Minutes for the
Basic Energy Sciences Advisory Committee Meeting
February 16-17, 2006
Marriott North Bethesda Hotel and Conference Center,
North Bethesda, Maryland

BESAC members present:

Nora Berrah
Sylvia Ceyer
Peter Cummings
Frank DiSalvo
Mostafa El-Sayed
Laura Greene
Bruce Gates
John Hemminger, Chairman
Eric Isaacs
Walter Kohn
Gabrielle Long
William McCurdy, Jr.
Daniel Morse (Thursday only)
Martin Moskovits
John Richards
John Spence
Kathleen Taylor

BESAC members absent:

Sue Clarke
George Flynn
Anthony Johnson
Kate Kirby
Ward Plummer
Stanley Williams
Mary Wirth

Also participating:

George Crabtree, Director, Materials Science Division, Argonne National Laboratory
Patricia Dehmer, Associate Director of Science for Basic Energy Sciences, USDOE
Mildred Dresselhaus, Institute Professor of Electrical Engineering and Physics, Massachusetts Institute of Technology
Harriet Kung, Office of Basic Energy Sciences, USDOE
Robert Marianelli, Basic Energy Sciences, USDOE, retired
Frederick M. O'Hara, Jr., BESAC Recording Secretary
Raymond Orbach, Director, Office of Science, USDOE
Eric Rohlfing, Acting Director, Chemical Sciences, Geosciences, and Biosciences Division, Basic Energy Sciences, USDOE
Karen Talamini, Office of Basic Energy Sciences, USDOE

About 80 others were in attendance in the course of the two-day meeting.

Thursday, February 16, 2006

Before the meeting began, each of the attending BESAC members was individually sworn in as a special government employee by a staff member from Human Resources, Office of Science (SC), U.S. Department of Energy (DOE).

Chairman Hemminger called the meeting to order at 10:01 a.m., congratulated the members on becoming special government employees, had the Committee members introduce themselves, and welcomed the new members (Ceyer , DiSalvo, and Spence).

He acknowledged Rick Smalley's passion for science, commitment to getting science right, and development of correct understanding. He called upon Vice Chair Moskovits to introduce the speakers honoring Rick Smalley.

Moskovits said that the Committee members had been saddened and upset by Smalley's untimely death. Smalley made fundamental advances in chemistry and served on this Committee. He called on the first speaker, **Mustafa El-Sayed**, who had known Richard Smalley since he was a graduate student, to speak about Smalley.

Smalley was born in Akron, Ohio, in 1943 and moved to Kansas City at the age of three. He was infected with science by his mother; by an aunt, a chemist who was among the first women professors in the United States; and by the launching of Sputnik. He spent 2 years at a small college and got his B.S. from the University of Michigan in 1965. He became a research chemist at Shell for 4 years. He got married, and his wife's pregnancy saved him from the U.S. Army. He got his master's degree in 1971 and his doctorate in 1973 from Princeton University. He was a postdoctoral fellow at the University of Chicago from 1973 to 1976, and his research proposal was on molecular beams. He mastered supersonic-pulse laser-beam techniques and joined Rice University in 1976 because of its abilities in high-resolution gas-phase molecular spectroscopy.

Smalley connected his laser-ablation nozzle-expansion system to a time-of-flight mass spectrometer, working with small clusters of three to four molecules. He contracted with Exxon to build a similar system for uranium clusters and began vaporizing materials to make and detect cold materials, mostly metal and semiconductor clusters. Rohlfing, Cox, and Kaldor were the first to detect fullerenes by vaporizing carbon in 1984, producing the first C_{60}. Kroto and Curl convinced Smalley to vaporize carbon and produce small carbon clusters. In September 1985, they used an improved system and saw an unusually strong mass peak for C_{60}: fullerene. This peak was highly enhanced by operating the system under high helium pressure.

Smalley, Kroto, and Curl spent 5 years trying to convince the world of the buckyball structure. The independent theoretical prediction of the stability of that structure was provided by Tony Haymet at the University of California at Berkeley. The very unreactive nature of C_{60} with many gases supported an unusual stability. Heath showed that an atom of lanthanum could be enclosed in the buckyball cavity, thus revealing the size of that cavity. In 1990, Huffman and Kratschmer were able to make C_{60} in large quantities. It took five years for the Nobel committee to become convinced of the significance of C_{60}.

From 1980 to 1985, Smalley conducted research on small metal clusters with a nozzle beam. From 1985 to 1992, he researched buckyballs' reactivity and self-assembly and began working on single-walled nanotubes (SWNTs). From 1992 to 1994, he investigated doping buckyballs, producing SWNTs, and using a laser-oven method. In 1996, he received the Nobel Prize and produced buckyballs by the high-pressure carbon monoxide (HiPco) method. From 1997 to 2005, he investigated the synthesis and properties of SWNTs and carbon fibers.

Smalley's research areas included fullerene nanostructures; the synthesis, purification, chemical cutting, and alignment of SWNTs; SWNT single-crystal growth; and SWNT applications to energy technology. From 1992 to 2002, he was the most cited author in nanotechnology.

Some significant contributions of Smalley to nanotechnology were (1) codiscovering a new form of an important element (carbon); (2) discovering the single-walled nanotube, studying its synthesis, chemical properties, and physical properties; (3) developing the HiPco method of SWNT production; (4) founding a company to make SWNTs in high quality and large quantities; and (5) testifying before Congress about the need for a national nanotechnology initiative.

Smalley's company, CNI, has had more than 500 customers, including many commercial firms that are purchasing tiny amounts of nanotubes for testing products ranging from plastics to batteries to water-purification systems to applications in aerospace, defense, and space exploration. One corporate client, Samsung, is using CNI's carbon nanotubes to create a new generation of energy-saving flat-screen televisions. SWNTs have not led to new products but have improved many commercial items (e.g., scratch-resistant iPod covers).

Smalley fought to protect the image of nanotechnology. An often-cited worst-case scenario is the "grey goo," a hypothetical substance into which the surface of the earth might be transformed by self-replicating nanorobots running amock. The public negative reaction, including mass demonstrations, to this prediction worried Smalley. He entered into a long debate in the press about whether or not it is possible to assemble such nanorobots. He published an article in *Scientific American* with the title of "How soon will we see the nanometer-scale robots envisaged by K. Eric Drexler and other molecular nanotechnologists? The simple answer is never." More recently, new analysis has shown that this "grey goo" danger is less likely than originally thought, and its proponents have stated that an accidental "grey goo" scenario is extremely unlikely.

