deficit reduction policies are coloring the overall picture.

Question: How do program authorization levels specified in the America COMPETES Act Reauthorization compare with current appropriation levels?
Answer: In 2009, funding was very healthy; plus the Recovery Act helped with construction projects. This year the funding picture is very different.

Question: What about funding for research facilities?
Answer: Accelerators and microscopy are considered a research line item and should not be overlooked.

Question: Will the Senate appropriators support ARPA-E?
Answer: We don't know, but we are anxious for the Senate to move forward with its appropriations bill.

Comment: We need to address the House's dissatisfaction with research progress and squeeze on funding. BES researchers report a "here's what I did this year," kind of thing, but the unimaginative approach doesn't seem to work well for the core R&D and energy

research centers, where a critical item is the flexibility of the research teams to respond to new ideas and movement toward new directions. We must be able to explain to Congress that research organizations are able to respond quickly to national needs to maximize return on investment. We should revise the template for the reporting of these organizations.

Dr. Kung said we must revise how we communicate how basic research is managed. We've allowed our community to pursue the best and most exciting ideas. We evaluate how well they have utilized resources. On the detailed plan, we intend to include how we manage the research portfolio.

Question: Can you comment on the specific language from the House committee's mark regarding a report on performance for all ongoing multi-year research projects, comparing performance with multi-year goals?
Answer: We can't rank them one-by-one, but we do have peer reviews that rank on merit. That can serve as a basis to summarize and respond. We can also include a list of programs that we have terminated.

Question: Has NSF or NIH have had similar warnings?
Answer: No.

Question: Will the Senate appropriation language also reflect that of House?
Answer: We don't know.

Comment: This House language hurts; the Committee of Visitors (COV) process is one in which we believed. The COV process is highly regarded in the scientific community. Something's not quite working.

Comment: The website could be an effective communication tool.

Comment: Regarding EFRCs and the House language to evaluate them by March 2012: it takes time to put these centers together. There's a brainstorming period, hiring post-docs, etc. This censure is detrimental because some EFRCs are just coming together and beginning to be productive. It is important to communicate that collaborative efforts do take time.

Comment: The House language has created angst in the research community. There is concern about designing such a response before we understand from where the House language came. We have no idea, and we could guess, but we don't know.

Question: With the debt ceiling, what happens if our community gets hit with a 10 percent cut in the BES budget?
Answer: We can't make a general, over-arching decision just based on a number like a 10 percent cut, but there would be a major impact.

Comment: The community needs to be actively involved in communicating with Congress that such a cut would impact on U.S. competitiveness.

Comment: The emphasis should be on communications. What if we got together with the American Chemical Society and the America Physical Society held a National Energy Day, asking supporters to call their member of Congress, inviting members to visit and see what we're doing in the lab? It would be a lot of effort but may have more impact than traditional efforts. Seeing what actually goes on at the national labs or university labs could have more of an impact.

Dr. Hemminger said that was an upbeat comment and then called for a scheduled break at 10:11 a.m. The meeting was reconvened at 10:51 a.m.

Next, the BESAC discussed the Mesoscale Charge from SC. **Dr. Hemminger** reminded the committee that advance work had been requested prior to the discussion. Also, after the BESAC meeting, whomever wanted to be involved in the discussion to organize and provide guidance on how to move this forward was invited to stay a few additional hours. The breakout discussion would also determine who from the greater scientific community could be included. Similar to how it handled the Grand Challenges report, the BESAC would break into a smaller working subcommittee that would include the broader scientific community. It would meet several times at different places around the country, broadly soliciting input before assembling a draft in response to the charge. Tomorrow, there will be more discussion among those who would like to be a part of that. Dr. Hemminger volunteered to organize a lunch for interested BESAC members and asked members to please indicate who would be interested. Approximately 12 to 15 BESAC members volunteered. One person asked if that could occur after the meeting today. Dr. Hemminger said he would not try to organize a group today, but that discussions could certainly occur off-line this evening.

Dr. Hemminger noted that Tom Kalil of OSTP would discuss the materials genome initiative, and that would fit nicely with the mesoscale topic. He then asked the committee: what are examples of mesoscale properties that are dominant in a material?

Comment: We've accomplished a great deal at the nanoscale; now we are ready to study materials at this scale because of strides made at the nanoscale. We can do new kinds of experiments with new technologies.

Comment: Mesoscale makes the connection between macroscopic behavior and nanoscopic behavior by connecting phase coherence of a superconducting constant.

Comment: This is exploiting materials properties at a new scale.

Comment: What are the classes of properties we want to exploit that are relevant here? It could include mechanical and electronic properties and how they interact. It could include chemical or surface-related or interface-related properties. We could approach

the problem by taking a larger scale view of categories and representative examples of those things that stand out, and indicate why this is important.

Comment: Mesoscale describes new phenomena. Penetration depth and coherence length are macroscopic. There are new tools for fabricating new structures to explore a wider range of phenomena than before.

Comment: Mesoscale is relevant in biology: in programmed self-assembly, such as for membranes and in DNA organization. Mesoscale relates to the materials genome and in understanding DNA-DNA complementarity to build ordered materials. It is in protein associations and biological machines, in chloroplasts in photosynthesis, and of course in the cell. Mesoscale can be relevant to synthetic polymers: you can synthesize them and have them associate into novel structures. Silk is an example; a spider makes different kinds of silk. Mesoscale takes the principles of biology to assemble structures with resultant properties.

Comment: Mesoscale can be relevant to discussions on atmospheric modeling, especially relative to the carbon cycle.

Comment: Mesoscale could include nanoscale synthesis resulting in a more energy efficient function. It could be characterized by real-life catalysis, understanding how one or two individual molecules interact with a surface and translating that into a real-life catalysis situation. It is the study of molecules' collective behavior and the translation of that understanding to real life catalysis.

Comment: Mesoscale could also mean the study of mechanical or material failures over long periods of time over extreme conditions, important in nuclear research. It is the study of erosion properties. How we can experimentally model accelerated aging and stress testing will be key.

Comment: In biology, we don't just build and that's it; there are life cycles for molecules. In physics, and semiconductors, the study of life cycle and how you study that can be enabled by mesoscale.

Comment: Mesoscale describes photosynthesis; you have membrane assembly, protein transport, and interaction of quantum class machines.

Comment: What about dynamic imaging? We need better tools for imaging at the metascopic scale of greater than 100 nm. We need to be able to visualize thicker, bigger objects.

Comment: The world was captivated by the nanoscale discussion. It began with a small number of people talking about it and the idea of new experimental capabilities. We must consider examples of specific issues and experimental methods that don't ignore nanoscale fundamentals. We must consider multiscale kinds of theories. What about industrial science?

Comment: The materials and tools for mesoscale study are important. The synchrotron is ideal for science at the mesoscale. Battery research at General Electric is studying the behavior of the battery at the mesoscale. It could also describe current work at the DOE scientific user facilities: materials fracture, failure, and processing issues are mesoscale. Electron beam centers and moving resolution are at the subatomic scale, but what about studying materials at the mesoscale?

Comment: Mesoscale could include the science of molecular/ materials self-diagnosis and self-repair. Electrochemistry involves charge transfer and charge storage at the nanoscale. How the charge gets to the wires connecting the world could be a mesoscale study.

Comment: It could include multi-phase gases and coupling a surface property to a bulk property.

Comment: It could include stability and phase/ class transitions.

Comment: All of this should be considered in the context of better communication with policy makers. We need to convey the products that will come as a result of mesoscale science. Why is this exciting? There are so many products we take for granted that came as a result of basic research. Consider the catalytic converter: a catalyst sits on a substrate; there are crystals and ports, exhaust and thermal expansion of material. This is an example of controlling the mesoscale in essential and everyday processes.

Comment: It is important to look at how nanoscale developed, but we shouldn't get too wound up in that. There were a number of scientific advances that set the stage for the nanoscale discussion, from C60, to being able to make macroscopic amounts of it, and doing the scanning tunneling microscopy (STM) experiments. That happened over an extended period of time. I'm not sure the mesoscale discussion will develop like that, but there are issues at this scale that determine important material properties. Can we convince people that their quality of life depends on that? With recent work, do we have a better way of packaging that?

Comment: The mesoscale could describe the planetary sciences. Multiple scales interface here, such as mesoscale and nanoscale. In this area, mesoscale can describe how the materials are held together and consider complex materials such as meteorites. Mesoscale can also be used to better understand carbon nanotube material behavior.

Comment: I don't think the goal is to try to make mesoscale science like nano, which started as an inter-agency working group, then a workshop report. This is internal to the SC and is less ambitious than the nanoscience initiative or manufacturing materials science issues. We're struggling with the catchiest way to characterize mesoscale science. The whole STM process excited the field of nanoscale science.

Comment: Nanoscale science was a rallying cry; it represented a new scale of building blocks. You could mail a friend a research sample that was completely invisible. Mesoscale science represents a new building block. Molecular machines are at this scale.

Comment: Nanoscale science started with the use of a machine, and it was cheap. Not everyone can have a neutron source in their lab; that is more expensive. Is this an activity that will occur in BES or in the society? Planning will be different depending on the audience. Catch phrases could be: "Science at Scale," or "Integrated Science at the Mesoscale." Do we want to make this go viral as nano did?

