Minutes of the
Basic Energy Sciences Advisory Committee Meeting
March 17-18, 2011
Bethesda North Marriott Hotel and Conference Center
North Bethesda, Maryland

BESAC members present:

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

BESAC members absent:

Sue Clark	Cynthia Friend
Allen Goldman	Kate Kirby

Also participating:

William Brinkman, Director, DOE Office of Science
Wayne Eckerle, Vice President of Corporate Research and Technology, Cummins, Inc.
Linda Horton, Director, Division of Materials Sciences and Engineering, DOE Office of Basic Energy Sciences
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
Jim Roberto, Director of Strategic Capabilities, Oak Ridge National Laboratory
Marvin Singer, Senior Advisor, Office of Basic Energy Sciences

Approximately 110 others were in the audience in the course of the two-day meeting.

Thursday, March 17, 2011
Morning Session

Prior to the full Basic Sciences Advisory Committee (BESAC) meeting, a closed session was held and new BESAC members were sworn in.

The public meeting was convened at approximately 9:15 am. Rachel Smith of the Oak Ridge Institute for Science and Education (ORISE) made safety announcements. BESAC Chairman **John Hemminger** asked BESAC members to introduce themselves. He then gave an overview of the agenda.

Next, **William Brinkman**[1], Director of the DOE Office of Science (SC), welcomed all attendees and commented on the congressional Continuing Resolution and appropriations outlook for the year.

The Office of Science supports research at the frontiers of science, work that has led to over 100 Nobel Prizes during the past six decades – 22 in the past decade alone. It provides 45 percent of federal support of basic research in the physical sciences and key components of the nation's basic research in biology and computing. SC supports over 27,000 Ph.D.s, graduate students, undergraduates, engineers, and support staff at more than 300 institutions. It also supports the world's largest collection of scientific user facilities with over 26,000 users each year.

Major research themes for SC in 2012 include:

- Materials by design, using nanoscale structures and syntheses for carbon capture; radiation-resistant and self-healing materials for the nuclear reactor industry; highly efficient photovoltaics; and white-light emitting LEDs.
- Biosystems by design, including combining the development of new molecular toolkits with test beds for the design and construction of improved biological components or new biohybrid systems and processes for improved biofuels and bioproducts.
- Modeling and simulation to facilitate materials and chemistry by design and to address technology challenges such as the optimization of internal combustion engines using advanced transportation fuels (biofuels).

Regarding the SC FY 2012 budget request to Congress, the areas of advanced scientific computing research, basic energy sciences, and biological and environmental research received nearly a 20 percent increase relative to FY10. Most other budgets are flat except for nuclear physics because of building construction. Leadership in SC had to make difficult choices to prioritize focus areas. We hope those choices will be honored by Congress going forward.

[1] Dr. Brinkman's full presentation is available at: http://science.energy.gov/bes/besac/meetings/#0927

In FY 2012, BES will support the continuation of the Fuels from Sunlight Energy Innovation Hub, the "Joint Center for Artificial Photosynthesis," or JCAP. The JCAP mission is to demonstrate solar fuels generation that is scalable to manufacture using Earth abundant elements and produces fuel from the sun ten times more efficiently than nature does in a common leaf.

Begun in FY 2010, JCAP serves as an integrative focal point for the solar fuels R&D community. Formal collaborations have been established with 20 Energy Frontier Research Centers. The design of highly efficient, non-biological, molecular level "machines" that generate fuels directly from sunlight, water, and carbon dioxide represent a key challenge for our nation's future energy needs.

A new hub on batteries and energy storage will be initiated in FY 2012. Its mission is to transform the nation's electricity grid and also to electrify transportation. Improved energy storage is critical for the widespread use of intermittent renewable energy, electric vehicles, and efficient and reliable smart electric grid technologies. The Hub will develop electrochemical energy storage systems that safely approach theoretical energy and power densities with very high cycle life.

The Hub will link fundamental science, technology, and end-users, and it will collaborate with relevant Energy Frontier Research Centers, the Advanced Research Projects Agency-Energy (ARPA-E), and the DOE Office of Energy Efficiency and Renewable Energy (EERE).

In the area of Advanced Scientific Computing Research: DOE supports two Leadership Computing Facilities: one at Argonne National Laboratory, and one at Oak Ridge National Laboratory (ORNL). In terms of the most advanced scientific computer in the world, the United States lost the lead to the Chinese last fall. However, the Chinese machine is less easy to program and has not been used for much so far. The focus at the DOE is to run these machines well and continue progress in computational research focused on the Department of Energy missions.

Research supported by the Basic Energy Sciences division includes work in femtosecond x-ray protein nanocrystallography. The free electron laser (FEL) at Stanford is doing exciting work using nanocrystals. Researchers are able to record single-crystal diffraction data from a stream of crystals in a continuous liquid water jet that flows across the focused LCLS X-ray beam in a vacuum. In contrast to cryo-electron microscopy or standard crystallography on microcrystals, which require cryogenic cooling, these data were collected on fully hydrated, three-dimensional nanocrystals. This tool offers great promise in the area of nanoscale protein crystallography.

Through technology transfer, fundamental research has moved to products in cars on the road. Research in basic science helped to discover new composite structures for stable, high-capacity cathodes. Nanotechnology research enabled the tailoring of electrode-electrolyte interface. High energy lithium-ion cells were developed with double cathode capacity and enhanced stability. Partnerships ensued between Argonne National Laboratories and General Motors, LG Chemical, BASF, and other companies for the development of next-generation automobiles. Argonne science continues to work on a 20-year horizon to address these challenges, studying new chemistries and focusing on the electrode-electrolyte interface that allows for higher energy capacity.

Dr. Brinkman said that Energy Frontier Research Centers (EFRCs) have helped to advance energy technologies. As examples, he noted that the world's smallest battery placed inside an electron microscope yields images of electrochemistry at atomic scales, providing new insight into electrochemical processes.

Simulations revealed why nanostructured materials with a large number of grain boundaries exhibit increased tolerance to radiation damage, enabling researchers to design radiation damage-resistant materials.

Biological and Environmental Research is also an important program area supported by SC. Highlighted areas of research planned for FY 2012 include:

- Clean energy biodesign on plant and microbial systems through development of new molecular toolkits for systems and synthetic biology research.
- Research and new capabilities to develop a comprehensive Arctic environmental system model needed to predict the impacts of rapid climate change.
- Continued support for the three DOE Bioenergy Research Centers, and operations of the Joint Genome Institute, the Environmental Molecular Sciences Laboratory, and the Atmospheric Radiation Measurement Climate Research Facility.

The BioEnergy Science Center (BESC), the Joint BioEnergy Institute (JBEI), and Great Lakes Bioenergy Research Center are leading the way with research on genetically-modified switch grass with increased ethanol yields; microbes that produce biodiesel directly from biomass; and the impacts of biomass crop agriculture on marginal lands with downstream impacts relative to greenhouse gas emissions.

The Atmospheric Radiation Measurement Climate Research Facility (ACRF) is tackling major climate uncertainties, providing the world's most comprehensive 24/7 observational capabilities for obtaining atmospheric data for climate change research. The Atmospheric Radiation Measurement Facility operates highly instrumented ground stations worldwide to study cloud formation and aerosol processes and their influence on radiative transfer. In FY12, ARM will deploy a new suite of measurement capabilities to regions of high scientific interest, such as the Azores and Alaska.

Dr. Brinkman explained that work in Fusion Energy Sciences is focused on understanding matter at very high temperatures and densities and building the scientific foundations for a fusion energy source. Research highlights for FY 2012 include support for ITER, the international project to design and build an experimental fusion reactor. High energy density laboratory plasma (HEDLP) research will focus on fast ignition, laser-plasma interaction, magnetized high energy density plasmas, and warm dense matter. International activities are planned to be increased. SciDAC, DOE's Scientific

Discovery through Advanced Computing Program, plans to expand to include fusion materials. The Fusion Simulation Program will pause to assess its now-completed planning activities.