In 1999, just three years after receiving the Nobel Prize, Rick learned about his leukemia. He fought it as courageously as he fought for nanotechnology. Many obituaries were written about him, two of which said:

- "Rick was a proud scientist, proud of what he had achieved and particularly proud of any students in his group who had green experimental fingers similar to those he had himself. ... With his flamboyantly uncompromising and inspiring presentation style, he became the most visible champion of nanotechnology and its promise to lead to revolutionary sustainable technologies."
- "He was one of those rare scientists, especially rare for chemists, who captured the imagination of a wider audience. He was, as Robert Gower was quoted as saying in the obituary in the *New York Times*, 'a rock star in technology.' "

Moskovits introduced **Walter Kohn** as the world's most cited physicist. He was born in Austria, worked as a geophysicist in Canada, served in the Queen's Own Rifles of the Canadian Army, is a promoter of a sustainable energy future, and has a new film entitled "The Power of the Sun."

Kohn said that one of the best rewards for serving on this Committee is the development of friendships with the likes of Rick Smalley. Smalley's mother got her bachelor's degree in science when he was a teenager. He and his older sister took classes together. His aunt was a professor of chemistry. The buckyball geometry of C_{60} was his insight. The promise of carbon nanotubes to revolutionize the conduction of electric power was very interesting to Smalley and was an important reason for his gravitation to a concern about the global energy picture. He turned his attention to energy and global warming and published a major paper about the issue in the *MRS Bulletin.* There, Smalley refers to three changes: a Sputnik effect (inspiring new scientists and engineers), the replacement of dwindling fossil-fuel resources, and the solution of the problem of global warming. We are now in a situation that is analogous to World War II, a tremendous global threat. The world is now operating at the margin of available supplies of oil and natural gas. Smalley and others recognized this as a real problem.

The U.S. Geological Survey predicts that petroleum and natural gas production will peak sometime between 2026 and 2047 and then drop off drastically. The world has a huge infrastructure tied to oil; it is too late to replace this infrastructure with one based on other fuel(s) by 2037, the mean prognosis for the peak of oil production. After Sputnik, there was an urgency to steer the best minds into science. That is not what is happening now. The National Academy of Sciences (NAS) report on effects of climate change in California is alarming. Smalley dealt with that topic in his *MRS Bulletin* paper.

There is a lot of coal, and you hear a lot about clean coal, but you cannot remove the carbon from coal. It is not tolerable to go to a coal economy without sequestration. Smalley said, “At some point, almost certainly within this decade, we will peak in the amount of oil that is produced worldwide.” Smalley is more likely to be right than the Department of Energy is.

If one looks at the doctoral degrees granted in science and engineering, one sees that the number of Asian students quadrupled between 1987 and 2000, but the number of U.S. students remained flat. The United States needs to prepare scientists and engineers to deal with the problems associated with energy production, transmission, storage, and use.

If one looks at global temperature, atmospheric carbon dioxide concentration, and global population, one sees that they have all risen sharply during the past 100 to 200 years. The increasing temperature correlates with atmospheric carbon dioxide level and with population. To get an idea of the magnitude of the challenge, Smalley noted that “to give all 10 billion people on the planet the level of energy prosperity we in the developed world are used to, a couple of kilowatt-hours per person, we would need to generate 60 terrawatts around the planet, the equivalent of 900 million barrels of oil per day.” If solar energy were used to supply all energy needs, six zones around the world, each the area of New Mexico, would need to be covered with solar cells and each generating 3.3 terrawatts of electrical power.

Smalley said, “There has been a lot of talk about the hydrogen economy, which I believe is, despite its virtues, likely to remain a distraction from the real, practical solutions to our energy needs.”

Kohn referred back to the paper in the *MRS Bulletin*, where Smalley said that conservation and efficiency could not amount to much in addressing the energy challenge. Kohn disagreed. Rosenfeld considers it the most important influence on energy issues. Rick Smalley was very skeptical about biomass: it requires an enormous amount of arable land and of water. Storage of energy is a very important problem for many forms of energy. Smalley felt that solar energy would be the most important alternative source of energy. He also envisioned a distributed energy grid and local energy storage. Kohn had spoken with Smalley about nanotubes’ contribution to long-distance transmission of electrical power. This possibility should be explored.

Moskovits thanked the speakers and asked for a moment to silence in honor of friend and colleague, Rick Smalley.

After the moment of silence, Hemminger asked for questions or comments from the Committee. There were none. He thanked El-Sayed and Kohn for their presentations. A break before the working lunch was declared at 11:41 a.m.

Hemminger called the meeting back into session at 12:32 p.m. and introduced **Mildred Dresselhaus** to present a tribute to Richard Smalley.

Smalley had a large impact on the nano initiative and in energy. He died of leukemia at age 62. He was extraordinarily imaginative, intense, and passionate. He was very courageous in his science as well as in his life. He had an ability to explain science in a simple way. He could boil and down complex topics to their essences. He was the main person to show how important nanotechnology is; he played a big role in getting nanotechnology into the international perspective and vision.

The energy challenge was of interest to Smalley early in his career in the early 1970s. He was also very interested in K–12 education. He was able to convey the excitement of science to the general public. In this, he resembled Enrico Fermi. Smalley always wanted to work on high-impact science.

In studying ion-implantation and interpolation of carbon, it was noticed that the ions were knocking off carbon atoms as large clumps and were doing that with much less energy than was needed to break the carbon-carbon bond. We found even numbers of carbon atoms in the clumps. Smalley was interested in the higher-mass species, and he figured out how they were structured. He had intuition. He noticed features of the mass spectrum that everyone else missed. The infrared spectrum of C_{60} confirmed that Smalley's solution of a truncated icosahedron was the correct structure of C_{60}. Smalley was successful in making single-walled nanotubes (SWNTs) and was the first to publish results. It was 5 years before there was a large-enough sample of nanotubes to allow analysis of their properties. Smalley was able to make them in large-enough quantities, and he kindly and generously supplied them to numerous researchers for analysis.
He was convinced that the 10-10 metallic nanotube was special and would be produced preferentially at the expense of other structures. He was very disappointed when the spectrum showed this not to be the case.

He developed a fluorescence technique to show all the species of nanotubes in a sample (in competition with Raman spectroscopy). A person who does novel things often influences areas outside his or her own area.

He got back into the energy field because he thought nanotechnology would drastically influence energy production, transmission, and use. He was interested in energy conservation and transmission by nanostructures. He was amazing at making things work that others did not think would work.