Dr. Hemminger said we can use language that gets other communities excited; it helps to convince the government that mesoscale science is useful and helps solve important problems. The terminology we use may evolve as we go through the activity of trying to define mesoscale. There is nothing to force us to say mesoscale solves the world's problems, and we have flexibility. The scientific community has embraced the nanoscale revolution; tremendous knowledge has come from that. We should be looking for opportunities to use that knowledge to address challenges at different scales.

Comment: One issue is that of classification. Properties of materials, how they fail, and even transport across pores are determined by how structures at the nanoscale level are assembled. How materials are assembled represents mesoscale. Mesoscale researchers do work at the nanoscale and then put the pieces back together. Make a list of collective properties that depend on materials assembly. For biological assembly, it is information and regularity. Properties depend on how nature assembles components to get devices. For manmade materials, the lack of information, pattern, or structure may be a mesoscale study. For example, meso-porous materials that are crystalline have different properties from other manmade materials.

Comment: A second discussion point on how BES facilities can impact mesoscale science. In going from nano to a larger scale, if there are important problems to solve at this scale, BES facilities need to be able to address those. What can our facilities do to image or resolve problems at this scale?

Comment: Consider light sources and the LCLS. Mesoscale science could generate a renaissance in American manufacturing. Imagine better materials for roads. Think of the area of polymer science or of the materials genome initiative. Think of the manufacturing of new materials. It would be good to have light source directors come and discuss the practical applications of their work. This is to design materials with better properties; it applies to superconductors, semiconductors, polymers. Mesoscale science enables us to understand better and synthesize materials with desired properties.

Dr. Hemminger and others concurred.

Comment: Consider it in the context of working with neutron sources. Neutron scattering is a powerful component of mesoscale science.

Comment: Mesoscale science is about putting together nanoscale structures to assemble things at a higher scale. We don't want to lose the words "nano science."

Comment: There are multi scale phenomena to consider: it is a continuum description of matter that includes both quantum descriptions and mechanical descriptions. Mesoscale allows you to define those issues.

Dr. Hemminger, hearing no further comments, said about a dozen people would remain after lunch Thursday, maybe for an hour. He invited members of the BESAC to participate.

Comment: Please put a draft or something capturing these ideas on the board. People like to criticize much more than to produce an original document. Producing an initial draft will make progress.

Dr. Hemminger called for a lunch break at approximately 11:45 a.m.

Afternoon Session
Wednesday, August 3, 2011

The afternoon session was reconvened at approximately 1:32 p.m. **Dr. Hemminger** introduced **Dr. Patricia M. Dehmer**[2], Deputy Director for Science Programs and Acting Associate Director for Workforce Development for Teachers and Students (WDTS) at SC. Dr. Dehmer gave a report on WDTS focused on an update one year after the BESAC COV report.

The COV report ranked WDTS programs from excellent to poor. Several of the programs play a unique role in U.S. scientific workforce development. Several programs that the COV ranked as excellent have insufficient funding to reach their full potential. Furthermore, the COV determined that short and long-term assessments of the quality and impact of WDTS programs was inadequate.

In April 2011, Bill Valdez, the career official in that office, left, and Dr. Dehmer became acting director of WDTS. At that time, the team of 15 staff began an assessment of WDTS programs and business systems. This presentation serves as the 90 day progress report to the BESAC.

The unofficial mission of WDTS is to develop the next generation of scientists and engineers to support department missions, administer its programs, and conduct the research that will realize the nation's science and innovation agenda. It should be the standard for workforce development programs in a mission agency in which science and technology lie at the heart of that mission.

Current WDTS programs include:

[2] Dr. Dehmer's full presentation may be viewed at: http://science.energy.gov/bes/besac/meetings/#0928

- Student internship programs at DOE laboratories (one for 4-year institutions and one for community colleges) and a visiting faculty program
- SC Graduate Fellowship
- Albert Einstein Distinguished Educator Fellowship
- National Science Bowl

Other activities include an on-line business systems modernization effort and a program evaluation and assessment initiative. WDTS aims to support the DOE Strategic Plan, stated in May 2011 to sustain a world-leading technical workforce of scientists, technologists, and engineers. Investments in SC, and specifically WDTS, will enrich the diversity of the science, technology, engineering, and mathematics (STEM) pipeline so that it is more inclusive of women, minorities, and persons with disabilities while mentoring the next generation of scientists, technologists, and engineers. WDTS supports the department by fostering workforce development through education and training programs involving energy literacy and energy efficiency.

In its report, the COV recommended that WDTS:

- Focus efforts and resources on its strong programs that include:
    - Office of Science Graduate Fellowships (SCGF),
    - Science Undergraduate Laboratory Internships (SULI),
    - Community College Internships (CCI),
    - Einstein Fellowships, and
    - National Science Bowl (NSB).
- Redirect funds from the weak programs (ACTS, FaST, Undergraduate Research Journal, College Guide, RWDC, and PST) to funding the recommended changes and expansions in the strong programs.
- Add Ph.D.-level scientists to the staff who have experience in scientific research, educational outreach, and grants program management.
- Increase the level of interaction, cooperation, and coordination between staff in WDTS with Office of Science programs and program managers in Germantown.

The overall funding outlook for WDTS is poor. Although the FY12 President's budget request was for $35.6 million, the House appropriations committee marked its bill with only $17.849 million for WDTS programs. Priority funding should go to SULI and the SCGF. The NSB is a very popular program and should be supported.

In order to better evaluate its programs WDTS focused on program goals, scope, and definition as well as metrics of success for SULI, CCI, and FaST. In mid-July, program leaders hosted a meeting in Washington, D.C., with DOE laboratory education directors to further refine metrics for program evaluation. By mid-August, Dr. Dehmer and colleagues expect to finalize the process. By early FY12 (October 2011), they will commission new business system software that will incorporate participant applications, reviewer input, participant deliverables, and questionnaires. That data will be collected, analyzed, shared, and archived.

Dr. Dehmer provided overviews of SULI, CCI, FaST, SCGF, and the NSB programs, including when the programs began, how they operate, and basic funding profiles. Details may be found in her presentation.

The House appropriations committee mark for FY12 funds WDTS at $17.849 million, which is $4.751 million below FY11 levels and more than $17 million below the President's request. Within the funds provided, up to $5 million is for the SCGF program to fund the existing cohort established in FY10. If the House language is enacted, the department will be directed to submit to the appropriations committee, not later than 90 days after enactment, a 10-year plan outlining the long-term objectives for this program, the number of simultaneous fellowships the department plans to ultimately support under a flat-budget scenario for SC, and the funding needs under that plan. The plan should also justify to the Committee why fellowships should be funded within SC when other agencies, in particular the NSF, are the primary federal entities for such purposes.

What is the value of supporting 450 SC Graduate Fellows? The original goal for the SCGF was to support 450 fellows in steady state, i.e., each year's cohort would be 150 fellows. In FY09, SC supported about 4,500 graduate students through its research awards across the programs. For this new program, SC set a goal of supporting 450 fellows or 10% of the current programmatic support of graduate students. SCGF attracted more than 3,200 completed applications in its first year, with no advertisement or outreach. 450 finalists were selected based on a merit-based peer review process, 150 fellowships were awarded, representing a 4.6 percent success rate and high confidence of top quality fellows.

The House appropriations committee had asked why the SCGF should be a primary responsibility of DOE. One answer is that it is important to support and train students when they are young and to entice them to pursue research critical to federal agencies' missions. Nearly every federally funded scientific agency supports science education and training to grow the innovation workforce. The total number of graduate fellows supported by other federal agencies is about the same (about 5,000) with the following among the leaders:

- NIH (F31) about 1,800,
- DoD (Science, Mathematics & Research for Transformation Fellowship [SMART] and National Defense Science and Engineering Graduate Fellowship [NDSEG]) about 1,000,
- NASA (3 separate fellowships) about 1,000, and
- EPA Star and USDA about 400-450 each

Dr. Dehmer then relayed key recommendations of the COV, Part II. The COV recommended that WDTS:

- Improve the procedures used in the solicitation and selection of the Graduate Fellows, building on the experience learned in the first year.
- Work diligently and strategically in all programs to increase the participation of students and scholars from underrepresented groups.

- Develop and implement assessment and evaluation procedures for its programs that meet the standards of similar programs in other agencies such as NSF.
- Use these assessments on a regular basis to improve/modify existing programs.
- Follow the procedure that is routinely used in the Office of Science to develop new programs: specifically, new program development should involve careful planning before implementation, including a national workshop attended by stakeholders and a workshop report.

Dr. Dehmer thanked BESAC for the COV report. It is helpful to think about programs from a bottoms-up perspective. WDTS near term goal is to be a model program for energy science workforce development. Having the 17 DOE-supported national laboratories is an asset. She then concluded her remarks and invited questions and discussion from the committee.

Question: Can middle and high school STEM teachers do summer internships? Teachers at that level need to be able to explain to students what a career in this area would be like, and direct experience in the lab would help them do that better.
Answer: That program has been terminated due to financial constraints. Plus, it is not a key DOE mission to train teachers, and it would be difficult to measure success. The COV recommended discontinuing that program, rating it poor.

Comment: It is important to introduce students to the agency when they're young. Every student knows who provided their graduate funding. Dr. Dehmer remembered who gave her funding, and although she never worked for the agency, she did continue to keep up with them.

Comment: My graduate fellowship came from DOE, and I never forgot.

Question: What about the program in computational science?
Answer: No problem there. It is an excellent program and is not questioned.