Work on ITER has reached the construction stage, which is expected to take 10 years. Dr. Brinkman displayed an aerial photo of the site, in Cadarache, France. ITER's goal is to be the first demonstration of high-gain fusion energy production, generating fusion power 10 times greater than that used to heat the plasma. The U.S. is a member to the ITER partnership, formed by seven governments representing more than half the world's population. This past year, the U.S. led initiatives to put in place a world-leading management team for the construction phase of ITER and to establish the cost and schedule baselines. The United States will be involved in the development of the central solenoid. U.S. researchers at the DIII-D tokamak invented a new method for mitigating potentially damaging transient heat fluxes (Edge Localized Modes) by precision manipulation of the magnetic field. This work can have an enormous positive impact for ITER. Researchers at the Max Planck Institute in Garching, Germany, recently were able to reproduce these results.

In Nuclear Physics, the research emphasis is on discovering, exploring, and understanding all forms of nuclear matter. FY 2012 research highlights include:

- A 12 GeV upgrade to CBAF, the Continuous Electron Beam Accelerator Facility in Newport News, Virginia. The upgrade will allow the study of exotic and excited bound systems of quarks and gluons and the force that binds them into protons and neutrons.
- The design of the Facility for Rare Isotope Beams to study the limits of nuclear existence.
- The operation of three nuclear science user facilities –
    - Brookhaven's Relativistic Heavy Ion Collider - RHIC;
    - CEBAF; and
    - The Argonne Tandem Linac Accelerator System, ATLAS.
- Research, development, and production of stable and radioactive isotopes for science, medicine, industry and national security.

Dr. Brinkman reported that the Holifield Radioactive Ion Beam Facility at ORNL would be closed. We are facing tight budgets for the next few years, he said.

A new super heavy element (SHE) with atomic number 117 was discovered by a Russian-U.S. team with the bombardment of a Berkelium target by Calcium-48. The existence and properties of SHEs address fundamental questions in physics and chemistry, such as:

- How big can a nucleus be?
- Is there an "island of stability" of yet undiscovered long-lived heavy nuclei?
- Does relativity cause the periodic table to break down for the heaviest elements?

The work of the isotope development and Production Program, within Nuclear Physics, aims to make hundreds of isotopes available to the community for science, medicine, industry and national security. Isotopes are generated by universities, national laboratories, and industry – all over the country. Overall decision-making for the program is guided by strategic planning with federal agencies, community, and peer review mechanisms. SC is coordinating with other federal agencies to address shortages of critical isotopes such as Helium-3 and molybdenum.

In High Energy Physics, work is focused on understanding how the universe works at its most fundamental level. FY 2012 highlights include:

- Support for U.S. researchers at the Large Hadron Collider.
- The research, design, and construction for several experiments as part of a program of high energy physics at the intensity frontier.
- Research in accelerator technologies, including superconducting radio frequency and plasma wake field acceleration work.
- U.S. participation in several international collaborations pursuing dark matter, dark energy and neutrino physics.

The Fermi Gamma-Ray Space Telescope, (FGST) has uncovered many unexpected findings about the gamma ray sky. DOE partnered with NASA on the fabrication of the Large Area Telescope (LAT), with contributions from France, Japan, Italy and Sweden. The LAT is the primary instrument on NASA's FGST, launched in June 2008. SLAC managed the fabrication and now hosts the LAT Instrument Science Operations center. In March 2010, results from experiments utilizing the FGST showed that less than 1/3 of gamma-ray emission arises from black-hole-powered jets in active galaxies. Particle acceleration occurring in normal star-forming galaxies or gamma-ray production from dark matter particle interactions may be the cause. In August 2010, the Fermi LAT detected gamma-rays from a nova for the first time overturning the long-held assumption that novae explosions lack the power to emit such high-energy radiation.

Dr. Brinkman briefly reported on Fermilab's Tevatron and on the Large Hadron Collider (LHC), located beneath the Franco-Swiss border near Geneva. Both are running well, but funding for continued operation of the Tevatron beyond 2011 was not included in the FY 2012 President's budget request.

The Workforce Development for Teachers and Students program seeks to encourage and support the next generation of scientific talent. For FY 2012, SC will:

- Continue to support graduate fellowships. These are three year fellowships for candidates to purse advanced degrees in areas of research important to SC. The Goal of the SC Graduate Fellowship Program is to support a total of 450 fellows in steady state, with a new cohort of 150 fellows each year.
- Continue to support The National Science Bowl, with participation of 22,000 middle- and high school students from 1,500 schools to encourage them to pursue careers in science.
- Continue to support trainees through research experiences at DOE national laboratories. These experiences include the Science Undergraduate Laboratory Internship; Community College Institutes; and Academies Creating Teacher Scientists for middle school and high school educators.

Referencing Section 103 from the America COMPETES Reauthorization Act of 2010, Dr. Brinkman described a new BESAC charge[2] with a report to be submitted by July 1, 2011:

- Describe current policies and practices for disseminating research results, including written findings and digital data, in the fields relevant to the Basic Energy Sciences Program.
- Identify which dissemination models, if any, successfully maximize the potential benefit of research results in a way that is sustainable within the research community.
- Identify any opportunities where public access policies or practices could enhance the discovery potential of Office of Science research results.

Dr. Brinkman summarized his remarks by saying that SC had to set priorities this year in an austere funding environment. The energy challenges of the U.S. are serious because they are a hallmark of international competitiveness. Other nations have already focused on this area for the long term, developing 30 year plans. We need to compete in that world and see that we drive the US into a more competitive position.

Dr. Brinkman responded by questions from the BESAC.

Question: Regarding science and technology graduate students working here who are non-U.S. citizens: more than half of them are ineligible to work in this country. We are investing a lot in them. Is the DOE doing something systematically about this?
Answer: Most foreign graduate students are from China and India. In the past, the top of the class would come to the U.S. to study sciences; that's not happening anymore. Bright young people are allured by the potential of wealth from start-up companies and are pursuing entrepreneurship, rather than pursing advanced degrees. At the same time, China's education system is improving, so more of their bright students will choose to remain there instead of contributing to the U.S. research enterprise.

Question: The recent SciTech report has had a positive impact within the Department of Energy. What, if any, is its impact on the SC budget situation?
Answer: It all helps. There is an effort within DOE to improve coordination of work among different divisions in the department. It is properly done from the bottom up, utilizing knowledgeable people who have a better understanding of the research done at DOE, more so that in the past.

Question: Have the federal budget constraints impacted the scope of the DOE research hubs?
Answer: As long as we continue operating under a Continuing Resolution, there will be impacts to the scope of our research hubs. We cannot support a new hub until FY 2011 appropriations come through. There are three proposed hubs: batteries, critical (rare

[2] See COMPETES Charge to all SC advisory committees: http://science.energy.gov/bes/besac/reports/

earth) materials, and power grid. The scope of research done at these hubs depends on funding support we receive from Congress.

BES Director, **Harriet Kung**[3] reported on the activities of the Office of Basic Energy Sciences (BES). Dr. Kung noted the reports that had been prepared as part of BES's strategic planning activities, and highlighted three that had recently been completed:

- Carbon Capture Beyond 2020[4];
- Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science[5]; and
- Science for Energy Technology: Strengthening the Link between Basic Research and Industry[6].

Dr. Kung discussed the FY 2012 BES budget request. The total BES request is $1.985 billion and includes funding for:

- Two Energy Innovation Hubs: continuation of the Fuels from Sunlight Hub and initiation of the Batteries and Energy Storage Hub.
- Continued support for Energy Frontier Research Centers. The EFRCs represent an important research modality for BES, bringing together the skills and talents of a critical mass of investigators to enable energy relevant, basic research of a scope and complexity that would not be possible with standard single-investigator or small-group awards.
- Construction and instrumentation. Major projects within this area include:
    - 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

The concept of "materials by design" is a key BES area of focus. Research to establish materials design rules will help launch an era of predictive modeling, changing the paradigm of materials discovery from serendipity to rational design. The discovery of new materials has been the engine driving science frontiers and fueling technology innovations. The U.S. has the world's most powerful suite of tools for materials synthesis, characterization, and computation. For FY 2012, the $40 million request would support research in synthesis; characterization and testing; and theory/ simulation and would include partnerships with the National Institute of Standards and Technology (NIST) and the Department of Defense (DoD).