She quoted three colleagues on Rick Smalley:

- Naomi Pellet – He was always an iconoclast.
- Bob Curl – His mind was like a searchlight.
- Mostafa El-Sayed – Nanoscience and nanotechnology have lost a great champion.

Hemminger opened the floor to comments. Rohlfing noted that Smalley had been contracted by Exxon to help in uranium-isotope separation. Funding went away when the uranium market declined and Exxon Nuclear went belly up. *The Most Beautiful Molecule* is a good book on the discovery of buckyballs.

Moskovits noted that, in those days, people vaporized many things into inert gases to take their spectra. The infrared spectrum of C_{60}, indeed, clearly demonstrated the structure of C_{60} as Smalley had asserted it to be.

Spence noted that Mike Keith also recognized the buckyball structure and is mentioned in the book.

Kohn asked in what practical applications would the low weight-to-conductance ratio (in comparison to copper) play a role. Dresselhaus responded that a number of industrial applications require a high carrier density, and one has to have some mechanism to maintain high mobility and have high carrier density at the same time. The early papers were on experiments with short lengths with ballistic transport. The ballistic-transport regime has to be extended to long distances. She did not believe that that was possible.

Moskovits said that another individual at Exxon was Terry Baker, who did exquisite experiments with metal beams eating through carbon, producing carbon nanotubes. Dresselhaus said that Baker was the first to observe multiwalled nanotubes (MWNTs), and he figured out the mechanism of their growth. His work is not as well known as it should be. Gates said that Baker also made MWNTs catalytically. Dresselhaus cautioned that MWNTs are made catalytically but are not catalysts. She went on to say that Smalley mentioned several applications of nanotubes, one of which is their use in lithium-ion batteries, which use has been picked up by Japanese manufacturers who use the mechanical properties of the nanotubes to extend battery lifetime and improve performance.

Hemminger suggested that Dresselhaus had given the Committee a charge to make an impact on energy production and use in United States. He again thanked the speakers for their tributes and reminiscences about Richard Smalley.

Kohn said that the President's state of the union address was very promising. However, it was all goals, and it needs scientific input from this Committee and other sources. At the National Renewable Energy Laboratory (NREL), a concern is that much of the budget increase would come under the direction of industry. Scientific input could be greater than is currently called for.

Dresselhaus said that the National Academy of Sciences report, *The Gathering Storm*, should be acted upon, and BESAC has a role to play in responding to and implementing that report.

Hemminger asked **Patricia Dehmer** to update the Committee on the activities of the Office of Basic Energy Sciences (BES). She said that she will not talk about the Spallation Neutron Source (SNS), the five nanoscience research centers, or the Linac Coherent Light Source (LCLS). She will concentrate on the 2007 budget and the President's competitiveness initiative.

The BES portfolio should balance key components that together create a uniquely DOE program. It should support fundamental research to provide a decades-to-century energy-security plan and to produce discovery science that enables the mission, including the support of a critical mass of principal investigators who are a great "discovery machine" that is no less important than the big machines built for researchers. It should also aim for world leadership by the construction and operation of forefront scientific user facilities for the nation.

The DOE FY07 budget requests $23.6 billion, the same amount as the FY06 appropriation to DOE. However, the amount for SC increases a half-billion dollars from $3.6 billion to $4.1 billion. National security is also up slightly, and energy and environment are down. Core research is just about flat. Hydrogen research increases 54%. Solar energy has no presidential initiative, but it does have $34 million in new research. Advanced nuclear energy systems has new research funding of $12.4 million. Ultrafast science gets a new $10 million for LCLS instrumentation and tabletop lasers. There is $10 million to support a solicitation for midscale instrumentation. And there is $5 million apiece for chemical imaging and complex systems/emergent behavior. This adds up to a jaw-dropping 25% increase for the SC budget. In addition, there are (1) the major instrument initiative, which will receive a 10% increase for instrumentation construction, and (2) facilities operations, which will receive a 44.5% increase, most of which comes from the start of new facilities and some construction at the SNS. The upgraded National Synchrotron Light Source (NSLS-II) and LCLS were stressed in previous years, and some of the facilities' operations funds attempt to make up for those past shortfalls. All in all, there are significant increases across the board for BES. In construction funding, there is a dropoff because of the completion of construction of the nanoscience research centers and the completion of the SNS. There are increases in construction funding for the LCLS and for the R&D and design for the upgrade of the NSLS-II, the highest-rated SC facility.

The BES core research activities are slated to receive a little more than $100 million above their FY05 funding, with materials science and engineering research and chemical geophysical and biological research seeing about a 25% increase in funding and with facilities-related R&D seeing a 21% decrease.

Many supporters deserve our thanks in DOE, the Executive Office of the President, the Office of Science and Technology Policy, the Office of Management and Budget, Congress, National Academy of Sciences, and the science communities.

The story of these increases begins with the report *U.S. Competitiveness 2001*, which said, "given the rising bar for competitiveness, the United States needs to be in the lead or among the leaders in every major field of research to sustain its innovation capabilities." That report made several recommendations:

- Increase national investment in frontier research,
- Strengthen support for fundamental disciplines that have been neglected,
- Expand the pool of U.S. scientists and engineers,
- Upgrade K–12 mathematics science education, and
- Modernize the nation's research infrastructure.

The Council on Competitiveness began the National Innovation Initiative, which called for increased investment and infrastructure. In the spring of 2005, the National Academies were charged by Congress through two letters, one from senators Lamar Alexander and Jeff Bingaman and one from representatives Sherwood Boehlert and Bart Gordon, to address the study of America's competitiveness. The National Academies' Committee on Science, Education, and Public Policy (COSEPUP) established the Committee on Prospering in the Global Economy of the 21st Century: An Agenda for American Science and Technology. The committee of 20 members was chaired by Norman Augustine, retired chairman and CEO of Lockheed Martin. The committee assembled issue papers and convened focus groups in K–12 education, higher education, research, innovation and workforce issues, and national and homeland security. The key thematic issues underlying their discussions were the nation's need to create jobs and the need for affordable, clean, and reliable energy. It had one meeting in August, and the report was released on Oct. 12, 2005, after being vetted by 200+ reviewers. Congress had asked for 10 actionable recommendations. They came up with 4 overarching recommendations and 16 sub-recommendations.