Comment: It is important to support the graduate fellowship program, even with a flat budget, because it is an essential effort to help build the workforce.

Question: Is this a priority for SC funding?
Answer: Yes. However, the National Science Bowl is more challenging. Every child in school took spelling, and many are familiar with the geography bee. But the Science Bowl is not that well known relative to other similar programs.

Question: Can foreign students come to national labs?
Answer: It depends on the country.

Comment: Another issue is that the younger generation thinks that being a scientist means being poor. Their idea of us scientists is that we don't make much money.

Comment: Both DOE and NSF programs attract other outstanding students. That raises visibility of DOE research. It has a leverage effect that expands the power of one fellowship to a larger group of people.

Comment: The BES community believes this is a very important program. There is also a political issue: if BES core program money is used to help students, then Congress believes BES has extra money and could reduce the budget accordingly. If we could have faith that Congress won't take the money away, then we could be more inclined to invest.

Comment: We have one shot in this report with congressional staff to make the case that these are programs of value.

Dr. Hemminger said it would be useful for BESAC to see the report to help make that case to Members of Congress. He then thanked Dr. Dehmer, and introduced **Dr. John Tranquada,** a physicist at the Condensed Matter Physics & Materials Science Department at Brookhaven National Laboratory, to discuss "Public Access to Research Results: Response to BESAC Charge."[3]

The charge was to describe current policies and practices for disseminating research results in the fields relevant to the BES program. Additionally, the report was to be sensitive to the differences between written findings and digital data. The driver was language from the America COMPETES Reauthorization of 2010, Section 103, requiring the formation of a working group on the dissemination of data. Members of the BESAC discussion group included Drs. Barletta, Bare, Hammes-Schiffer, Hall, Kirby, and Tranquada. They participated in a June 30 conference call with subsequent contact via email. The requested report deadline was July 1, 2011.

Dr. Brinkman of SC had provided a series of specific points to address. First were the criteria for dissemination of data and who makes this determination. Researchers determine what and when to publish. A strong motivation is the concept of "publish or perish" that is pervasive in academic settings, especially in hiring, promotion, and other key career-affecting decisions. This satisfies DOE and user facility policy requirements that peer-supported research results must be publicly disseminated. Peer review establishes that a level of supporting data and analysis required to substantiate a conclusion exist. Scientific journals also perform this peer-review function. Editors also play a role. They are often recruited from the research community and specify publication standards and scope. They select peer reviewers and rely on them to help enforce these quality standards.

For raw digital data, public dissemination is not currently required by the research community. Selections of data presented in graphical form are generally sufficient. Sharing of digital data between groups is typically done informally. For example, computational chemists frequently provide all necessary information to reproduce experimental results in the published supplementary material.

[3] Dr. Tranquada's full presentation may be viewed at: http://science.energy.gov/bes/besac/meetings/#0928

Access to experimental data in BES is provided and controlled in specific ways. For example, access to peer-reviewed research papers is provided through journal web sites and in print, where content can be freely searched. However, full-text viewing may require a subscription. Access to single articles can be purchased. In some research communities, manuscripts may be posted on open-access preprint servers (e.g., arXiv). This is acceptable to many publishers.

The working group explored whether increased data access comes with additional functionality. Common features might include hyperlinks for references; lists of later papers that cite a given paper; and articles in portable document format (pdf) that are easily printable. Regarding the version of the written material or data provided, the version of record is controlled and stewarded by the publisher.

On whether peer review is a condition of data dissemination in the BES community: the answer is yes. It is the standard of formal data sharing. Manuscripts often are made available prior to peer review, but the process of peer review enables experts to validate the results. The publication of research results is a fundamental process of the research community. This common practice satisfies the policies of institutions, DOE facilities, etc. There currently are no requirements to publicly disseminate digital data.

On the issue of long-term stewardship: journal publishers current provide long-term stewardship of publicly-available research data. Most have made all back issues available on the journal website. Data sustainability depends on maintaining a viable economic model. Public archives, such as arXiv, need public support to be maintained to provide long-term data stewardship.

Dr. Tranquada said that the working group discussed the issue of raw digital data. This kind of data likely has only a finite useful lifetime. Current data retention practices include keeping it for more than 1 year but probably for less than 10 years. The group concluded that old data are not sacred, especially because research emphasizes better-quality samples, measurement techniques, etc. In time, newer, better-quality data supplants the old. One example of a data archive is the Protein Data Bank. It stores three dimensional atomic coordinates for proteins, not raw data. The challenge is to transform the atoms into an atomic model. So the diffraction patterns are less important than the atomic model itself.

ScienceInsider reported on July 27, 2011, that the United Kingdom Parliament reported positively on the issue of peer review. Its report recommended that “all data should be fully disclosed and made publicly available at time of publication, particularly if it is the outcome of publicly funded research.” That recommendation, according to *ScienceInsider*, has prompted some concern. "In our experience, most misunderstandings from scientific research come from an absence of meaning and context. “Preparing and scrutinizing papers for publication is a vital part of establishing the meaning and context," says Tracey Brown of the pressure group Sense About Science. "It is not clear from the Committee's report what the problem is that would be addressed from raw data

publication nor the other costs and effects of demanding it." With that, Dr. Tranquada concluded his presentation.

Dr. Hemminger invited questions from the BESAC, reminding the committee that the aim is to accept this report and transmit it to SC Director Dr. Brinkman.

Question: How does this compare with the NIH guidelines on data transparency?
Answer: We did not compare the two.

Dr. Hemminger said that SC leadership recognized it was useful to have input from the BES community as to what happens now. An interagency working group will be formed, and it will have a solid foundational perspective from BES for subsequent discussions.

Comment: The NIH has been making all their research results publicly accessible for three or four years. That is one policy model. We in the BES research community should be concerned with how costly that would be to do for our data. There was a group that tried to use the Freedom of Information Act (FOIA) to determine how much money was being spent on data storage with the PubMed system. It was many millions of dollars per year.

Comment: We should consider the effects of scientific publishing on scientific start-up companies or other small research organizations. Locking up information is a way to protect companies' business models.

Dr. Hemminger: The goal is not to produce recommendations on the future but rather to provide SC with information on what is done at the moment by this community regarding data transparency.

Comment: The America COMPETES Act authorized this work but there is no specific appropriation for it. It is an unfunded mandate. Also, the open publishing model pushes the cost into the P.I.'s research portfolio. For NIH, people can afford to devote thousands of dollars for data storage and archiving, but for us at DOE, that's the cost of a graduate student or post-doc. There are scientists who could not publish if it weren't for publishers who didn't charge authors for the cost of publishing the work.

Comment: The way we do it now is fine. If DOE is being forced to report the way we do things now, then the implication is that something is wrong with what we are doing.

Comment: You can't compare the NIH and DOE because the pharmaceutical industry cares much more about the NIH data being available. For DOE, the demand is different.

Dr. Tranquada noted that at the end of the report is a link by Fred Dilla that lists many of the different ways publishers are exploring this data access issue. One way is that some is at public libraries and is free. The taskforce tried to be careful in how it describes these things; competition between journals is good. No recommendations are in the report; we

did say that for BES, the current system works well. Any recommendations for policy changes should consider unintended consequences.

Dr. Laura J. Biven, of SC's Office of the Deputy Director for Programs, provided an update on the activities of the inter-agency working group on research data transparency. The context of the effort includes consideration of how the report will be used. The motivation for the report was the America COMPETES Act Reauthorization and a congressional interest in public access to research results. The working group devised a straightforward charge to receive reports from various scientific communities in a timely manner. Two White House National Science and Technology Council (NSTC) subcommittees (data and publications) have been formed.

The publication subcommittee has discussed different models and ways of engaging publishers. Interagency discussions have occurred with a broader view of data. They are pre-decisional but here are some ideas that have been discussed. The notion that physics and chemistry raw data isn't so valuable is helpful. The subcommittee is also discussing unique challenges that arise with the higher volume of data relative to decades ago. Reports will be used as input for broader discussions on large-volume data.

There is an internal SC working group focused on digital data. The White House Office of Science and Technology Policy (OSTP) wanted to understand this initial information and recommendations that have been provided and will then follow up on issues they see from the committees that report back to them. This is the first iteration in a continuing conversation the interagency committee intends to have with DOE and BES.

All of the SC advisory committees, including BESAC, received this request for information. Each of those communities is a little different.

The committee had comments and questions for Dr. Biven.

Comment: Some scientific organizations are very worried about these data management plans. Data is supposed to be kept secret pre-publication. Information Technology (IT) policies could become complicated.

Comment: We should consider how the data is coming in. Is this a data storage issue or a data management issue? The economic impacts on the scientific community could be severe as we consider the unintended consequences of unfunded mandates.

Dr. Biven noted other committees had raised the issue of the costs to make data available. The interagency committee does not have a process for collecting figures for that.

Dr. Hemminger invited the BESAC to provide Dr. Biven with direct feedback. He announced a break beginning at 3:02 pm and reconvened the group at 3:29.

Dr. Henry Kelly[4]**,** Acting Assistant Secretary for Energy Efficiency and Renewable Energy (EERE) presented an overview of EERE's activities and potential areas of collaboration with the Office of Science. Dr. Kelly said EERE was looking forward to working with the SC. In terms of renewable energy research and development, the difference between where we're trying to go and where we are now is huge. Most energy is consumed by buildings, transportation, and electricity generation. To change this scenario into something that is affordable and economically viable, we need new, basic ideas.