The SciTech report helped set priority research directions in nine areas: solar electricity from photovoltaics; advanced nuclear energy; carbon sequestration; electrical energy

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[3] Dr. Kung's full presentation is available at: http://science.energy.gov/bes/besac/meetings/#0927
[4] http://science.energy.gov/~/media/bes/pdf/reports/files/CCB2020_rpt.pdf
[5] http://science.energy.gov/~/media/bes/pdf/reports/files/cmsc_rpt.pdf
[6] http://science.energy.gov/~/media/bes/pdf/reports/files/setf_rpt.pdf

storage; electric power grid technologies; advanced solid state lighting; biofuels; efficient energy generation and use; and scientific user facilities. The report identifies areas where additional investments will help expand BES reach. Funding increases were prioritized in major areas such as non-carbon sources, carbon capture and sequestration; transportation and fuel switching; transmission and energy storage; and efficiency.

The complete FY 2012 budget request for Basic Energy Sciences can be found at the DOE website: http://science.energy.gov/budget/fy2012/.

Dr. Kung then discussed BES appropriations, specifically, the impacts on research activities when there is a discrepancy between the President's budget request and the actual appropriation of funds. She compared budget requests versus appropriations between 1996 and the present. In FY07 and FY08, there were $170 million and $230 million respective differences between requested funds and actual appropriations. As a result, research grants were not awarded, and major research programs were delayed. Research facilities got a level of financial support that allowed them barely to remain in operation. Funding for FY 2011, as well as for the next few years may be similar, and it will be valuable to review steps taken in FY07 and FY08 to mitigate the negative impacts. FY 2011 has already been impacted, as research programs are operating under last year's funding levels, so inflationary impacts and FY 2011 plans have been delayed.

Dr. Kung briefly presented several program updates, including:

- Energy Frontier Research Center (EFRC) highlights, upcoming Summit & Forum;
    - Dr. Kung invited the audience to an EFRC summit and forum to be held May 25-27 in Washington, entitled "Science for our Nation's Energy Future." The forum is intended to promote further collaboration across the energy science enterprises.
- The Joint Center for Artificial Photosynthesis (JCAP);
    - Begun in FY10, JCAP serves as an integrative focal point for the solar fuels R&D community. And formal collaborations have been established with 20 Energy Frontier Research Centers.
- Linac Coherent Light Source (LCLS) early science results;
    - The LCLS is the world's first hard x-ray laser. Within six months of completion, the laser is being used to study a wide array of science topics, including hollow atoms; magnetic materials; the structure of biomolecules in nanocrystals; and single shot images of viruses and whole cells.
- National Synchrotron Light Source II (NSLS-II) progress;
    - The project is 50 percent complete.
- FY 2010 Scientific User Facilities Statistics;
    - BES Synchrotron Light Sources have been valuable to the user community. There have been more than 13,000 users of these facilities in 2010 alone. Many users represent Fortune 500 companies. In fact, more than 30 industrial users come from these top companies. These facilities represent a high impact, valuable resource for cutting-edge research.

Next, Dr. Kung provided a staff update for BES, indicating key positions filled recently (See presentation)[7]. She thanked BESAC for its support in highlighting staffing needs to help BES improve the management of its research portfolio.

BES strategic planning activities are focused on three areas: science for discovery; science for national needs; and national scientific user facilities. The BES brochure is being updated. It is important for justifying the value of basic research. Linda Horton was part of the original writing team. She accepted the invitation to lead the update of the brochure and will report tomorrow on progress in that area.

Dr. Kung thanked the Committee for its guidance and support. She then answered questions posed by the panel.

Question: What has been the impact of the suite of reports from BES? Have they helped BES?
Answer: Dr. Kung said that the reports helped BES prioritize investments in critical areas. They also facilitate connections between core disciplines to applications so that when new funding opportunities arise, science leadership is ready to present something visionary, compelling, and a good use of taxpayer money.

Question: For divisions that do not have a director, what is the plan?
Answer: Dr. Kung said that an individual would be the "acting" leader of the division until someone could be hired. She expects to conduct a nationwide search for a new director.

Question: At the NSLS at Brookhaven National Laboratory, about 2,000 users would need a home to go to in short order. How are you planning for that?
Answer: Dr. Kung responded that Brookhaven lab was involved in discussions on the transition from NSLS I to NSLS II. Resources and capabilities continue to be major concerns. The budget uncertainty further compounds the issue. It is important to plan for the trnasition, as there will likely be research disruptions.

Question: Are the EFRCs and Hubs users of BES user facilities?
Answer: Of the 46 EFRC grant recipients, 20 of them propose to use the SC-supported user facilities. However, so far we only have anecdotal evidence to answer the above question.

A break was called at 11:10, and the meeting resumed at 11:35.

BESAC Chairman John Hemminger announced that the DOE Office of Science (SC) had given the BESAC a new charge: provide initial direction on mesoscale science – the size regime of hundreds of nanometers. In a letter dated February 14, 2011[8], SC asked BESAC to:

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[7] See: http://science.energy.gov/bes/besac/meetings/#0927
[8] See: 2011 Charge to BESAC: http://science.energy.gov/bes/besac/reports/

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

He added that SC has also asked the BESAC how to respond to the America COMPETES Act with respect to disseminating the results of its federally funded research.[9]

A central theme of BES reports is the importance of an understanding at the atomic and molecular scale of how nature works and how this relates to advancing the frontiers of science and innovation. BESAC should extend this work by addressing the research agenda for mesoscale science: the study of particles in the size range of hundreds of nanometers, where classical, microscale science and nanoscale science meet. The study, structured around the above two themes, could encourage a national discussion of mesoscale science to the level comparable during the initial formulation of the National Nanotechnology Initiative a decade ago.

Many of the properties of materials that are important for macro function occur at the next scale above nano, which is mesoscale. In the late 1990s, following national discussion on nanoscale science, the BES created and supported federally funded nanoscience research facilities. The result has been dramatic in terms of acceptance of nanoscience as a fundamental science topic worldwide, with the United States taking on a leadership role. The number of research publications in nanoscience escalated from 1,500 in 2001 to more than 7,000 in 2010. The number of nanoscience-related patents grew from less than 25 between 1985-1989 to more than 1,800 in the U.S. alone in 2005. Japan ranks second, followed by Germany, in number of nanoscience-related patents.

The leading idea behind the "Meso Charge" is how to get materials from a computer's design or prediction into one's hand – or into real life. Dr. Hemminger queried the BESAC for initial thoughts and discussion.

Comment: We should begin by defining "meso scale." What phenomena and applications involve mesoscale?

Comment: The name itself might not captivate the imagination like nano did. Researchers have already begun thinking in terms of the mesoscale. Anything larger than a molecule is meso.

Comment: We should use what we've learned from the nanoscience effort.

Comment: Perhaps "Materials by Design" is better terminology. With meso scale, scientists can understand how to design materials. Meso is about considering structural properties at various scales. Properties of interest deal with structural and physical properties at scales much greater than at the nanometer scale.

[9] See COMPETES Charge to all SC advisory committees: http://science.energy.gov/bes/besac/reports/

Comment: We should provide some good examples. The line between micro, meso and macro scale is blurry. Meso materials are much more complex than materials at the nano scale. And, making the link between meso and energy applications would be important.

Comment: The justification for nano science was that one could see dramatic changes in physical and chemical properties, even with small structural changes at the nano scale. Can one make such a concise case for the potential benefits of mesoscale science? If you consider an example, such as for the photosynthetic apparatus discussed earlier, there are molecular and nanoscale phenomena that are integrated. In the language of chemical engineering, reactor design is the integration of phenomena occurring at the molecular level. Perhaps this would help define mesoscale.