- Increase America's talent pool by vastly improving K–12 science and mathematics education.
- Sustain and strengthen the nation's traditional commitment to long-term basic research that has the potential to be transformational to maintain the flow of new ideas that fuel the economy, provide security, and enhance the quality of life.
- Increase the federal investment in long-term basic research by 10% a year over the next 7 years.
- Create in the Department of Energy an organization like the Defense Advanced Research Projects Agency (DARPA) called the Advanced Research Projects Agency-Energy (ARPA-E).
- Make the United States the most attractive setting in which to study and perform research so that we can develop, recruit, and retain the best and brightest students, scientists, and engineers from within United States and throughout the world.
- Ensure that the United States is the premium place in the world to innovate; invest in downstream activities (such as manufacturing and marketing); and create high-paying jobs that are based on innovation by modernizing the patent system, realigning tax policies to encourage innovation, and ensuring affordable broadband access.

Many on the committee spent a lot of time briefing Congress, agency heads, and Executive Office of the President personnel from October to December 2005. Something changed in the administration. In late January, President Bush announced the American Competitiveness Initiative (ACI) to encourage innovation throughout our economy and to give our nation's children a firm grounding in math and science. He proposed to double the federal commitment to the most critical basic research programs in the physical sciences over the next 10 years. This funding will support to work of America's most creative minds as they explore promising areas, such as nanotechnology, supercomputing, and alternative energy sources.

The President's ACI describes a broad program to increase America's economic strength and global leadership. Such strength and leadership depend in large measure on our nation's ability to generate and harness the latest in scientific and technological developments and to apply these developments to real-world applications. These applications are fueled by scientific research, which produces new ideas and new tools that can become the foundation for tomorrow's products, services, and ways of doing business; a strong education system that equips our workforce with the skills necessary to transform those ideas into goods and services that improve our lives and provide our nation with the researchers of the future; and an environment that encourages entrepreneurship, risk-taking, and innovative thinking.

These themes came from the *Gathering Storm* report. The ACI also doubles, over 10 years, funding for innovation-enabling research at the federal agencies that support high-leverage fields of physical science and engineering: the National Science Foundation (NSF), the DOE/SC, and the National Institute for Standards and Technology (NIST) within the Department of Commerce. It modernizes the research experimentation tax credit by making it permanent and working with Congress to update its provisions. It strengthens K–12 mathematics and science education. It reforms the workforce-training system to offer training opportunities to some 800,000 workers annually. And it increases our ability to compete for and retain the best and brightest high-skilled workers from around the world by supporting comprehensive immigration reform.

The ACI acknowledges that sustained scientific advancement and innovation are key to maintaining our competitive edge and are supported by a pattern of related investments and policies. One of those is federal investment in cutting-edge basic research whose quality is bolstered by merit review and that focuses on fundamental discoveries to produce valuable and marketable technologies, processes, and techniques. This is what BES has been trying to do over the past 4 years. Another is federal investment in the tools of science (facilities and instruments that enable discovery and development), particularly unique, expensive, or large-scale tools beyond the means of a single organization. That is another thing that SC and BES do.

The ACI also provides for the construction of a number of cutting-edge scientific research tools with direct implications for economically relevant R&D, including the world's most powerful civilian supercomputer and an X-ray light source user facility with world-leading capabilities to study materials, chemicals, and biological matter at the scale of the individual atoms.

Many of the ACI recommendations speak to DOE SC/BES:

- world-class capability and capacity in nanofabrication and nanomanufacturing that will help transform current laboratory science into a broad range of new industrial applications for virtually every sector of commerce, including telecommunications, computing, electronics, health care, and national security;
- chemical, biological, optical, and electronic-materials breakthroughs critical to cutting-edge research in nanotechnology, biotechnology, alternative energy, and the hydrogen economy through a central infrastructure, such as the NSLS-II and the NIST Center for Neutron Research;
- overcoming technological barriers to the practical use of quantum information processing to revolutionize fields of security communications, as well as quantum mechanics simulations used in physics, chemistry, biology, and materials science (these hearken back to reports that BES and BESAC have issued);
- overcoming technological barriers to efficient and economic use of hydrogen, nuclear, and solar energies through new basic research approaches in materials science; and
- improving capacity, maintenance, and operations of DOE and NIST laboratories.

In 2007, the ACI proposes overall funding increases for NSF, DOE-SC, and NIST core research of $910 million or 9.3%. To achieve 10-year doubling, overall annual increases for these agencies will average roughly 7%. The ACI doubles total research funding; individual agency allocations remain to be determined and will depend on the performance of each agency.

At this time last year, the American Association for the Advancement of Science (AAAS) provided out-year projections based on the FY06 President's budget. No detailed out-year projections were released with the FY06 President's budget; AAAS relied on FY05 projections. In an analysis, nondefense discretionary funding continued to decrease. We now have a different picture with total R&D, defense R&D, and non-defense R&D being flat for 3 years. Some agencies go up significantly, and others do not do as well. The news in the administration is quite good for SC/BES.

Congress has put together the National Innovation Act of 2005. It responds to recommendations contained in the *National Innovation Initiative Report* of the Council on Competitiveness, focusing on (1) establishing the Innovation Acceleration Grants Program, which encourages federal agencies funding research and science and technology to allocate 3% of their R&D budgets to grants directed toward high-risk frontier research and (2) increasing the national commitment to basic research by nearly doubling research funding for the National Science Foundation by FY2011.

There is also a bill for Protecting America's Competitive Edge Through Energy (PACE). It reintroduces mathematics, science, and engineering education at DOE, providing for specialty schools for mathematics and science, experiential-based learning opportunities, graduate research fellowships, summer institutes, distinguished scientists, and other activities complementing what other agencies do. It also calls for DOE early career research grants, authorizes the ARPA-E to support ground-breaking energy research, and doubles authorized funding levels for basic research in the physical sciences.

Three bills have been introduced in the House of Representatives:

1. Sowing the Seeds Through Science and Engineering Research Act, which authorizes 10% increases each year and funding for basic research in the physical sciences, mathematical sciences, and engineering at the principal federal agencies supporting such research; and
2. 10,000 Teachers, 10 Million Minds Science and Math Scholarship Act; and
3. Establishing the ARPA-E.

With all of these legislative initiatives, both the House and the Senate along with the administration have responded to the NAS report.

To encourage and sustain such public support, the scientific community needs to make a strong connection between scientific frontiers (nanoscience and technology; complexity; theory, modeling, and simulation; materials probes and atomic-scale visualization; ultrafast science; and national facilities) and societal needs (defense, economic security, energy, water, food, health care, and environment). Two high-level ACI investment goals are

- federal investment in cutting-edge basic research whose quality is bolstered by merit review and that focuses on fundamental discoveries to produce valuable and marketable technologies, processes, and techniques and
- federal investment in the tools of science, particularly unique, expensive, or large-scale tools beyond the means of a single organization.