Petroleum is one of the hardest issues to address in terms of efficiency and alternative fuels. The biggest users of energy in the transportation sector are lightweight vehicles and heavy trucks. There seem to be many different approaches to address this problem, many of which may be competitive in 15 years or so assuming costs decrease. Metal-hydride batteries to lithium-ion batteries are a success story. More detail on this will be provided tomorrow. In manufacturing, much energy goes to process heat in fabricating things.

EERE has a two-pronged approach: to develop both new processes and new materials that are lower cost. In buildings, where most electricity is used, existing buildings are a big issue. A large amount of the energy is going into heating and cooling using the same technology as was used 40 years ago. And buildings turn over at a rate of only one percent per year.

Another major issue for EERE is how to decrease energy consumption even with a growing economy. The main challenge is doing it cheaply. Unless a new technology can compete with natural gas, it will be in "the land of perpetual subsidies," and not economically viable. Take SunShot, an ARPA-E development, for example. How do you install it? How do you get the right permits and inspections? There are many impediments to long term success.

For wind energy, a focus is to install turbines off-shore. The costs for installing turbines in deep water are off the scale. It is a multi-faceted problem. We are trying to develop ways to build off shore while not killing birds, considering ocean bottom and surface effects, wind, weight, etc.

In the area of biofuels, there are a variety of approaches that can produce substitutes for jet fuel, diesel, and gasoline. However, all of the approaches currently have tremendous price challenges, and some have technical challenges.

Enhanced geothermal technology development is in progress. An important R&D question is how to drill deep enough to capture heat from deep in the earth.

Since the Recovery Act, EERE has funded a large amount of hydro-kinetic or "ocean technologies." There are a basketful of new development technologies.

[4] Dr. Kelly's presentation is available at: http://science.energy.gov/bes/besac/meetings/#0928

Regarding fuel cells, we are moving toward applications like forklifts and reversible fuel cell storage. We are developing cheaper, more effective catalysts.

EERE's work has been "a complete experiment." EERE leaders have considered the real problems this office can help solve.

A potential top-ten list for "Energy Efficiency" includes:

1. Durable membranes that transport only H_2O (for cooling/ dehumidification)
2. Room temperature separations (replace distillation etc.)
3. Thermoelectric device with ZT (a measure of thermodynamic efficiency) greater than 3
4. Magnets for motors and generators that operate at room temperature without rare earth materials
5. Glazing materials with controllable properties (transmissivity, reflectivity, emissivity)
6. Fast synthesis of Lithium-electrolyte interface layer
7. Low cost insulating materials with low conductivity/cm-thickness
8. Low cost sensor for measuring air quality (CO, CO_2, particulates, hydrocarbons, bacteria)
9. Low cost, low embedded energy substitute for concrete
10. Multi-photon phosphors

A potential top-ten list for "Renewable Energy" includes:

1. Methods for accurate prediction of wind speeds on land and in the ocean (minute scale to monthly scale)
2. High-efficiency biological pathways for converting biomass to materials now made from petroleum (bacteria, enzymatic processes)
3. High-efficiency non-biological or bio-mimetic pathways for converting biomass to materials now made from petroleum (electro-fuels, sunlight-to-fuels)
4. Low cost, durable materials with high optical transmissivity and high electrical conductivity
5. Inexpensive production methods for high-efficiency III-V photovoltaics
6. Low-cost, durable membranes that transport only hydrogen and require little or no rare materials (flow batteries, fuel cells)
7. Inexpensive methods for locating geothermal resources
8. High band gap semiconductors (power conditioning/controls)
9. High growth rate algae or other materials that convert more than 80 percent of their mass to lipids
10. New membranes and/ or chemistries for utility-scale flow batteries

This summarizes the major issues currently being considered by EERE. Dr. Kelly concluded his presentation and invited questions and discussion from the BESAC.

Question: For outside the U.S., there has been more successful implementation of renewable energy technologies. Why?

Answer: European countries have been more aggressive at addressing climate change, with high carbon emission standards and steeper tariffs for transgressors. That idea has been difficult to apply in the U.S.

Question: Why are coal-fired turbines absent from the "Top Ten Research Problems"?
Answer: That is because the EERE lists are forward-looking.

Comment: The BESAC and EERE should be in better communication.
Dr. Kelly: How we can facilitate that? How can EERE put the big challenges out to research communities that are not accustomed to tackling them?

Question: This is a nice list of things to be accomplished. What about building an economic engine of the future? What about China: what is it doing in this area?
Answer: In terms of low-cost production and subsidizing renewable energy and energy-efficient technologies, China is already ahead of us. The U.S. went from 40 percent to 5 percent market share in these technologies due to competition by China. Our technology dominance in this field is under threat as the Chinese invest heavily in energy efficiency research institutes.

Comment: China has for centuries had low-cost capital. The U.S. has long term technology investments, but the Chinese have low cost labor as well as technology deployment. They have the ability to scale technology deployment that far outmatches the U.S.

Dr. Kelly: We are looking for ways to get low-cost manufacturing production here. The Valley of Death – when a start-up company runs out of initial investment money and needs to build a production facility – is still a problem. It is a significant and painful gap in the United States.

Comment: Regarding the top 10 lists: they're not on the EERE website. It might be nice to have them on the website. Many of the scientists in our research area are ignorant of what EERE does.

Dr. Kelly: EERE needs BESAC's help to put those goals and ideas into terms that are understood by BESAC scientists.

Comment: Just put them up on the EERE website. You could call them "Big Challenges."

Dr. Hemminger added that Dr. Kelly's presentation would be up on the BESAC website[5].

Comment: We really need financially feasible solar cells on roofs. Europe seems to have more political will than the U.S. for EERE R&D.

[5] See http://science.energy.gov/bes/besac/meetings/#0928

Dr. Kelly: Technology development has seen a major shift toward China for production of solar voltaics, despite the fact that China's weather often is not conducive for solar energy generation.

Question: A difference between the U.S. and Europe is that in the U.S., it is possible to obtain venture capital to get started. How difficult is it to get venture capital in China?
Answer: The U.S. still has more venture capital than anywhere else. The challenge is in the funding gap that occurs when the venture capital money has gone through the third round of technology development.

Comment: That is the next phase of building our capability. If we as a nation aspire to produce a million electric vehicles by 2015, the largest producer will make vehicles for $30,000 apiece at a total cost of $200 million. It's not the first $50 million in venture capital that's the problem, it's the next $4 billion required to generate a critical mass in the auto market.

Question: What population of scientists and/ or engineers do you support in terms of research grants?
Answer: EERE doesn't support much basic research. The work EERE supports is more applied research and development– such as something that is closer toward a practical demonstration of a device. If you consider Technology Readiness levels: basic research is 1. Taking something out into a field is 9. Our projects are between levels 2 and 5. There are a lot of different programs, and the national labs do a lot of it, and the rest is divided among industry. There are bottlenecks. We do a lot of work with biotechnology companies. We would like to support a biotech valley – like a Silicon Valley – to work on these issues.

Question: Do you support SBIR – the Small Business Innovation Research program that supports early-stage technology development? Europe doesn't have this. China, sort of does, but not really. SBIR could support commercial starts for some of these ideas.
Answer: Yes, we do.

Dr. Hemminger then thanked Dr. Kelly for being at the meeting and said that the BESAC would welcome continued discussions in the future.

Dr. Bruce Gates[6] then presented the COV report on the chem-biosciences division.

The BESAC was reminded that it had seen the draft, detailed, written report and had already heard about the plans at the last BESAC meeting. The COV met in April for 2.5 days of intense work in Germantown, Maryland. There were seven panels; the total panel membership was 37 people. Some had been on COVs before. Panels and members are listed in the slide presentation. Three BESAC members participated: Drs. Bare, Berrah, and Kirby.

Panels were organized in the following areas:

[6] Dr. Gates' presentation may be viewed at: http://science.energy.gov/bes/besac/meetings/#0928

- Atomic, Molecular and Optical Sciences
- Chemical Physics
- Solar Photochemistry
- Biosciences
- Catalysis Science
- Heavy Element Chemistry/ Separations & Analysis
- Geosciences

Panels included scientists with diverse experiences in academia, national laboratory settings, and in industry. The groups were hard-working and insightful in doing the review.

The scope of the committees' evaluations covered core research programs, including: (a) base program awards to universities and DOE labs; (b) the Single-Investigator and Small-Group Research (SISGR) program in FY09; and (c) renewals of awards made in earlier BES solicitations including the Hydrogen Fuel Initiative (HFI), Solar Energy Utilization (SEU), Nanoscale science (NSET), and Chemical Imaging (CI).

The evaluations did NOT cover EFRCs, SC Early Career Awards, the SC Graduate Fellowship Program, the BES Equipment Supplement Program, or the Fuels from Sunlight Energy Innovation Hub.

The panels examined and discussed the issues, and they formulated comments and recommendations. Major discussions and ideas emerged and became the product of the COV.