Comment: With nanoscience, scanning electron microscope images brought the field to life. With meso scale, we are trying to think about the way we understand materials and molecules.

Chairman John Hemminger announced the commencement of the lunch break at 12:12.

Thursday, March 17, 2011
Afternoon Session

The meeting reconvened at 1:38. Rachel Smith of ORISE made a few brief logistical announcements.

Jim Roberto[10] of the Oak Ridge National Laboratory discussed a recent report, "Computational Materials Science and Chemistry,"[11] that resulted from the July 2010 workshop jointly supported by DOE's Office of Advanced Scientific Computing Research (ASCR) and Basic Energy Sciences (BES).

The goal of the report's authors was to be informative, accessible to lay readers, and national in context. Advances in materials and chemistry have enabled technological revolutions that have shaped the course of history. Materials lend their names to ages: e.g., the stone age, bronze age, silicon age. Energy technologies are currently limited by the availability of advanced materials and chemical processes. None of these technologies is close to meeting its potential. Scientists still need to make progress to improve solar cells, electric cars, and rechargeable batteries. Transformational advances in materials and chemistry are needed to resolve scientific and industrial challenges. But both are fundamental to our industrial competitiveness.

As we move toward these advances, materials and chemistries become increasingly complex. Achieving performance gains requires exploiting many degrees of freedom in

[10] Dr. Roberto's full presentation is available at: http://science.energy.gov/bes/besac/meetings/#0927
[11] See the full report at: http://science.energy.gov/~/media/bes/pdf/reports/files/cmsc_rpt.pdf

composition and structure. An industry example: the parameter space for advanced steels has increased a million-fold compared to early steels. There are billions of chemical combinations and structures for new catalysts. New superconductors and high-field magnets are much more complex than their predecessors. Intuitive, “trial and error” discovery is impractical.

Dr. Roberto explained that to move forward in the area of computational materials sciences, we must transform the discovery process. Over the past two decades, the U.S. has developed and deployed the world’s most powerful collection of tools for the synthesis, processing, characterization, and simulation and modeling of materials and chemical systems at the nanoscale. Examples include:

- World-leading x-ray and neutron sources;
- Nanoscale science centers; and
- High-performance computers.

For the first time in history, we are able to synthesize, characterize, and model materials and chemical behavior at the length scale at which this behavior is controlled. The scale and quality of U.S. scientific infrastructure currently convey a significant competitive advantage. This can pave the way toward exciting new discoveries at the nanoscale. The key will be harnessing the predictive power that one can achieve through simulation-based engineering and science (SBES). Over the past decade, computing power has increased by a factor of 1,000, with the U.S. owning many of the top machines in the world. In the same period, software advances have added another factor of 1,000 for many applications. This million-fold increase in effective capability provides access to length scales, time scales, and numbers of particles that transform our ability to understand and design new materials and chemistries with predictive power. There are profound implications for the pace of discovery and the creation of new technologies and impacts the innovation cycle, from discovery to product development. Companies such as Boeing, Cummins, Goodyear, Ford, and GE/P&W were mentioned as businesses that have attained competitive advantages as a result of SBES.

A Workshop on Computational Science and Chemistry for Innovation was held in Bethesda, MD, from July 26-28, 2010. The premises were:

- Advances in computing and computational science offer the potential for predictive capability in many areas of science and engineering;
- Experimentally validated simulations will accelerate discovery and innovation;
- This provides a competitive advantage for both science and technology.

The approach taken was to assemble experts in materials, chemistry, and computational science to assess the potential of experimentally validated simulations to accelerate discovery and innovation. Discussions would build on ideas of existing reports: Basic Research Needs (BRNs) reports, Grand Scientific Challenges, Exascale, and Federal Technology Advisory Committee (FTAC) reports. The team would assess the potential of experimentally validated simulations to accelerate discovery and innovation. A report would then be prepared describing the challenges and opportunities as well as focusing on potential impacts in scientific fields related to energy technologies. There were 160 invited participants and observers representing 69 organizations. Of those, 41 were universities; 21 were DOE national laboratories; 4 were industry; and 3 were federal agency representatives.

Dr. Roberto further described discussions that occurred at the plenary session. Topics covered included the basic energy sciences (BES) context; the computational sciences context; the industrial context; computational design of materials; and how to accelerate the innovation cycle.

Seven foundational topics framed the subsequent breakout session. These included materials for extreme conditions; chemical reactions; thin films, surfaces and interfaces; self-assembly and soft matter; strongly correlated electron systems; electron dynamics, excited states, and light-harvesting materials and processes; and separations and fluidic processes.

Key questions addressed in the breakout sessions included the following:

- What is the state of the art in each subfield of materials and chemistry?
- What are the most significant research opportunities/barriers in science and technology, particularly related to energy?
- How can experimentally validated computational models and simulations accelerate discovery and innovation in these areas?
- What computational and experimental challenges must be overcome to enable this acceleration?

Workshop participants concluded that we are at the threshold of a new era where predictive modeling will transform our ability to design new materials and chemical processes. The time is ripe to pursue research in materials and chemistry by design, as experimental and computational facilities are in place and capable.

On average, it takes two decades for an idea to progress from the initial discovery to commercialization. Innovative products such as Teflon, Velcro, titanium, polycarbonate, and lithium-ion batteries have all followed such a timeframe. The Materials Genome Project at Massachusetts Institute of Technology is accelerating the design of new materials. Many materials properties can be predicted from first principles. With computational advances we should be able to compute these properties for all inorganic compounds (approximately 100,000). This will allow us to discover new structures and chemical classes and to synthesize and characterize the most promising materials. Early results of the Materials Genome Project included the discovery of 200 new ternary compounds. All were discovered hundreds of times faster than with conventional approaches. The phrase “software equals infrastructure” means that we now possess the software infrastructure that allows us to study more complex systems.

Attendees of the workshop discussed the foundational challenges that currently exist in predictive materials science and chemistry – topics later translated into the report. These include the following:

- Predicting and optimizing structure

- Understanding and controlling self-assembly
- Light harvesting
- Controlling chemical reactions
- Separations and carbon capture
- Designer thin films and interfaces
- Predicting and controlling electronic structure

The overall conclusion made at the workshop was that we will create an innovation ecosystem. The goal will be to accelerate discovery and innovation through predictive materials science and chemistry. To get there, we will need to develop computational approaches that span vast differences in time and length scales. Systems need to be in place to validate and quantify uncertainty in simulation and modeling. We must retain a robust computational infrastructure that includes software and applications. Finally, SBES technologies must be efficiently transferred and incorporated into industry. Seizing the opportunity requires integrating SBES across the discovery, development, and technology deployment enterprises.

Dr. Roberto concluded his remarks and invited the group to ask questions.

Question: What are other agencies doing to contribute to this initiative?
Answer: This is indeed a cross-agency initiative. OSTP plays a coordinating role. Four years ago, NSF, DOE, NIH, NIST, and DoD program managers initiated an international comparative study and workshop similar to the nano initiative. OSTP set up a fast track committee to integrate the reports. NSF has already established multiple working groups to outline what a national initiative would look like. It appears that NSF and DOE will be the major players.

Comment: Computational power is now a key factor in experimental design. More than 200 compounds have been discovered using SBES. While SBES will certainly not replace experimentation, it will increase efficiency, guiding researchers into fruitful directions. The workshop did not discuss the specific link between computational abilities and synthesis of new materials, but perhaps SC should help guide the direction of synthesis.

Question: It is challenging to determine how to allocate funding resources between prediction/modeling and synthesis. Some compounds are created under conditions in which they are not thermodynamically stable. The kinetics of those things really matter. Are we able to address the time factor?
Answer: We can actually calculate the rates to determine how fast a compound can be synthesized. It is like using a really big hammer to get at a really complex problem.