BES and BESAC have initiated a series of workshops on societal needs that can be addressed by scientific research that include

- Basic Research Needs to Assure a Secure Energy Future,
- Basic Research Needs for the Hydrogen Economy,
- Basic Research Needs for Solar Energy Utilization,
- Nanoscience Research for Energy Needs,
- Basic Research Needs for Superconductivity,
- Basic Research Needs for Solid-State Lighting, and
- Basic Research Needs for Energy Storage.

Other workshops have been conducted or are planned with colleagues and other agencies:

- Advanced Computational Materials Science: Application to Fusion and Generation IV Fission Reactors,

- The Path to Sustainable Nuclear Energy: Basic and Applied Research Opportunities for Advanced Fuel Cycles,
- Advanced Nuclear Energy Systems, and
- Combustion of Alternate Fuels.

These activities reflect research directions that speak to societal needs and cross-cutting scientific research areas. The Committee should start with frontiers of science and relate them to societal needs. Taken together, these workshops have contributed to a comprehensive decades-to-century energy plan.

On February 6, 2006, Secretary Bodman announced a $250 million FY2007 request to launch the Global Nuclear Energy Partnership (GNEP). This new initiative is a comprehensive strategy to enable the expansion of emissions-free nuclear energy worldwide by demonstrating and applying new technologies to recycle nuclear fuel, minimize waste, and improve our ability to keep nuclear technologies and materials out of the hands of terrorists. SC is not part of the GNEP, but in anticipation of this initiative, BES will sponsor a workshop on basic research needs for advanced nuclear energy systems from July 31 to August 2, 2006, in Bethesda, Maryland. The workshop is in the early planning stages and will cover such topics as:

- materials under extreme conditions;
- chemistry of the 5f elements;
- separations science;
- advanced nuclear fuels;
- waste forms; and
- theory, multiscale modeling, and simulation of materials, separation processes, and performance of materials and systems.

The workshop will have standard elements, such as a technology factual document, plenary-session briefings by representatives of DOE technology programs, multiple breakout sessions, and a detailed report within two months of the meeting. As always, BESAC members are invited.

New funding for core research, hydrogen, solar energy utilization, advanced nuclear energy systems, ultrafast science, and midscale instrumentation will be distributed by issuing solicitations and reviewing proposals. A solicitation for proposals for chemical imaging just closed. The amount of money available for complex systems/emergent behavior is not enough to warrant a solicitation; it will be distributed among proposals on hand. Each solicitation will have an announcement of intent to issue solicitations, a posting on the SC web site, a preapplication deadline, notification to principal investigators (PIs) about preapplication decisions, a full-proposal deadline, and announcements of rewards.

For the midscale instrumentation solicitation, about $20 million will be available for instrument upgrades, instrument replacements, and new instrumentation in two categories: (1) X-ray and neutron scattering instrumentation, including the development of new instrument concepts and (2) other midscale instrumentation, including electron microcharacterization and scanning-probe microscopy, laser-based systems for ultrafast science, tabletop X-ray sources and diagnostic applications, high-field nuclear magnetic resonance (NMR), electron spin resonance (ESR), specialized mass spectrometers, high-field magnets, computer clusters, etc. The basic research for the hydrogen economy solicitation will enhance basic research with an additional $17.5 million. The Basic

Research for Effective Solar-Energy Utilization solicitation will provide a little more than $34 million. The Basic Research for Advanced Nuclear Energy Systems solicitation will be initiated at a level of $12.4 million after the report on this topic comes out.

Many of our power sources in the United States are rooted in century-old technologies. 21st-century technologies will exert control at the atomic, molecular, and nanoscale levels. They will be things like high-Tc superconductors, solid-state lighting, and many other applications of quantum confinement, bio-inspired nanoscale assemblies, and petascale computing. These are technologies that were unknown 20 years ago.

She ended by pointing out that there are three high-level positions in the Office of Basic Energy Sciences that are currently vacant and for which candidates are being sought.

Kohn said that he was happy to see the ARPA-E proposal. A condensed-matter program (MASON) was convened for defense, and at that time (during the 1970s), it was said that a similar program should be convened for energy. Chevron has changed its viewpoint 180 degrees on oil production and consumption, now calling for a decrease of reliance on petroleum products. Significant nuclear energy will be needed in the next decade. However, we are on a path toward a huge increase in nuclear energy. The French did it. But satisfying global energy needs will require 20,000 GW of new nuclear power. He expressed concern about that because of the possibility that those nuclear power plants will be used for the production of materials for nuclear weapons. The Hydrogen Initiative was announced before it came to this Committee. The scientific community should provide scientific information before funding is decided. Storage is a key issue for many different forms of energy.

Isaacs noted that Dehmer and her team at BES deserve a lot of credit for the changes that are occurring. Fundamental science has to have economic effects. Dehmer noted that there would be a new Undersecretary for Science in the Department and that transferring information to the industrial community will be an important role for that new position.

DiSalvo said that science, technology, and followers need a bigger share of the pie, not a redistribution of the current level of funding.

Gates said that the Committee needs to consider the possibility that institutions will use incremental funding to cover what they have been doing recently, increasing the cost of doing research.

Hemminger noted that the proposed budget for BES has a decrease planned for research except for two research programs. Dehmer replied that that is correct; without those two programs, research funding is flat.

Hemminger asked for a report on upcoming workshops. **Harriet Kung** initiated the discussion.

The world consumes 13 TW of electrical energy; that will double by 2025. The report *Basic Research Needs to Assure a Secure Energy Future* will be used to lay out the blueprint for a comprehensive decades-to-century energy-security plan. The report from the Workshop on Basic Research for Hydrogen Production, Storage, and Use identifies gaps and opportunities and indicates a path forward. It engaged the research community and informed the foundation of the discovery machine.

The next workshop will be on basic research needs for superconductivity. The world has seen tremendous advances in the past century, starting with the discovery of the conductivity of mercury in 1911 and progressing through the definition of thermodynamics in 1933, cuprate high-temperature superconductors, and the theory of the phenomena from 1950 to 2003. Four Nobel Prizes were garnered in a short time in a small field. The electricity grid loses more than 10% of all electricity generated, and transmission limitations increase the risk of blackouts. Superconductors offer great benefits for overcoming these problems. Already, they have been used in power generators and motors for transportation needs, but they have a long way to go.