Several major findings of the COV include:

1. The quality and impact of the science is excellent. The COV strongly praised BES researchers as well recognized and highly honored.
2. Management of BES programs is excellent and specifically, the work of the program managers was recognized. BES program managers were regarded as hard working, highly skilled, competent professionals. A correlation exists between the effectiveness of the program managers and the high quality of research supported by BES.
3. The use of White Papers that program managers can evaluate rapidly was commended. Program managers consult with colleagues on what kind of research is mission-critical and can quickly make a judgment on whether to encourage the PI to proceed to write the proposal, or to change the target because it does not support the DOE mission.
4. Records: record-keeping in BES is done via hard copies and paper. Files the committee investigated were hard copies. The COV heard comments by Linda Blevins on the desire to put a data management system called PAMS in place. The COV supports that move.

The COV offered three major recommendations. First, program managers are encouraged to attend more national and international scientific conferences in their

program areas and also to visit researchers in their programs, not just at the DOE national labs. Second, the committee recommends the continued policy of considering white papers of research ideas and plans to promote rapid evaluations that encourage researchers to either submit full research proposals or consider modifying their plans. Finally, the COV recommended improving the BES web sites to reach out more effectively to the general public and to encourage those who might be interested in applying for funding and/or participating in programs.

Other consensus comments included the opinion that the PAMS system for data management should be developed promptly. There was also agreement that the BES program should strive for more visibility. A number of committee members also felt that it would be beneficial to fund longer-term projects (such as four-year projects) in appropriate cases when reviews are extraordinarily positive. The COV believes BES staffing has reached a level sufficient to carry out the mission but cautions that detailees are needed and that program managers and staff have their hands full. Progress was noted from a 2008 report recommendation for proposals for national lab projects to put more emphasis on research plans and less on prior research accomplishments.

Concluding his remarks, Dr. Gates thanked all COV members for their work. He thanked Drs. Kung, Rohlfing, and John Miller. He also thanked Linda Blevins and all of the program managers and staff, as well as Diane Marceau. Then he invited questions and comments from the BESAC.

Question: Were you provided with the BES response to the last COV?
Answer: Yes, the COV panels were assigned to read those. They were given background information by Drs. Kung and Rohlfing.

Question: Were you expected to give sub-grades, or just four overall grades?
Answer: There was substantial discussion among the panels on how to interpret that part of the charge and how to assess grades. Detailed comments and recommendations may be found in the appendix, in the back of the report. That is the raw information from the panels. How to interpret the charge was more complex because of the words that were in the charge template. Dr. Rohlfing and colleagues will be putting thought into how the template may evolve and be improved.

Dr. Brown: For the 2008 report – I chaired the COV in 2005. We discussed that a bit. Sometimes people had not performed well in past DOE grants. I hope the new recommendation does not ignore previous COV work.

Dr. Hemminger then noted that the BESAC needed to formally approve the report.

Dr. Brown offered a motion to approve the report.

Drs. DiSalvo and Kay seconded the motion.

Dr. Gates said there were typos and wanted to fix them. The report was approved pending the stated refinements.

Next, **Chairman Hemminger** welcomed Tom Kalil of the White House Office of Science and Technology Policy (OSTP).

Mr. Kalil thanked the BESAC for the invitation to share OSTP's perspective on the Materials Genome Initiative and described a June 24 meeting covering the topics of manufacturing, IT, advanced materials, robotics, and biotechnology. The President's Council of Advisors on Science and Technology (PCAST) including the presidents of the Massachusetts Institute of Technology (MIT) and Dow Chemical would ensure industry remained involved in the partnership.

Mr. Kalil stated that he wanted advice from the BESAC regarding the Materials Genome Initiative. The Initiative aims to reduce the time and cost for manufacturing new materials. The administration will devote $100 million to help launch the initiative, including $40 million in BES, $20 million in EERE, and the remainder of funds in NIST, DOD, and NSF.

What motivated the administration to make this a priority was the idea that advanced materials are essential to competitiveness. Our nation must successfully transition to a lower carbon economy, using less oil and reducing greenhouse gas emissions. New materials will be essential to get us there. It is a problem we must solve in a short period of time. The status quo of 10 or 20 years to develop and deploy advanced materials is not acceptable.

The research community has begun to propose a number of ideas on how this cycle could be dramatically improved – including a National Academy of Science (NAS) report on materials in engineering. The use of data mining as a tool used by the research community could accelerate the process of discovery of new materials. Streamlining the materials development process via improvements in computational science and engineering leading to a more predictive approach might finally be within reach. Those are some of the factors that convinced the administration to support this in the FY12 budget.

DOE organized a workshop in computational science and engineering. The NSF and other science agencies have demonstrated a willingness to get involved.

The Materials Genome initiative has three priorities:

1. Infrastructure for modeling, simulation, and integrating digital data. Tools for data mining. Synthesis and experimentation technologies.
2. Identifying important national problems to identify as test beds. Ideas could include treatment for traumatic brain injury or design of lightweight materials for the transportation sector.

3. Investing in the next generation workforce. Specifically, identifying changes will be required to enable students to work across the boundaries of computation, experimentation and engineering.

OSTP has helped convene the agencies participating to develop consensus on future investments for the project. In the coming weeks, they will move from talk to initial action.

Mr. Kalil asked the BESAC how the informatics portion should be structured. What can we learn from the successes/ failures from the structural genomics consortium? What did we learn from the Alzheimer's Disease Neuroimaging Initiative (ADNI)? How did we identify biomarkers from Alzheimer's and can we do that faster and more efficiently using IT? How can we capitalize on NIH investments in bioinformatics like GenBank?

He continued, what levers does the government have to encourage data sharing within the research community? NSF says that PIs who are competing for grants must develop data management plans. How can we encourage a culture of data sharing? How do we get industry to participate? In a restricted fiscal environment, we are especially interested in leverage and cost sharing in federal investments. How can government help industry and motivate research projects? Also, in the areas of computation and informatics – how to tie in with experiments that are currently ongoing? How do we develop large databases for the materials genome?

Finally, he asked how to leverage investments that agencies have already made. DOE saw Recovery Act investments in energy frontier basic research needs such as solar fuels and materials discovery and development. How do we take advantage of these investments to jump start the Materials Genome Initiative?

Members of the BESAC then began a discussion with Mr. Kalil.

Comment: On data sharing, "encouraging" is a good thing to do. "Requiring" that all data be accessible in an arbitrary way will incur an incredible expense for BES scientists. For genomics, there is a large volume of data that will not necessarily be usable. For high throughput experiments, there are items researchers might miss, so we can understand the advocacy for making some primary data publicly available. It's good to do these things, but don't put too much effort only into high throughput synthesis because some aspects of high throughput synthesis are unclear and difficult to control.

Mr. Kalil referenced the Bermuda Principles on genomic sequencing and how to have relevant research communities get together to help the federal government distinguish between the wheat and the chaff.

Comment: Begin by asking researchers what data they might be able to use. What do they want to study? They don't want to waste their time looking through things that are not useful.

Question: Earlier we discussed how plans can evolve. Can you contrast current plans for the Genome Initiative with the National Nanoscale Initiative (NNI)?
Answer: The NNI was announced by President Clinton at CalTech. The initial federal investment in nanoscale research was $270 million. Now, expenditures are closer to $1.8 billion. More important than increased investment, many universities have started programs in nanoscale, and we see more collaborative programs including successful startup companies like A123 addressing important societal problems. I was involved in this successful effort in 1999 and 2000, and we held workshops to motivate the initiative. There was also strong support for NIH: Congress was midway through its effort to double the NIH budget from $14 billion to $28 billion. The situation has not been the same for the NSF and physical sciences –so this current effort has put more emphasis into the physical sciences and helped capture the public's imagination.

Question: What happens next with the initiative?

Answer: We will have to see if Congress provides the funding. Our hope is that they will and agencies will have funding to support items in the report.

Comment: We are concerned with the analogy between the Genome Project and applying that toward Materials Science.
Answer: We're not talking about bioscience. The term "Materials Genome" is more general audience friendly compared with "Materials Science and Computational Engineering." We are aware that it's not the same as genome research.

Comment: There is low-quality data that accrues over time – such as weather – that may be useful to store and archive.
Mr. Kalil: Or synoptic digital sky surveys that are transforming astronomy. Management, visualization, information extraction, data mining, and the integration of data are becoming a forefront issue of science.

Comment: We hope this will be based on a theoretical understanding of fundamentals.
Mr. Kalil: Yes.

Comment: Materials science is so much more multi-dimensional than anything you would study in genome research.
Mr. Kalil: The sequencing of the human genome is not just the end of the story for biology, and the biologists in the room will tell you they're dealing with some pretty complex systems as well in trying to move the field forward.

Dr. Hemminger then invited open questions from audience:

Comment: communication with Congress is critical. We should better engage our scientific fellows who work on Capitol Hill to carry on this message for us. A second issue is regarding mesoscale: how you get the public to support this challenge? Let there be a similar Hollywood analog like self-assembly of smaller particles into a larger entity.

Maybe we can engage Hollywood to partner with us to get the public excited about mesoscale science.

The meeting was adjourned at 5:13 p.m.

Wednesday, August 3, 2011
Morning Session

The meeting was called into session at 9:04 a.m. **Dr. Hemminger** invited **Dr. Daniel Hitchcock**[7]**,** Acting Associate Director for Advanced Scientific Computing Research (ASCR), to provide an overview of ASCR activities.

ASCR supported research aims to deliver world leading computational and networking capabilities to extend the frontiers of science and technology. Major scientific challenges include delivering next-generation applications using today's petascale computers. Another challenge for this division is to support the discovery, development, and deployment of tomorrow's exascale computing and networking capabilities as well as to develop, in partnership with U.S. industry, the next generation of computing hardware and tools for science. ASCR also aspires to support the discovery of new applied mathematics and computer science for the ultra-low power, multicore computing future. Another challenge is to provide technological innovations for U.S. leadership in I.T. to advance national competitiveness.