Next, **Chairman Hemminger** announced that **Chi-Chang Kao**[12] of the Stanford Synchrotron Radiation Lightsource would discuss the issue of scientific facility user access policies, specifically at synchrotron and neutron facilities.

[12] Dr. Kao's full presentation is available at: http://science.energy.gov/bes/besac/meetings/#0927

Dr. Kao began by saying that a facility user access policy defines the ways in which scientific user community can access the facility. Such a policy should contain elements to ensure open and fair access to the facility as well as promote the safe and efficient use of the facility. The goal is to maximize the scientific productivity and societal impact.

A well-written facility access policy should encompass various modes of user access:

- general users,
- partner users,
- proprietary users, and
- discretionary users.

It should include:

- proposal review and beam time allocation processes,
- advisory bodies,
- define the roles and responsibilities of users, and
- include policies on beam time specifically for facility staff as well as reporting requirements.

In the early 1980s, Participating Research Teams (PRTs) were created at the National Synchrotron Light Source (NSLS). These teams brought external funds to build, maintain, and operate facility beam lines. They managed up to 75 percent of the beam time for their scientific program and supported the remaining 25 percent of beam time for use by general users. Such teams were typically given three year renewable terms and approved by a Scientific Advisory Committee. In the mid-1990s, Collaborative Access Teams (CATs) were created at the Advanced Photon Source (APS) with terms similar to PRTs at the NSLS.

There exist several issues regarding the above arrangement. It is becoming clear that having the majority of beam time in the facility controlled by PRTs and CATs is not a sustainable model for the facility, as the user community has expanded quickly over the last two decades. The complexity and scale of new beam lines make it increasingly difficult for small research groups to build and maintain them. The PRT and CAT approach does not allow facilities to take advantage of economies of scale and is difficult to enforce standards (hardware, software, etc.) across facilities.

In the early 2000s, Approved Programs (APs) with a “partner user” were introduced at the Advanced Light Source (ALS) to transition PRTs to facility beam lines. With this arrangement, an investigator or a group of investigators received an assured percentage of beam time for a period of a few years to carry out an extended research program. It was then expected that investigators would bring in resources that enhance the capability of the facility. In contrast to PRTs and CATs, the AP model created a partnership with the facility by providing instrumentation, staffing or scientific expertise. Each AP is peer reviewed and has a limited life time. Similar partner use programs were adopted at the APS and NSLS synchrotron facilities.

In the mid-2000s, the Spallation Neutron Source (SNS) adopted a fully facility-owned and operated model. There were no PRTs and CATs. Up to 20 percent of the beam time is allowed for partner users. APS and NSLS also adopted this model and moved to convert PRTs and CATs to facility-operated beam lines. The Stanford Synchrotron Radiation Lightsource (SSRL) has always operated in this model.

Today, the facility owned and operated model has been adopted by all facilities. The transition from PRTs and CATs to facility beam lines at NSLS and APS continues. It is resource-limited. PRTs and CATs still exist under special circumstances, in particular beam lines funded by NIH and NSF. Partner user programs have been integrated successfully and the user community can be engaged without the problems of raising large quantities of money for funding an entire beam line and/or sector.

Dr. Kao concluded his presentation by noting that there are several issues to consider in developing a scientific facility user access policy for synchrotron and neutron facilities. Policies should contain uniformity, leaning toward BES guidelines but containing enough flexibility to allow for some facility discretion. Policy drafters should also consider what incentives best attract partner users and investments. Also, how would a user agreement for industry users be structured, i.e., how would intellectual property and review processes be arranged? DOE mission needs are another key consideration. Finally, now that many or most users are "remote users," how will they be counted? User access policies should be drafted looking outward, rather than inward.

Chairman Hemminger invited the BESAC to ask questions following the presentation.

Question: Regarding the counting of users at a facility, do you count the users who show up on site, at the facility, or all the names on a proposal, and what about remote users? Answer: DOE counts a user only if the user comes to the facility. For remote users, one user per project is counted. Mail-in users are not counted. And no matter how many times a user visits the facility, he or she is counted only once per year.

Comment: User facilities are especially important to industry, as the fruits of those labors translate directly into jobs. An example is a battery manufacturing plant being built in New York State. The underpinning technological input came from a DOE user facility. Management at the user facilities should consider what capabilities are most useful for industry and try to make those accessible to industry.

Comment: It is also important to have competent technical support people at facilities to help maintain the beam lines. The SciTech report said that industry demand for user facilities had increased. The counter point was made that for the NSLS-II there was no incentive for corporate investment. Not one proposal was submitted that was industry-based. The message needs to come from the top, from DOE – that we want to encourage partnership between academia and industry; then put support staff there to make it work.

Comment: Support staffs are very important and perhaps shouldn't be called 'support staff' because their role is essential. Modern synchrotrons are becoming incredibly complicated. Operating them requires detailed and deep knowledge.

Comment: Policy development should be peer reviewed. There was broad concurrence on this point.

Question: Will formal input be requested from BESAC?
Answer: Chairman Hemminger said that he would leave to BES management the question of more formal input from BESAC.

A break was called at 3:14 PM.

The meeting was reconvened at 3:48 PM. The concept of open access to federally funded research data was raised. (See BESAC Charge Letter[13]). There will be increased interagency discussions on how this will be addressed by the federal government. The BES community needs to discuss current practices and ideas for making research data more accessible in the future. In the BES research community, this is handled in a variety of ways. The physics community has an archive structure where information is put on the internet. The chemistry community appears to have no such strategy.

Question: What constitutes "archival data"?
Answer: We should say what we think it is and what we plan to do rather than let someone tell us.

Comment: Some user facilities operate is if the facility owns the data rather than the user. One situation to avoid is where the facility is protective about the data and/or may also give user data away without user permission. Pre-publication data should not be shared because it poses too great a risk to the career progression of postdoctoral fellows and graduate students.

Question: What is the origin of this push toward more sharing of data and transparency?
Answer: The pharmaceutical industry thinks that detailed, primary data is tremendously valuable. Also, Congress feels that research funded with taxpayer dollars belongs to the public and should not be hidden. DOE would be well-served to develop a proactive stance on this issue rather than a defensive position.

Comment: Federally funded research data should indeed belong to the public, especially for anyone wanting to confirm an experimental result. Also important is the issue of how data is disseminated. Should the public have to pay twice when scientific journals levy burdensome subscription fees? Whatever is adopted as a policy needs to be consistent so that publishers can sustain the cost of maintaining archival quality information. Pay structures can be built into research grant proposals, but for people in the developing

[13] See COMPETES Charge to all SC advisory committees: http://science.energy.gov/bes/besac/reports/

world, addressing such costs becomes more complex. NIH has a publication policy for grants it funds. The DOE should look into its own policies in greater detail

There was additional discussion among BESAC members from various technical backgrounds. Individuals spoke of personal experiences in the chemistry, physics, and biology communities on publication policies and data transparency. NIH has fairly strict rules about the imperative of sharing data that is funded through NIH. In the chemistry field, American Chemical Society members can request crystal structure data by checking a form and receive data a year later. Another individual had served as a journal editor for a year and did not receive one data request. Most committee members concurred that a systematic policy should be put in place. Some BESAC investigators had received requests for original lab data; others had not. There was discussion on what volume of original data should be kept. Original data, archived properly, can prevent scientific misconduct such as falsifying research results. In corporate America, there are often extremely strict retention time policies for data ranging from email to papers.

Comments: It is important to enumerate the actual costs for archiving and properly saving research data. Also, the value of the time required to archive data should be evaluated. From an industry perspective, six months may be long enough. For those in academia, that time frame may be much, much longer. Another consideration is that primary, or technical data might be in a different class from published data.

As DOE requested a response on ideas regarding data transparency by July 1, 2011, John Hemminger stated that his initial idea was for the BESAC to form a subcommittee to produce recommendations on the subject. He asked for volunteers to assist in devising a response on behalf of the BESAC. Someone suggested that both academic and industry voices should speak within such a working group. Another added that representatives of the DOE-supported national laboratories should also contribute. Regarding intellectual property, someone said BESAC should consider that issue within the context of published or unpublished data. There may be a special set of rules in cases involving intellectual property. Another person added that journal editors' voices should also contribute to such an advisory panel.