The superconductivity workshop is to identify basic research needs and opportunities in high-temperature superconductivity with a focus on energy-relevant technologies, including electrical transmission and the electric grid. Breakout panels will address fundamental material issues, physical phenomena, and cross-cutting theory and applications. Planning for this workshop began in October 2005. Panelist invitations and a briefing to the Technology Office were done in February 2006. The workshop will be held May 8-10, 2006, and a final workshop report is planned to be released in August 2006. The workshop will be held at the Sheraton National Hotel, in Washington, D.C. The plenary speakers will be Paul Chu, George Crabtree, Z. X. Shen, Mike Norman, and Alex Malozemoff.

Another workshop will be held on the basic research needs for solid-state lighting. Lighting accounts for about 20% of electricity consumption, yet has very low efficiency. Incandescent lighting has about a 5% efficiency, fluorescent lighting 25%, and metal-halide lighting about 30%. Light-emitting diodes (LEDs) can significantly contribute to the 2025 target of a 50% luminous efficiency if basic research needs can be addressed successfully. Semiconductor-based lighting technology offers great potential. Inorganic LEDs offer III-V semiconductor-based devices, high-brightness point sources, and a potential high efficiency and long lifetime. Organic LEDs (OLEDs) offer organic-semiconductor-based devices, large-area diffuse sources, thin and flexible applications, and ease of fabrication. The current barriers are that current LEDs are (1) predominantly in monochrome or niche applications and (2) high-brightness, broadband white light is needed for general-illumination applications. The workshop will have breakout panels on LED science (LED synthesis and properties; carrier transport, injection, doping, and recombination; light extraction and stimulated emissions; wavelength conversion and color mixing; and materials packaging issues), OLED science (OLED synthesis and properties; carrier energetics, injection, and transport; photophysics; and device architectures and light management), and cross-cutting and novel materials and techniques (tools for solid-state lighting and research; photon manipulation and management).

Planning for this workshop began in October 2005; panelist invitations and panel structure were set in February 2006; a Technology Office briefing will be held March 2006; and the workshop will be held May 22-24, 2006. The output of the workshop will be to produce concise and authoritative reports (1) giving overviews of technological challenges, scientific challenges, and scientific gaps and (2) identifying the basic research grand challenges.

Kung introduced **Eric Rohlfing** to speak about the Workshop on Basic Research Needs for Clean and Efficient Combustion of Alternative Fuels. Planning has been progressing on this workshop for about two weeks. Alternative fuels will be defined as those fuels other than the ones produced by refining light, sweet crude oil. Alternative fuels include those derived from renewable resources, such as biodiesel or ethanol, and fuels obtained via Fisher-Tropsch chemistry applied to heavy crude, shale oil, tar stands, and coal. The United States is likely to use these fuels in internal-combustion engines for transportation after traditional fuels (such as gasoline and diesel fuel) are exhausted and before hydrogen can be utilized. DOE and other agencies are supporting research into enhancing the production of alternative fuels from renewable sources (ethanol from biomass). However, the impact of the widespread use of these fuels in terms of efficiency and emissions is unknown, particularly for the next-generation of high-efficiency, low-emission internal-combustion engines. A basic research program is needed on the cleaning and efficient combustion of alternative fuels that assesses their potential impact on modern internal combustion engines.

The basis of this workshop is the strong BES program in gas-phase chemistry, combustion diagnostics, and combustion simulation.

Three examples provide tools to study the combustion of alternative fuels:

1. New experimental tools reveal new class of flame intermediates to diagnose the complex chemistry of combustion. Enols are alcohols within an adjacent double bond; they were postulated in 1880 by Erlenmeyer and seen by nuclear magnetic resonance in 1973 and in the gas phase in 1976. Enols are not currently in flame-chemistry models. Work by a team of BES-funded researchers is using molecular-beam flame sampling with tunable vacuum-ultraviolet (VUV) photoionization, revealing the presence of enols in many flames. New chemistry is needed to explain the role of enols.
2. New simulation tools for turbulent combustion include the world's largest simulation of combustion in turbulent flow. Molecular mixing is determined by turbulence, which is not complete. This simulation uses about 30 terabytes of data. One has to do preliminary calculations and then mine the data. This technique will be used for benchmarks for larger simulations.
3. Laser diagnostics can be applied to real diesel engines. Multiple-laser-induced fluorescence/incandescence reveals the evolution of diesel-spray combustion.

About 75 participants are expected at the workshop in the fall of 2006, which will be held in the Washington, D.C., area. The workshop will be coordinated with the Office of Energy Efficiency and Renewable Energy's (EERE's) Office of Freedom Car and Vehicle Technologies.

Hemminger pointed out that Dehmer had mentioned a nanoscience workshop and these three others. All have the potential for large impacts. All BESAC members should consider getting involved. He declared a break at 3:20 p.m.

The meeting was called back into session at 3:44 p.m., and Hemminger asked **George Crabtree** to report on the activities of the Laboratory Working Group (LWG) and its assessment of DOE's applied-energy portfolio.

The motivation for this analysis comes from David Garman, Undersecretary for Energy, Science, and Environment, who said in his Senate confirmation hearing, "we have not done as good a job as we should coordinating the activities of the ESE [energy-science-environment] offices. We have not done as good job as we should in performing the cost-cutting analysis we need to justify all budgets to the Congress." He put this working group in motion and asked it to look at DOE's applied energy R&D portfolio. That portfolio constitutes $1.4 billion of funding, of which energy represents $2.5 billion, science represents $3.6 billion, and environment represents $7.8 billion. That funding is spread across 21 program units in 4 offices: Energy Efficiency and Renewable Energy; Fossil Energy; Nuclear Energy, Science, and Technology; and Electricity Delivery and Energy Reliability.

The charge to the working group was to deliver improved analysis and decision-support material to senior management for the FY08 budget process through a focused effort with an emphasis on simplicity, timeliness, clarity, and relevance; a focus on impacts and risks; and a reliance on the best available knowledge and capability from DOE and the national laboratories. The working group was also to develop a sustainable long-term portfolio-analysis capability and process.

The context is embodied in advancing four, broad national energy policy goals:

1. diversify our energy mix and reduce dependence on foreign petroleum;
2. reduce greenhouse-gas emissions and other environmental impacts;
3. create a more flexible, more reliable, and higher-capacity U.S. energy infrastructure (e.g., electric grid); and
4. improve the energy productivity of the U.S. economy.