FY12 ASCR research highlights include:

- Research in uncertainty quantification for drawing predictive results from simulation
- Co-design centers to deliver next generation scientific applications by coupling application development with formulation of computer hardware architectures and system software
- Investments in U.S. industry to address critical challenges in hardware and technologies on the path to exascale
- Installation of a 10 petaflop low-power IBM Blue Gene/Q at the Argonne Leadership Computing Facility and a hybrid, multi-core prototype computer at the Oak Ridge Leadership Computing Facility

Tomorrow's computers will be different from those of today because of developments in materials science. ASCR provides high-end computing facilities to scientists, where they develop research and evaluation prototypes. The Energy Sciences Network (ESnet) links it all together. Substantial innovation is needed to provide essential system and application functionality in a timeframe consistent with the anticipated availability of computing hardware. The following ASCR programs provide forefront research

[7] Dr. Hitchcock's presentation is available at: http://science.energy.gov/bes/besac/meetings/#0928

knowledge and foundational tools: Applied Mathematics; Computer Science; SciDAC, and Next Gen Networking for Scientists.

ASCR frequently evaluates requirements for what programs need to do and looks toward the future of computing and data management. One case example is computer chip capacity. Throughout the 1990s, application rates ("clock rates") increased. The typical computer server chip currently has about 8 cores; a laptop has about 2 cores. The power of a chip increases as a square of the frequency. By 2020, computer chips developed through ASCR-supported research will have about 400 cores on them, with laptops having approximately 100 cores.

Tomorrow's chips must be energy efficient. A key challenge will be dissipating the heat off the chip, which will also take energy. Concurrency, or doing things in parallel more effectively, will be a key development and currently is a significant algorithmic, mathematic and technological challenge. ASCR supports some of the world's most powerful high speed supercomputers, with names like Hopper, Jaguar, and Intrepid. Titan, at ORNL, will be coming online shortly. It is a heterogeneous, 20 petaflop system.

SciDAC is DOE's Scientific Discovery through Advanced Computing initiative. SciDAC institutes, university-led centers of excellence, have been consolidated to deliver advanced math and computer science more effectively to the applications community. The official announcement on the website is occurring at present. The goal of SciDAC institutes is to deliver tools and resources to lower barriers to effectively use state-of-the-art computational systems and create mechanisms to address grand challenges across different areas of science. SciDAC institutes aim to incorporate basic research results from applied math and computer science into computational science challenge areas. In summary, SciDAC institutes aim to grow the nation's computational science research community. SciDAC awards in the amount of up to $13 million per year over five years are currently available to support between one and five institutes. Eligible applicants for these awards include DOE national labs, universities, industry, and other organizations. The first awards will be given at the end of FY11. More information may be found at: http://www.scidac.gov/institutes.html

One SciDAC institute is called SUPER: the Institute for Sustained Performance, Energy and Resilience, which partners with the University of Southern California. Another institute, FASTMath – Frameworks, Algorithms, and Scalable Technologies for Mathematics – is paired with Lawrence Livermore National Laboratory. QUEST, or Quantification of Uncertainty in Extreme Scale Computations, is associated with Sandia National Laboratories. These institutes are just beginning to start up, working with scientists with the ultimate aim to make software run as fast as possible.

A complementary effort that ASCR supports is joint funding opportunities with other SC programs. Characteristics of those initiatives include pairing the best applied math and computer science with the best software applications and people to address strategic questions with BES. ASCR leadership wants to know: what are the big scientific

questions that BES really wants answered? ASCR is trying to plan the initiative in collaboration with Dr. Kung and her staff in a way that makes the most sense.

Computers can provide important research tools – one can for example put diagnostics into computer applications rather than putting a laser into a material. The future of computing is really about energy efficiency. One can build an exaflop computer today assuming enough floor space and the availability of two to three gigawatts of power for it. Right now, a gigawatt of power is cost prohibitive due to energy costs. A crucial goal of exascale computing is to decrease power usage. Energy efficiency will have a tremendous future impact on advanced scientific computing in our country.

What do ASCR-funded research projects indicate about the future of high-speed computing applications? Locality and not moving the data are important. Most numerical analysis for the past 80 years has been based on counting operations. The future instead is about not moving the data. For some applications it may not matter, but for a branch, it does matter. Incorporating advanced uncertainty complication methods may now be possible. Radiation and chemistry computational processes could occur at the same time if one did not need to move the data. Exascale computing is concerned with what architecture to leverage the most desired research.

Computer scientists focus on co-design to increase our understanding of advanced computing technology and advance future applications and application readiness. The goals of co-design are to:

- Understand how to allocate complexity between hardware, systems software, libraries, and applications
- Modify application designs at all levels
- Understand reformulating as well as re-implementing tradeoffs
- Explore uncertainty quantification, in line data analysis, and resilience in applications
- Co-adapt applications to new programming models and perhaps languages
- Realize the impact of massive multithreaded nodes and new ultra-lightweight operating systems.

Three exascale co-design centers have received funding awards: the Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx), and Los Alamos National Laboratory; the Center for Exascale Simulation of Advanced Reactors (CESAR), at Ames National Laboratory; and the Combustion Exascale Co-Design Center (CECDC), at Sandia National Laboratory. Each center fosters collaboration between multiple DOE national labs as well as university and industry partners.

ASCR wants to chart a path for science application developments to follow. All research trends push toward data driven science and call out for faster computers with more memory. The complementary metal–oxide–semiconductor (CMOS) is a technology for constructing integrated circuits. CMOS technology is used in microprocessors. Data capacity from instruments is still on an 18-24 month doubling path. Our ability to make

sensors is outpacing the ability to process and archive the data. Fiber optic networks with increased capacity are on the horizon: 100 gigabit per second per lambda (wavelength), multiplied by 128 channels on the fiber. Each channel can carry 100 gigabits per second. Currently, launching a petabyte file on someone's laptop is a hostile thing to do. Current internet protocols were never designed for that. Disk read and write rates will fall further behind processors and memory. However, capacity is not the biggest challenge. It is getting the data back off the disk. Getting data off the computer is not feasible because the disk read/write rates are too slow. Figuring what data one wants to transfer is the question. Saving all primary data and analyzing it later is probably not realistic. This changes how we think about our advanced computing facilities.

ASCR wants to work with BES on these and other technology challenges. There will be a workshop on October 24 and 25, 2011, on data communications for BES to communicate what kind of data capacity its science requires so that we at ASCR can enable a data rich future for BES and other SC divisions. Peter Nugent of NERSC and Michael Simonson of SNS will be the chairs.

Additional information, including ASCR leadership and staffing information, is on the website. With that, Dr. Hitchcock concluded his prepared remarks and answered questions from the Committee.

Question: One concern that BES had over the last few years regarded a desire for better detectors. Should we not be concerned?
Answer: Integrated detector and hardware design are critical. But it's important to think about the entire work flow. Automatic feature detection work means scientists don't have to actually look at all the data, but instead they are cued when the data exhibits interesting patterns. But one caveat is in the locality of analytical facilities. Transferring large amounts of data is currently prohibited by technological limitations, so a lot of the high-throughput computing and/or data manipulation must occur at the home institution. One must ask: where is the right place to put all of that? We as scientists can figure out ways to deal with the data, but we must also determine how to optimize the system from end to end.

Comment: It is wise to consider facilities energy management issues. High performance computing really does handle an incredible amount of data and utilize a lot of memory. SLAC has a really good computer system, but this is needed. These ideas are great.

Dr. Hitchcock: A decade ago in ASCR, we realized that for multi-scale systems, one will never be able to compute everything from the lowest scale. Some scientists had physically linked the scales together and gotten non-physical systems. We learned that as one links across scales, it is important to ensure that one is not violating some physical property of the system. Five years ago, we started thinking about the mathematics of large data sets. System developments we have in the pipeline will hopefully help with this problem. Really, it is an end system problem in which you cannot send the data to the users. Thus, where to keep the data becomes important.

Question: Which SC division will be impacted most by the multi-division funding from ASCR?
Answer: ASCR is seeking joint funding opportunities (FOAs) with all SC offices. An FOA from the Fusion Energy Science program (FES) will hit the street this week. FOAs from Nuclear Physics and Biological and Environmental Research (BER) will also be announced this week. ASCR wants to form individual partnerships with each of the offices. We tried a general collaborative grant solicitation before, but it was too vague and hard to respond to.

Comment: One must rethink the way we do experiments from the ground up. Experiments need to be carefully thought through to decide what is chaff and what wheat is. The BES community will need help from your experts in algorithmic processes for data and the mechanism of how you move, store, and process bits of data. A challenge is to understand how to set up the experiments. For next generation light sources, data rates can be enormous, but it's the culture of the experts in how they do science. Yes, this is an important partnership.