Chairman Hemminger, noting that the meeting had only a few minutes' discussion time remaining for the day, asked the group to consider what "mesoscale" really means. Is it the study of things ranging in length from 10 to 1,000 nanometers? Is it the idea that a molecule's structure at this scale truly controls its physical properties? He charged the group to think about terminology that may better describe the concept of meso scale. He then invited the audience to comment.

Comment: Dr. Greg Exarhos from the Pacific Northwest National Laboratory suggested that H. Frederick Dylla, Executive Director and CEO of the American Institute of Physics (AIP) be invited to share the publishing industry perspective. He added that the emphasis of materials by design is an important issue: a great deal of the patent literature contains those references. Processing by design is another concept to consider. Can we design different processing routes or give insight to what parameters are important in processing to achieve those structures?

Comment: Dr. Robert Moore, from SLAC, said it would be important to consider where large volumes of raw data and information would be stored. For example, the LCLS instrument alone produces terabytes worth of data in a day or two.

Discussion was concluded for the day at approximately 4:56 p.m.

Friday, March 18, 2011
Morning Session

The meeting was called back into session at 9:02 a.m. **Wayne Eckerle**[14] of Cummins, Inc. was asked to provide an update on the Workshop on Predictive Simulation of Internal Combustion Engine (PreSICE).

Our nation's energy security is tied to transportation. Two-thirds of America's crude oil is imported from other countries. Two-thirds of that oil is used for transportation. Improving the technology of the internal combustion engine is a significant opportunity. Enhanced engine efficiency can lead to reduced fuel use. Currently, an internal combustion engine's thermodynamic limit is 60 percent. The average current gasoline engine efficiency is 30 percent. Improvements to greater than 45 percent are achievable, as are fuel economy improvements to more than 50 percent. Therefore, there is potential for a 50 percent reduction of fuel use from cars. That reduction has the potential to save four million barrels of oil per day.

Computational, predictive modeling will help to accelerate the achievement of greater levels of fuel efficiency. It is the key to rapid combustion optimization in a non-linear parameter space. Cummins has been an early industry leader in science-based engine design, developing a new diesel engine with computer modeling. Reducing the time and cost to design diesel engines while boosting fuel efficiency and lowering emissions is a major accomplishment in the automotive industry.

Cummins achieved this goal with its ISB 6.7 liter diesel engine, manufactured since 2007 at the company's Columbus Midrange Engine Plant in Indiana for the Dodge Ram pickup truck. In addition to a more robust and efficient diesel engine, relying solely on computer design reduced development time and cost by an estimated 10 to 15 percent and avoided the need for prototype testing. More than 200,000 Ram Heavy Duty pickups with the ISB diesel have been sold. Cummins' early adoption of science-based engine design has made the company more competitive while helping the environment. It has blazed a trail that other engine makers are now keenly following.

The success of the computer design approach was possible because of a solid foundation of fundamental research on combustion chemistry, including laser diagnostics to

[14] Wayne Eckerle's full presentation is available at: http://science.energy.gov/bes/besac/meetings/#0927

accurately measure reaction details. Complete modeling of diesel fuel combustion demands an accurate description of nearly 10,000 distinct chemical reactions involving 1,000 different compounds, all taking place in a swirling flow of fuel spray and hot gases. Not only must this be studied at the scale of molecules, where chemistry occurs in nanoseconds, but also at the scale of engine pistons and cylinder cycle times measured in seconds. And turbulence can exert a profound influence upon the combustion outcome.

This basic research underpins the ongoing development of numerical simulation tools to model, and advanced laser diagnostics to measure, turbulent flames in real, in-cylinder engine combustion. While the computational simulation Cummins used for the ISB engine is fairly crude by current standards, its early success points the way to more sophisticated, science-based engine design in the future.

Cummins' success traces to technology transfer from the SC Office of Basic Energy Sciences and the Energy Efficiency and Renewable Energy (EERE) Vehicle Technologies program. These offices sponsored basic and applied R&D at Sandia National Laboratory's Combustion Research Facility including partnerships with other national laboratories and multiple U.S. universities.

The PreSICE workshop represented the culmination of a year of DOE-fostered community engagement. Discussions were facilitated at Sandia National Laboratories, the University of Michigan, and in the Chicago area. They involved more than 28 different entities, including representatives from DOE-supported national labs, academia, federal agencies, and industry.

Workshop participants identified industry barriers to the development of advanced engines. They concluded that all could be mitigated or overcome through science-based modeling. Of five barriers identified, those of highest priority included:

1. The effect of stochastic nature of in-cylinder flow on engine combustion, performance and emissions; and
2. Spray modeling and experimentation in dense spray and nozzle internal flow regions, including physics like cavitation and flash boiling

The PreSICE workshop was charged to answer four questions:

- Why is investment in pre-competitive R&D for predictive engine simulation needed?
- Why is now the opportune time to develop predictive simulation tools for advanced engine design?
- What are the critical needs in basic and applied R&D in chemistry, physics, and engineering required for the successful realization of predictive combustion simulation for engines?
- What is the potential impact on the U.S. automotive and engine industries if new simulation tools are developed?

Held March 3, 2011, in Arlington, Virginia, the PreSICE Workshop was co-chaired by Wayne Eckerle of Cummins and by Chris Rutland of University of Wisconsin. There were two breakout groups. Chairing the “Sprays” group were Caroline Genzale of Georgia Tech and Joe Oefelein of Sandia National Lab. The “Stochastic In-Cylinder Processes” breakout group was co-chaired by Dan Haworth of Penn State University and by Volker Sick of the University of Michigan. The workshop was invitation-only and included 63 participants, including significant representation from industry. The first day was structured for discussion and information gathering, while the second day was utilized for information compilation and initial report drafting. The goal was to complete the 20-page report by March 31.

Attendees surmised that a “hierarchy” of software tools is needed, including those for direct numerical simulation (DNS); high-fidelity large eddy simulation (LES); engineering LES; and Reynolds-averaged Navier Stokes (RANS) approaches. Critical research going forward will include the development and validation of models to enable simulation of stochastic or random processes. Examples include sub-grid scale models for unresolved processes; reduced chemical kinetic mechanisms; and new theoretical frameworks and efficient numerical approaches. The fundamental goal is to improve model accuracy and to minimize uncertainty. In the area of spray dynamics, one critical research direction will be modeling the more detailed treatment of fuel delivery systems such as fuel rail and internal injector flows. Better modeling will enable optimization of fuel-preparation strategies, such as in-cylinder injection, mixing and combustion.

Pertaining to engine development, Dr. Eckerle said that once fuel gets to the combustion chamber there are processes and models that need to be improved at that stage. Modeling and simulation can help us better understand what occurs near the wall of the engine block. In-cylinder fluid-wall interactions and heat transfer are ripe areas for improved simulation capability, as fuel impingement on engine cylinders degrades engine performance, emissions and durability. Surface temperature variations create similar problems.

PreSICE workshop participants also identified cross cutting research needs. These include the chemistry of complex systems, i.e., methods to obtain chemical force fields, rate representations, and automatic mechanism generation. Efficient, on-the-fly kinetic mechanism reduction as a function of local conditions will be needed to enable cost-effective simulation of combustion. Another cross-cutting research need will be in uncertainty quantification.

Participants identified two major research areas going forward:

- model development, and
- tool infrastructure development.

In the area of model development, validation, and reduction, benchmark experiments will need to be supported as a source for validation of the data. A companion high-fidelity LES will be needed for detailed model development and reduction. LES and RANS would need to be engineered for engine cycle optimization and analysis, for faster solution times. Finally, DNS will be needed for the analysis of small-scale turbulence-chemistry interactions.