The Science and Technology Laboratory Working Group has ad hoc S&T analysis teams that it can call on. There is also a parallel S&T Integration Working Group. These working groups report to an R&D Council made up of representatives from EERE; Fossil Energy (FE); Nuclear Energy, Science, and Technology (NE), Electricity Delivery and Energy Reliability (OE), and SC, which Council in turn reports to the under secretaries for science and technology. It is a multiyear process that started last year. In FY05, it looked at applied-energy programs and the qualitative impact of the budget. In FY06, it is looking at quantitative impact, relation to science, and risk. Next year it may add a model analysis. Its tasks are (1) an energy R&D innovation strand, (2) innovation-strand impact analysis, (3) integrated portfolio assessment, and (4) recommendations for an enduring R&D assessment process.

The innovation strand is subdivided into (1) supply, (2) distribution, and (3) use. The supply strands come from advanced nuclear, alternative liquid fuels, zero-emission fossil electric generation, renewable energy, bioenergy/chemicals, and fusion energy. The distribution strands come from electric grid of the future, fuel grid of the future, and gaseous fuel grid (including the hydrogen infrastructure). The use strands come from industrial technologies, advanced building systems, and vehicle technologies. The working group looked at three rollups of the strands: (1) future electricity systems, (2) future liquid fuels and transportation, and (3) future hydrogen and gas systems. It then added cross-cutting and enabling science and technology opportunities and challenges. These topics were rolled up across the energy chains (combinations of supply, distribution, and use) to simplify analysis.

Among the general observations are that earmarks had a large effect on the applied-energy side. Of the 21 programs, transmission reliability R&D, HFCIT [Hydrogen, Fuel Cells, and Infrastructure Technologies], Generation-IV nuclear energy, nuclear hydrogen initiative, and advanced fuel cycle initiative all went up to twice in 2 years. Most of the programs did not go up or go down in the past 2 years. Biomass, vehicle technologies, and industrial technologies went down twice in 2 years.

Several technical challenges warrant focused attention. Energy storage at every scale is a critical issue in multiple technology strands. Electrochemical conversion (at high and low temperature) is a key issue. New materials for extreme environments are required across many technology areas. And real-time adaptive control of large-scale or complex systems is required at multiple scales (computational sensing and algorithmic control).

Several areas of science have particularly high enabling potential. Nanostructured materials will have a transforming impact in the near, mid, and long terms. Catalysis advances will enable many things to happen, including energy conversion, zero-emission hydrocarbons, and biomass. Advances in systems biology can "change the game" for biofuels and bioproducts through engineered feedstocks and bioprocessing technologies. Advances in high-temperature superconductivity are important for both the grid and for fusion. And high-end computational modeling and simulation has very high potential.

He offered four tenets on the role of science:

1. Incremental advances in the state-of-the-art of existing energy technologies will not meet the nation's future energy- and environmental-security challenges.
2. Revolutionary innovations are needed, both in the energy technologies themselves and in our understanding of the fundamental science that enables their operation.
3. Vibrant fundamental science programs generate revolutionary innovations in two ways: (1) by discovery-driven advances at the frontier of knowledge, enabling new paradigms and unexpected opportunities for disruptive energy technologies and (2) by use-inspired research that targets specific areas where incomplete understanding blocks technological progress. Here DOE should maintain strong programs in both areas that sustain U.S. leadership in science.
4. Basic–applied interactions are a fertile source of innovation. DOE should develop new ways to stimulate translational research and creative connections across the basic–applied interface.

The Working Group defined some basic science frontiers: high-performance materials; science at the nanoscale; dynamics of physical, chemical, and biological phenomena; emergent behavior and complex systems; catalysis and control of chemical transformation; a molecular- to systems-level understanding of living systems; biomimetics and photobiological energy conversion; molecular-scale understanding of interfacial science, separations, and permeability in physical systems and membranes; and new tools for in situ molecular characterization, theory/computations/numerical applications, and biomolecule production and characterization.

The Working Group produced a chart for each of these basic science frontiers that showed the research directions, scientific challenges, potential impacts, and timescale. For high-performance materials, the research directions were seen to be stability in extreme environments (temperature, corrosion, and radiation) and greater functionality (fast, small, strong, smart, efficient, and multifunctional). The scientific challenges were seen to be understanding structure–function relationships at all scales, stimulating and modeling behavior from first principles, and creating properties through nanoscale design. The potential impacts were seen to be next-generation materials for nuclear reactors; high-temperature thermochemistry; superconductivity; catalysis; biomimetics; and energy conversion among photons, electrons, chemical compounds, and heat. The timescale was seen to be continuous. Advances are interdependent. A discovery in one class of materials triggers breakthroughs in another.

The interaction between basic and applied research needs to be enhanced between SC and the applied-energy offices.

The goals for the basic–applied research program are at least two: (1) to translate applications from basic to applied (e.g., a 50% efficient quantum-dot solar cell and a cost-competitive superconducting wire) and (2) to develop a disruptive approach to grand energy challenges. Bell Labs set out to make an electronics switch and came up with the transistor, diodes, etc. and started the information revolution. Two grand challenges for DOE might be to store 24 GWhr of electrical energy for 24 hours and to produce personal transportation at one-tenth the cost of cars.

To accomplish these goals, it is important to

- have integrated basic–applied PI teams,
- have integrated basic–applied management teams,
- tap the best scientists and engineers,
- be innovation driven and not time-scale driven,
- have a stable program with a 10+-year life,
- engage an international network of workshops and visitors to create community and to stimulate fresh perspectives,
- set up periodic reviews by top scientists and engineers from outside DOE, and
- examine other innovation machines for organizational inspiration [e.g., DARPA, Bell Labs, Google, Microsoft, Apple, and Xerox Palo Alto Research Center (PARC)].

DiSalvo said that this is a terrific goal. Those examples (e.g., Bell Labs and PARC) can also provide examples where integrated teams did not work.

Gates commented that the goals based on hope should be critically assessed and cut off when not productive.

El-Sayed said that workshops might be helpful. Also, he asked if any current scientific efforts could be expanded. Crabtree responded that the workshops were a good effort to bridge the gulf between the applied and research sides. Biology is coming as a cross-disciplinary element. One or two targets may be approached on a pilot scale.

Berrah asked about international collaboration. Crabtree replied that that was a superb comment; DOE does not tend to work that way.

Greene observed that technology transfer did not work well. Ways to do that are still being looked for. The approach presented here is exciting.

Isaacs said that there is no industrial outreach in these programs. The customers have to come in and tell DOE what is needed. Crabtree said that that was an excellent observation. Transfer is two-stepped, going from research to development and then to the marketplace.