Question: These ideas apply to correlation analysis, which studies patterns as data accumulates. We have learned to better manage the volumes of data. In our field, the person who makes the sample owns the data. So what happens when a granting agency tells the user she must buy tapes and make copies of data, and then they may not discard it before a certain time point? What's your view on long term data storage?
Answer: We tell users if they want a backup copy, they have to keep it. We don't throw it out because tape densities have been increasing fast enough that the effort of finding, throwing out, and repacking the tapes is a bigger effort than stringing high density tape. This is entirely an economic decision. Most of the data will probably never be accessed or wanted again, but it is such an effort to get rid of it, and scientists are reluctant to agree to get rid of it. Currently our strategy/ economic tradeoff analysis is that it doesn't pay to do that. We are trying to get scientists to curate this raw data or give up computer time; this made no impact on their behavior. For now, we live with this form of data archiving.

Question: In the area of advanced scientific computing, where is the U.S. in terms of competitiveness? How does the U.S. fund science in this area relative to other nations?
Answer: The fastest computer in the U.S. is number 3 on the top 500 list. China is working hard to establish leadership via hardware and people investments. It has stated a goal of one million experts in high performance computing by the next decade. A lot of the computation work people do at our facilities is energy related. We are one layer removed from the people who are doing the energy related computing research at our facilities. Our industrial users such as the Smart Truck are doing energy related work. The Smart Truck program's goal was to increase fuel economy by 7 percent. This research was done at Oak Ridge National Laboratory. Air flow re-directed around the rear axle helped increase fuel economy. At $4 per gallon for diesel, that really adds up for the trucking industry. We utilized mathematics and computer science that make that work possible. The design of trucks for fuel economy is not intuitive. For example, a truck with tarp on its cab will experience greater wind resistance than one without a tarp.

As wind passes over a truck bed with no tarp, an eddy of air forms in the bed that smoothes the air flow.

Comment: Good points were made on data archiving and storage. We in BES keep our data about a year. It is expensive to store the data on large volumes of discs. After a year, access to data could be tricky if operating systems change or the volume is too large.

Dr. Hitchcock: In the world of tape density, the commercial sector has the same problem. So there is a drive to increase tape density and bring costs down. As for storing the data: costs are painful but manageable. One must budget for it, though. One cannot simply transfer the problem to our users; then the data will be stuck on some laptop that has died. Distributing data to end users is just not a stable situation. End users are not trained to maintain it. For electronic medical records, I once heard an agency person say that everyone should keep their electronic medical records at home. So every person is responsible for operating an IT center in her house? That is not going to happen. Computation facilities play a major role in archiving data. I do not see a good solution other than the facilities being the place for storage of data. It is the best of a bunch of non-ideal solutions.

Dr. Hemminger said that the committee looked forward to the BES workshop in October. He then invited Dr. Linda Horton to discuss the Battery Hub and R&D integration.

Dr. Linda L. Horton[8]**,** Director of the Materials Sciences and Engineering Division at BES began by saying that the battery hub has been around for quite some time. It is in the House mark for FY12 and there is optimism that it will continue to be supported.

Batteries are important in the transportation industry as well as to the electricity grid. Battery technology is important to scientists studying renewable power and storage issues. Society needs batteries with longer lifetimes and better storage capability, especially for vehicles. With the electricity grid, there exists a time lag between when the battery can send electricity and when one receives the power. It is undesirable for operations to be interrupted by a switch in power delivery. This is a key technical issue that battery research must address.

At DOE, BES is just one of the offices supporting batteries and energy storage research. Others include ARPA-E and EERE. DOE formed a team to focus on batteries for vehicles. The team coordinates research at EERE, ARPA-E and BES to align the research and development by reducing communication barriers among the different divisions. A seminar series is also ongoing to facilitate coordination. It attracts researchers from multiple disciplines and fosters collaborations across SC divisions. The team has also held joint international activities with the European Union and Asia. One set of activities that started with the hydrogen program are joint workshops and PI meetings to articulate shared program goals via workshop discussions. Meetings and

[8] Dr. Horton's presentation is available at: http://science.energy.gov/bes/besac/meetings/#0928

poster sessions are especially good for fostering collaborative, cross-disciplinary research partnerships.

An overarching battery goal called MyBattery2020 has arisen from the integrated technology team. Qualities such as battery cost per mile, battery size, battery cost, and charge time are major issues of R&D. Additional goals include battery life, energy density, and power density. Discussions on how to reach these battery capability goals are occurring across the DOE research groups.

DOE has been interested in moving battery technology forward for a long time. The BES interest in this effort really is at the Technology Readiness Levels 0-1 to include developments in structure, interfaces, and the study of phenomena. That is basic research that BES is well suited to support. ARPA-E and DOE's Vehicles Technology Program (VTP) are working at Readiness Levels 2-6 of the technology development cycle.

Funding for energy storage R&D has increased over the past three years, especially with support of EERE. Proposed funding for FY12 is about $35 million mainly because of EERE and ARPA-E. In addition, the Office of Electricity Delivery and Energy Reliability has about $10 million per year budgeted for grid storage research and demonstration project support. In addition to that is the FY09 Recovery Act (ARRA) funding for advanced battery manufacturing ($1.5 billion) and demonstrations ($400 million for transportation and $185 million for grid-scale).

There are current programs that are focusing on graphite and high voltage cathodes, graphite and nickel, manganese, iron cathodes, and others. Future near-term research will focus on graphite and high-voltage cathodes, while silicon/ alloy and high voltage cathodes are for medium-term research. In 2020 and beyond, the predicted focus will turn to lithium/ sulfur/ air and non-lithium battery designs. The ARPA-E program on Batteries and Electrical Energy Storage for Transportation (BEEST) is driven by energy capacity goals, selecting research ideas that are out of the box with specific energy and system cost goals (See slide 7). Total funding for BEEST is an estimated $52.8 million over three years.

The ARPA-E Gridscale Renewable Intermittent Dispatchable Storage (GRIDS) program studies the economics of pumped hydro and grid solutions that are deployable anywhere. Both EERE and the Office of Electricity have invested heavily in demonstration projects. This is a different space from where BES focuses its activities.

The Battery Hub seeks to develop devices for utility scale storage. DOE-sponsored national labs, universities, and small businesses conduct applied research to bridge the gap between BES and technology demonstrations. Large-scale energy storage cost, capacity, and cycle life developments require devices more advanced than Lithium-ion batteries. Hub-supported research projects are focused on the development and testing of prototypes of promising new technologies.

For BES, six of the Energy Frontier Research Centers have a major focus on energy storage. The core research portfolio is growing. A recent example is work by Dr. Nina Balke at ORNL who developed scanning probe techniques to look at Lithium flow. Another example, from Sandia National Laboratory, uses transmission electron microscopy to look at charge/ discharge on a small length scale. The core program emphasizes fundamental research to understand interface phenomena, new characterization techniques, etc.

What is the value of having a hub-level energy storage program? This is a competitive field. A fundamental science question is: what do we need to do to enable the next generation of batteries? Maybe we can get to a different type of energy storage technology than we now have. It requires fundamental science that is complementary and not duplicative. The hub is needed to gather what is currently done, support complementary work, and rapidly get us to the next generation of energy storage. A focus should be understanding hard science problems and impacts on current technologies. The Hub will foster incremental scientific advances that might help form a small business or improve an existing business. It will link fundamental science to applied research, resulting in rapid transfer of technology advances.

Much of the scientific basis for the hub came from EERE and the Office of Electricity. Improved energy storage is critical for the widespread use of intermittent renewable energy, electric vehicles, and efficient and reliable smart electric grid technologies. The Battery Hub, proposed for FY12, will develop electrochemical energy storage systems that safely approach theoretical energy and power densities with very high cycle life. These are systemic challenges requiring new materials, systems, and knowledge.

The Battery Hub will address key fundamental questions in energy storage including:

- Can we approach theoretical energy density?
- Can we safely increase the rate of energy utilization?
- Can we create a reversible system with minimal energy loss?

It will link fundamental science, technology, and end-users, and it will collaborate with relevant Energy Frontier Research Centers, ARPA-E and EERE. In summary, a Battery and Energy Storage Hub will move science and technology for electrochemical energy storage forward at a rapid pace to enable transformative developments for reliable energy supply and transportation systems.

Dr. Horton concluded her presentation and invited questions from the BESAC.

Question: To what degree is private industry investing in battery R&D?
Answer: At this early stage of basic research, the field relies on federal funding for research and development.

Comment: The initiative looks like a 6-2 type of creature.
Answer: It is a 6-1 creature that needs to go through to 6-2.

Question: Is there a formal mechanism that connects the organizations? We don't own the consumer.
Answer: The research proposal solicitation will specify how to do that.

Comment: While there is significant investment with private industry, another route is through the States. A number have tried to be a center for battery technology R&D – like the BEST consortium in New York State. An agency funded through a surcharge on people's utility bills could be used to fund university battery research.

Question: One priority choice is to answer the question: do we want to study energy storage or do we want to focus on energy generation? Also – the BESAC has not had hard discussions on shifts in priorities to address low cost natural gas. What is the impact of low cost natural gas on the nation's appetite for energy storage research? Will BES have a discussion on how to address that?

Dr. Kung: That issue will have a more immediate impact on EERE's program and less on BES. Proposals and research projects may be affected by this topic and natural gas as a diverse source of energy. We are open to ideas but there is no focus on it at this time.

Dr. Hemminger thanked Dr. Horton for her presentation and then introduced Dr. Rohlfing.

Dr. Eric A. Rohlfing[9], Director of the Chemical Science, Geoscience and Bioscience Division reported on developing communications plans for BES.