In the area of tool infrastructure development, software tools will be needed for advanced grid generation and grid quality assessments. Core solver development will be needed using science-based LES and engineering-based LES and RANS, followed by software tools for advanced model reduction and uncertainty quantification. Software tools will also be needed for post-processing, visualization, and data management for both science and engineering.

One key impact resulting from the development of new simulation tools would be that the design, testing, and calibration portions of the product development cycle can all be shortened. Subsequently, industry can then expand the design space to encompass a broad range of design concepts. Participants were hopeful that a further impact would be to reach the theoretical 60 percent limit on thermodynamic efficiency, thereby potentially saving the U.S. four million barrels of petroleum per day. A program based on PreSICE will enhance the competitiveness of and develop the future workforce for U.S. industry, improve U.S. energy security, and promote global environmental security.

Dr. Eckerle invited comments and questions from the BESAC.

Comment: Europe is ahead of the U.S. in diesel use. However, we are ahead of Europe in terms of analytic capability. Heavy duty engines here are more efficient than those in Europe. Also, Europe’s use of analytic techniques varies quite a bit.

Question: What is meant by “reduce chemical mechanism,” and can you comment on modeling capabilities for heat transfer? What is being modeled?
Answer: If one were to try and measure the chemical properties of a fuel, and then put that into computer code, it would take forever to do the calculations. We have to get that down to a size our numerics that we can handle. Today, we calculate flow coming into intake valves; then compression; compression stroke; expansion; and expansion stroke. There exists spatial heat transfer to the walls as well as heat distribution patterns. Within an engine, boundary conditions aren’t fixed. Currently, we are not able to make all of the calculations needed to design a more efficient engine.

Question: How are other companies competing in this field?
Answer: There are more and more examples of industry success stories. More companies are doing analysis for designs going into production. The key is the integration of the computational experts who run the codes with staff in product development. At Cummins, that is very well integrated. This is the key to its success.

Comment: Yesterday, the BESAC heard about increasing efficiency in trucks just by putting boxes underneath to improve aerodynamics. [Laughter]

Comment: That innovation won an award. Our target is to achieve 50 percent greater efficiency (10 miles per gallon) than we have today. Half of that can be attributed to better engine design, and half will be due to the improved design of other parts of the truck.

Question: What are the barriers to progress in large eddy simulation? Intellectual? Numerical?
Answer: It is both. A key challenge is how to model subscale processes. How can one design the computational modeling numerics to integrate all of these subscale processes and get reasonable computational output times? For a 360-degree, three dimensional simulation calculation, one cycle will take two to three days. LES calculations now take many days. For industry, that time frame is not realistic. Combustion chambers are designed sometimes within two to three weeks. Industry wants computational simulation to enable engineers to model and choose from thousands of different engine designs

Question: Is industry focused mainly on trucks or cars for this kind of innovation?
Answer: Both. Everything. When engines are inefficient, that is money lost. Remember the two-thirds of oil we as a nation import; we need to connect that support of this kind of research leads to greater energy security. However, the trucks are burning so much fuel.

Next, **Eric Rohlfing**[15], Director of the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division, described the planned Committee of Visitors (COV) review of the CSGB division.

A history of COVs in BES was presented. The first COV in SC was the review of the chemical sciences portion of the CSGB division in 2002. This will be the fourth review for CSGB and the tenth COV review in BES. Previous COV reports can be found on the BES web site in the archives section. COVs are now a standard practice. Their recommendations are taken seriously and have resulted in substantive changes. For example, as a result of this most recent set of COV recommendations, development of the Portfolio Analysis and Management System (PAMS), was begun.

Two standard COV charges are:

1. For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
    - (a) Solicit, review, recommend, and document proposal actions and
    - (b) Monitor active projects and programs.
2. Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
    - (a) The breadth and depth of portfolio elements, and
    - (b) The national and international standing of the portfolio elements.

In addition to the above elements, COVs are asked to provide input for the evaluation of Basic Energy Sciences progress toward the Government Performance and Results Act (GPRA) long-term goals. The COV rates each element of the division as excellent, good, fair, poor, or not applicable. GPRA long-terms goals for BES are:

1. Demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures,

[15] Dr. Rohlfing's full presentation is available at: http://science.energy.gov/bes/besac/meetings/#0927

including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.
2. Demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.
3. Develop new concepts and improve existing methods for major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.
4. Demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

In its review, the COV planned to cover core research programs, including base program awards to universities and DOE labs. It also would cover single-investigator and small-group research (SISGR) programs for FY 2009; and it would cover renewals of awards made in earlier BES solicitations: the Hydrogen Fuel Initiative, Solar Energy Utilization, Nanoscale Science, and Chemical Imaging. The review would not cover Energy Frontier Research Centers, SC Early Career Awards, the SC Graduate Fellowship Program, the BES Equipment Supplement Program, or the Fuels from Sunlight Energy Innovation Hub.

Chairing the panel would be Bruce Gates of U.C. Davis. The meeting was planned to span April 5-8, 2011, at DOE Germantown, Maryland. Thirty-nine COV panelists organized into seven panels would review the core programs within the division. Panelists represented academia, the DOE laboratories, industry, and other federal agencies. About half of the panel had received BES funding; half did not. There would be 21 males and 18 females in attendance.

Dr. Rohlfing then displayed an organization chart of CSGB, showing where the seven COV panel assignments fit. Dr. Rohlfing shared the anticipated COV agenda. Highlights will include an update on the management of the PAM system as well as CSGB review procedures. He concluded by saying that the COV was well-prepared and that he hoped for a good meeting.

Question: When will the COV report be finished?
Answer: The report will be completed and presented to the BESAC for approval at its summer 2011 meeting.

Comment: BES staff have insufficient computing and information management system capabilities.
Response: They are using the same systems from 2008. The Department is committed to implementing the PAM system. Iit takes time to ensure the program offices are confident with the system and that it interfaces correctly. It is not an easy thing to do.

Comment: There are concerns that the travel budget may be insufficient for all members to attend the meetings.

Response: The budget situation is improved. Staff are able to travel to a couple of meetings per year. On-site reviews and contractor meetings are costly but important. In FY11, travel funding will be at increased risk.

Chairman Hemminger said that the BESAC was working to prepare an updated report on the impact of BES research and that Linda Horton would discuss progress on that effort.

Dr. Linda Horton[16] relayed progress made on an updated report on the impact of BES research. She said that in 1995, BES had assessed the value of basic research. A BESAC subpanel chaired by economist John H. Moore of George Mason assessed "how the nation has received a return on the taxpayer's investment in the Basic Energy Sciences program." The subpanel visited the DOE-funded national laboratories to learn about technology and the impact of research. Team members included economists, industry professionals, academics, and scientists working at national labs. The team also collected over 800 paragraph-size highlights summarizing the impact of research from across all program and research performers. The outcome was a BES report on basic energy sciences with the tagline, "Serving the Present, Shaping the Future."

Dr. Horton showed a picture of the cover of the 1996 BES report on the impact of BES research. That report highlighted interactions involving BES researchers and industry ranging from informal arrangements among scientists to formal agreements between or among institutions. Its introduction describes BES, its stewardship responsibilities and research highlights. It also contained a section on user facilities. The report covered a broad range of topics, including technology areas such as energy efficiency, energy resources, ceramics, environmental technology, transportation, and manufacturing.

The plan is to update the document for 2011 with the tagline, "Science Serving the Nation." Serving as the foundation will be recent "success stories" from the national labs. Another key update will include information from the BESAC workshop: "Science for Energy Technology: Strengthening the Link between Basic Research and Industry[17]," as well as the set of Basic Research Needs (BRNs) reports[18].

So far, success stories covering the following technology impact topics have been collected or sought:

- Solar Energy
- Alternate Fuels
- Energy Efficiency
- Geosciences
- Extreme Environments
- Energy Storage
- Superconductivity

[16] Dr. Horton's full presentation is available at: http://science.energy.gov/bes/besac/meetings/#0927
[17] See report at: http://science.energy.gov/~/media/bes/pdf/reports/files/setf_rpt.pdf
[18] See: http://science.energy.gov/bes/news-and-resources/reports/basic-research-needs/

- Electronics
- Transportation
- Combustion
- Catalysis
- Chemical Processing
- Biotechnology
- Medical Technology
- Measurement and Analysis

Dr. Horton concluded her remarks and invited volunteers to become involved.

Comment: We just collected stories from all 39 user facilities from SC.
Response: The information already gathered will accelerate the production of the report. The timeline will be approximately six months.

Chairman Hemminger moved to the final discussion topic: to revisit the BESAC charge from Dr. Bill Brinkman regarding mesoscale science[19]. He asked the committee for their ideas on how to respond and move forward.

The 2007 Grand Challenge report has been impactful in Washington. Since then, however, terminology has changed. We should not feel constrained by the terminology of "meso." We can change it if we want. Hemminger said that the BESAC should consider terminology that captures the concepts best.

Question: A Google search of the word, "mesoscale" shows that the meaning of "meso" depends on the scientific research field. Meso indicates distances between 2 km and 1,000 km in the field of astronomy. In materials science, meso means distances between 100 nm and 1,000 nm. Why not just say, "between nano and microscale?"

Answer: Instead of a length scale, why not consider meso in terms of functional materials or functionality. We now have much detailed, interesting science at the nanoscale. Looking in the other direction, for macroscopic materials, scientists will ask from where their function comes. We discussed examples yesterday where the functionality comes from structure at this intermediate scale.

Comment: Size and also time are dimensions to consider. Google Earth allows one to fly all over the planet and also in time. So, there is a smart way that information is partitioned and then integrated holistically. Barriers are dimensional in nature and apply both to time and space.

Comment: A few possible terms are: connections interactions, integration, or perhaps "beyond the nanoscale." Computational science now has the capability to bring considerations in all of these scales together.

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[19] See: 2011 Charge to BESAC: http://science.energy.gov/bes/besac/reports/

Comment: The committee should consider what would be new with this type of scale. Examples could be the properties of a particle; decreasing melting temperature as a function of decreasing particle size; super-molecular materials; or superheating. For mesoscale, the idea is less about the size itself and more about new properties conferred by integrating nano materials into a new environment. Mesoscale is the study of meta-materials.

Question: Would research focus on a system of one material that is mesoscale in size or a collection of materials at the mesoscale level? The scale can include many components. That area should be clarified.

Answer: **Chairman Hemminger** concurred, adding that operationally, the BESAC would set up a subcommittee comprised of BESAC members plus people off the committee as discussions progress. Similar to a Grand Challenges report, there will be multiple discussions in the future. The intent is for the BESAC to provide initial direction.

Comment: The tools one uses to measure properties at the mesoscale are a key consideration. Electron microscopy allows scientists to zoom down to the nanometer. Perhaps we should take a step back and look at micron scale. It is studied by tools that readily obtain the information. The mesoscale contains subjects that would be fascinating to measure, but we don't have ability to zoom at these different length scales.

Comment: It is good to state the technical limitations that currently exist. Take an example of dissimilar materials, such as viral nano particles like tobacco mosaic virus in plants. These grow from individual proteins to micron scale cylinders without any human intervention.

Comment: Mesoscale is neither smallest nor largest in scale. Why would researchers care about interactions at this scale, and who would be the consumers of that research? Nobody gets excited about "medium." People are excited about origins and emergence; let's call it the emergence of function of materials. We want to carefully consider the anticipated research products and fish for intellectual excitement. We must choose a name that embodies what we're going to produce.

Comment: Think about what would be absent if the mesoscale didn't exist. Mechanical behavior spans from the nanoscale to the macroscale. For biology, there is communication across tissue. Traffic patterns are macroscale. There are even larger scale interactions in climatology. Consider social networking. Mesoscale can be a relative term.

Chairman Hemminger agreed that coupling the term to its use in other communities is an interesting idea.

Comment: Size and function are to be considered together, along with time. For example, biological "machines" can self-assemble into engines on a time scale of femtoseconds, process information, and heal themselves. Specifically, Photosystem 1 keeps replacing a key protein in every 20 minutes because the old one dies. Mesoscale is the study of the biological world from the nanoscale range to our macroscale world. Mesoscale brings science up to the world people can see and understand.

Comment: Mesoscale represents multi scale functionality beyond nano. Beyond nano is an important part of selling this.

Chairman Hemminger stated we should avoid giving the impression that we have finished research on nano.

Comment: We are far from realizing the full potential of nano. We now have researched interactions between nano particles, but we cannot design and construct nano systems based on blocks that we create. Working with that huge set of the right building blocks is what mesoscale represents. "Emergent" as a term is ok but has difficulties. In semiconductor fabrication, "emergent" is current because scientists are making systems from pieces.

Comment: If one thinks back to how nanoscale science was able to expand, one can track conversations back to President Clinton's visit to CalTech, encouraging the audience to imagine volumes of information comparable to the Library of Congress. What outcome statement will capture the imagination for mesoscale? Imagine a material that self-heals. Imagine being able to digitally send information regarding a scent, and a small company could rapidly produce that scent for you.

Chairman Hemminger noted that on the horizon is the research area of multi scale computational modeling. Researchers can explain what materials go with what macroscopic function, but often we don't understand how to make the materials. We can't couple the modeling with how to make the materials; so mesoscale will play a critical role in materials synthesis.

Comment: Mesoscale defines properties that come out of collective behavior that are not easily identified from the nanoscale components. Photosynthesis is a good example of a mesoscale research area.

Comment: In understanding photosynthesis or how a catalyst works, the link is transport phenomena, or the study of how electrons or molecules move from one place to another.

Comment: Mesoscale science could help research take an inexpensive material like silver and fabricate it on a larger scale. He cited one research project involving scintillation properties of materials and detectors. Mesoscale is the bridge that brings science from fundamental calculations to materials useful for macroscopic applications like detectors. The BESAC should identify a token project that helps define work at the mesoscale.

Comment: The committee should clearly define the value of mesoscale science, asking, what would be the exciting outcomes if we did this? The area of electrochemical energy is all about charge transfer. At the nano scale, we know about how charge is stored and transported, but not about how a fuel cell works. Mesoscale helps scientists understand how a nano device is connected to the outside world. It can help researchers design better devices.

Comment: The committee needs to recommend to BES where new opportunities are and how to focus limited resources for mesoscale science. There is no real unifying theme; one can call it "meso" but the meaning is not immediately clear. The BESAC must identify that unifying theme.

Chairman Hemminger said that he would get a group of people together who might like to be involved in developing a more specific directive. He entreated the BESAC to give the idea of mesoscale science more thought. He announced that the date for the summer BESAC meeting had been set for August 2 and 3. He then invited members of the audience to provide additional comments.

Dr. J. Charles Barbour, Director of the Physical, Chemical, and Nano Sciences Center at Sandia National Laboratories, noted that mesoscale science seeks to understand how properties of smaller scale molecules get expressed in an average onto a larger scale. He pointed to the interfacial force microscope at Sandia National Lab as an example of relevance. In his research experience, there is knowledge to be gained by studying an individual unit. When molecules are put together, they behave differently.

Dr. Alex Malozemoff from American Superconductor Corporation said that the SciTech report was exciting. He said he was hopeful regarding prospects for budget increases to address the research proposed in that report. A byline for the report was strengthening the link between basic research and industry. There was underlying novelty in the report. Iit contained a great section on the combustion and modeling interface with industry. Key energy challenges can be addressed by more effective collaborations.

Dr. Duane D. Jonson, Chief Research Officer at Ames Laboratory, commented that if it mesoscale science is so important, why isn't industry paying for it? The BESAC should articulate the potential benefits of mesoscale research that so that others will see that these issues are important.

As no other discussion ensued, John Hemming declared the meeting adjourned at 10:58 AM.

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

(Edited: 6/03/11, MIS)