Congress and others have indicated that in the energy sciences, there is opportunity to improve communication of discoveries and innovation. BES needs to communicate why it funds what it DOEs, what it funds, how it DOEs business and especially, the impact of BES research. The objective of the communications effort is to improve transparency through better communication with all BES stakeholders, including DOE, the Office of Management and Budget (OMB), OSTP, Congress, the broader scientific community, and the public.

The communications plan will include multiple, complementary message pieces. BES has sufficiently communicated why energy research is important, but it could improve in communicating the impacts of BES research. A 1996 report[10] highlighted the formal and informal interactions between BES researchers and industry and featured specific success stories that demonstrated the impact of BES research investments on energy technologies. Congressional staffs have pointed to this document as a good example of what BES should be doing to better communicate research impacts. In the past, BES produced "research summary books" containing abstracts of BES research projects at universities and DOE labs. Currently, the availability of this information is not uniform across BES. The Materials Science and Engineering division maintains a searchable abstract database

[9] Dr. Rohlfing's presentation is available at: http://science.energy.gov/bes/besac/meetings/#0928
[10] See "Basic Energy Sciences – Securing the Present, Shaping the Future," at http://science.energy.gov/~/media/bes/pdf/brochures/files/spsf_brochure.pdf

for grants and separate listing for DOE laboratory projects. Both research divisions put the reports from principal investigator meetings on line

Providing more details on the "Science Serving the Nation Update" report, Dr. Rohlfing said that the update would include impacts over the last 15 years. It would emphasize how BES research has translated into technological advances. A working group will select highlights, consolidate input, and draft individual sections. A contractor will provide technical editing, layout and production.

The SC website's home page depicts real, ongoing research in a way that is accessible to the public. The Dodge Ram pickup truck, for example, provides a real-life story of BES research at work. These are the kinds of stories that the task force will be collecting. In addition, the BES Annual Report for FY11 will contain a layperson summary of energy research in a brochure format. It will include an overview of the BES mission, organization, research, and planning initiatives. It will also feature descriptions of the BES research portfolio, with representative research highlights for FY11. This information piece will serve as a gateway to more detailed information about energy science.

Dr. Rohlfing then gave some examples of research projects from the FY12 budget request. They include titles such as: "Smallest Superconductor Discovered," "A Protein that Protects Photosynthetic Apparatus Critical to Algal Survival," and "High Brightness Beams Obtained with Low Charge Injection." These are fairly technical. When rolled into the brochure, they will be more layperson friendly and will also include graphics. The plan is to have searchable pdf files summarizing the 1,400 research projects supported by the BES core programs. Each program will have information on the principal investigator, research institution, funding source(s), abstract, and more. This information will be collected via a web based system run by a contractor. A solicitation for information call will go out next week. The working group hopes to collect approximately 1,400 abstracts. With that, Dr. Rohlfing concluded his presentation.

Comment: When you put data on the website, please ensure that it is easy to download or link to later. The web page address (URL) should be short enough to easily be cited later on. Also, it is important to keep these URLs stable over time. We want to point this data out to people and don't want to have to spend hours hunting for it.

Question: Have you had a focus group to determine the most interesting and relevant information that stakeholders would like to see? Also consider having an active versus static web site featuring monologues or short movies. That can bring the science to life.

Answer: The task force has broadly engaged stakeholders, received input from the COV and congressional staffers. Its focus is on demonstrating the impact of investment in energy science research. Regarding the comment for a more dynamic web presence, BES did that for the EFRCs, holding a video contest. BES has partnered with the ACS on early careers and EFRCs. The FY11 project summaries will be more static.

One BESAC member commented that he had served on an NSF panel to review NSF operations. He observed that many scientists and engineers can't explain their own projects to one another. The task force must write these stories so one's grandmother or Congressman can understand them. He recommended hiring a professional science writer so the vignettes could be understood by a broader audience. This is especially pertinent in mathematics. It is extremely important that BES try to fix any potential communication issues.

Dr. Rohlfing commented that the task force will employ a science writer to help translate the abstracts/ vignettes, yet not lose the meaning of the actual science. It can be very challenging to translate basic energy research topics for a layperson's understanding. The task force is aware of some easily-translatable research areas; others are nearly impossible to simplify.

Question: Can BES scientists directly utilize this contractor to translate our work?
Answer: PI meetings are excellent vehicles to show to our colleagues what we are doing and provide opportunities to practice explaining our work to a broader audience. The abstracts from those are publicly available. However, we want to retain the flavor of those meetings and not divert them to communications meetings. The abstract tools are great but not as accessible.

Comment: We really need to ask, "What's the core message?" and then devise a communications strategy to engage the public. A crucial core message is to determine what is fundamental research and to articulate its role leading to technology development. BES scientists are the headwaters that flow into the development of new technologies.

Comment: The APS held public focus groups and asked for people's perceptions on basic research. The public asked, "Why are you doing basic research and not advanced research?" So, there is a public perception that basic research is somehow not sophisticated or advanced. The public favors the term scientific research.

Dr. Rohlfing: Language matters.

Question: When do you envision this report going out?
Answer: The report is scheduled to be completed by the end of the calendar year and before the FY13 budget is introduced next February.

Question: It is great to increase the availability of information on the web. But the web is more of a passive approach. Are we doing other things to reach out to the public?
Answer: A brochure will be printed and available for SC to take to the Hill or to anyone else.

Question: The national labs have open houses. The public visits, scientists demonstrate what we do, and it is incredible because people get excited when they see energy research first-hand. Why not do an open house?

Answer: You've been to Germantown, right? [Laughter.] Conferences held by scientific organizations like the American Association for the Advancement of Science (AAAS) have lots of colorful displays and foster interactions with broader audiences. The notion of bringing people to Germantown may be more challenging.

Comment: One message we should all take home – and many of us in the room are BES PIs – is that we should respond rapidly to Dr. Rohlfing's request.

Comment: We already have the request out to the National Labs for the "Science Serving the Nation" initiative as well.

Dr. Rohlfing: The email should already be coming out soon from our contractor.

After that, **Chairman Hemminger** moved to begin the discussion on mesoscale science. Three comments were recorded from the previous day's discussion. BESAC members provided many examples of phenomena driven by meso length scales. The response differed from that at the previous BESAC meeting because people had been thinking about the question in advance.

The committee also appeared to be in consensus that terminology and the name "mesoscale" is a significant issue. The name on this project can be determined as we go along. There are lots of other terms we can use to describe the science, such as "systems, transition, multi-scale," etc. In the short term the goal should be to identify new areas where fundamental research (versus applied or later-stage research) can have a significant impact in the energy arena. Ideas on mesoscale science are at an early concept stage.

Dr. Hemminger: There were about a dozen people from BESAC who would like to discuss this more over lunch. Thank you for your comments and participation, tremendous attendance.

To accommodate members' requests, we have scheduled the meetings farther out into the future so people can plan. The next meetings will be February 22-24, and July 26-27. With respect to the process that we will use for the mesoscale discussion: I hope to form a subcommittee willing to be aggressively active that will include BESAC members plus members of community outside BESAC. This subcommittee will hold small meetings around the country that generate something for people to review and also create opportunities for local stakeholders to provide input. The process will be similar to the Grand Challenges process from a few years ago.

Chairman Hemminger invited anyone on the BESAC or in the audience to provide comments. Noting an earlier-than-anticipated conference adjournment, he also invited the committee and audience to join in subsequent mesoscale science discussions over lunch. He invited further comments and suggestions from the committee.

Comment: We really need to listen to Dr. Rohlfing's point on effective communication. We don't know how to communicate. We really need some guidance with examples of

how to communicate better. We don't want to lose support for basic energy science as a result of communication issues.

Comment: Some of the national labs have excellent science writers.

Comment: SLAC offers a two to three hour workshop on effective writing. It was difficult. We had to do an exercise on how to communicate. It should be part of graduate training, so by the time students earn advanced degrees, they have the ability to give a 30-second elevator speech effectively explaining their work to anyone. Universities must work this out.

Comment: If we PIs don't know how to do it properly, it is hard to teach our students.

Comment: This issue is not only about communication, but also about increased engagement. In industry, a recent focus has been on open innovation. At an industrial fellows' forum to be held later this year, there will be a session on open innovation and research transparency. Innovation in the 21st Century will be done in totally different ways than in the past. Proctor and Gamble, IBM, and others are holding "innovation jams." These events engage stakeholders to think about innovation for the future. Stakeholder and public engagement should be considered.

From the audience, Michael Lubell, Director of Public Affairs for the American Physical Society commented on Dr. Rohlfing's presentation regarding the collection of abstracts and vignettes on energy science. As a caution, be careful not to water down the research too much in the descriptions. It can lead to undesirable consequences. Jazzy titles can be misconstrued and create problems down the line. Also, on the issue of having a web presence – people have to come to you to learn about energy science. Congressional staffs want tweets from Twitter; consider employing social media. Four focus groups were recently carried out by two organizations with experience in science. The good news is that the public thinks the U.S. is a world leader in science. The bad news is that they don't know why. The public thinks too much money is being spent on science, and they don't understand the impact. They do see value in energy research. BES should build on that. Remember that the take-home message is not in what is said, but is in what is heard.

As no other discussion ensued, Dr. Hemminger declared the meeting adjourned at 10:58 a.m.

Respectfully submitted,
Joye E. Purser, PhD
Technical Writer and Recording Secretary
September 15, 2011

(Edited 11/01/2011, MIS)