Cummings said that the working group might want to look at the National Institutes of Health (NIH) and base solicitations on grand challenges.

Taylor suggested that the working group might want to look at models from the big world and see what it can learn from their successes and failures.

Spence noted that some companies pay for postdocs to work in their laboratories and then make job offers to them afterwards. Crabtree replied that the best technology transfer is people transfer.

Hemminger noted that workforce-development issues are not in the mandate of this working group, but it would be a mistake to ignore them. Crabtree suggested that one workforce-development task might be educating the next generation of engineers in energy. Hemminger asked what the products from this effort are. Crabtree replied that the working group was told not to write a report but to make a presentation. It will brief the R&D Council about what it found and then brief Sullivan and Decker and then Garman and Orbach. Then those people will do what they will with that information. The working group is looking at potential R&D, not at the programs or offices.

El-Sayed said that, if one came up with a product, DOE would not make it. Crabtree agreed. The market would have to pick it up and market it.

Hemminger said that the Committee will review the charge to consider grand challenges on the following day. That charge was sent to the Committee the previous year but was suspended when the lawyers got involved in making Committee members special government employees. This new charge is different from the workshops that have been done. The Committee needs to decide how to proceed with the charge.

Hemminger introduced **Ray Orbach** to give an update on the activities of the Office of Science.

The President's budget has made a tremendous commitment. That potential advance is now ours to lose, and we do not want to do that. The PACE Bill now has 62 sponsors. In the State of the Union Address, President Bush said "I propose to double the federal commitment to the most critical basic research programs in the physical sciences over the next 10 years. This funding will support the work of America's most creative minds as they explore promising areas such as nanotechnology, supercomputing, and alternative energy sources." This is a historic opportunity for our country, a renaissance for U.S. science and continued global competitiveness. Senators have referred to this as a "second-Sputnik" response. This opportunity will not be given again. This proposal could double the SC budget from $3.6 billion in FY06 to $27.2 billion in 2016. In contrast, the FY95 level plus inflation would amount to an 18% increase after earmark removal. However, one should note that this proposal would double the sum of the budgets of the four basic-research agencies. If DOE does not respond, the monies will go to other agencies. Earmarks will decrease the level of funding in the current year and in future years as well. The core support and the facilities need to be maintained. A 10-year projection has been made, and it shows an increase in BES's budget of 25% to about $2.1 billion in 2016.

The consequence of the FY07 budget is that half goes to facilities and half to research. Some of the highlights of that budget are

- The International Thermonuclear Experimental Reactor (ITER) is fully funded. It will be the model for all future large-scale collaborations.
- In high-end computation, more than 250 teraflops will be provided on the floor in Oak Ridge, and 100 terra flops on the Blue Gene P at Argonne; the capacity of the National Energy Research Scientific Computing Center (NERSC) will be increased to 100–150 teraflops. At these speeds, scientific discovery can be done in many fields in which it could not be done before.
- Linac Coherent Light Source (LCLS) construction continues; it will provide an order of leadership beyond any other facility in the world and allow single-molecule structure determinations.
- The Spallation Neutron Source (SNS) is being completed on-time and on-budget.
- Four of five DOE nanocenters will begin operations in 2008, providing the United States with resources unmatched anywhere in the world.
- The International Linear Collider (ILC) would give the United States world leadership in the study of particle physics in the next decade at Fermilab. Killing

the Superconducting Super Collider (SSC) offshored high-energy physics research. It is imperative to bring the ILC to the United States and maintain collaboration with colleagues in other fields.

- The Continuous Electron Beam Accelerator Facility (CEBAF) and the Relativistic Heavy-Ion Collider (RHIC) are the primary high-energy physics programs in the United States. The upgrade of CEBAF will double its energy.
- The NSLS-II is slated to get $45 million for R&D and design in the FY07 budget, allowing it to leapfrog the third-generation accelerators and be the first fourth-generation machine with a 1-nm spot size. Nanoparticles will be grown in situ, and their properties studied. Stability is the challenge.

BES is slated to get a $286,423,000 increase in budget from FY06 to FY07. BES will run the Stanford Linear Accelerator Center (SLAC) and would take on other mortgages, a 25% increase in budget. In all of SC, one sees an increase of $505,319,000, a 14% increase (18% if one takes out the Office of Biological and Ecological Research earmarks).

The increase in funding is distributed between research (47%) and facilities (51%). At the SNS, the second target and power upgrade, it is hoped, will give a slow-neutron flux that is comparable to that of the Institute Laue Langevin (ILL) reactor.

In closing, Orbach quoted what he had said the previous day at the Congressional hearing on the budget: "We are indebted to the President for his foresight in recognizing the vital importance of America's continued leadership in the physical sciences to our nation's global competitiveness position in our quest for greater energy security. We are committed to holding up our end of the bargain by delivering truly transformational science and technologies – breakthrough advances that will provide new pathways to energy security and ensure America's continued global economic leadership in the years ahead."

Berrah asked what is happening to the RHIC. Orbach replied that it does not show up but *is* in the budget. A choice had to be made between RHIC and NSLS-II. Three other facilities in the world do what RHIC does. Money has been set aside for exotic beams. The United States will probably partner with one of the three machines elsewhere, but there are things that RHIC can to that others cannot. It is hoped that more will be learned about the design of such machines during the next 5 years and that the nation can proceed with RHIC then.

Richards asked how one prevents earmarks. Orbach responded: by supporting the President's budget. Our message to Congress should be that we have a commitment from the President that we want to support.

Greene observed that ITER keeps coming up as something that will take funding away from other activities. Orbach said that the budget is constructed with ITER in there. This is a period of transition for the fusion community. Like accelerators before them, a large machine will shut down small machines. Greene said that she did not want to see research leaving this country and for core research to be lost. Orbach said that 750 Americans are at CERN [Conseil Européen pour la Recherche Nucléaire, now Organisation Européenne pour la Recherche Nucléaire] working on the Large Hadron Collider (LHC). In fusion, ITER is an experimental device, and it is not known what science will develop. Our researchers and students need to be involved. He said that her caution is well taken and that research is quite strong in the FY07 budget.

Ceyer asked how likely this budget is to be passed given that increases at DOE come at the expense of other agencies. Orbach replied that other agencies are taking a hit; DOE got a significant increase because of strategic investment opportunities. The NIH hardly went up.

Gates asked if it is important that momentum be maintained. Orbach replied that four senators met with the President about the PACE Bill and there are now 60 senators (roughly 50% Democrats and 50% Republicans) that are sponsoring the PACE Bill. That bill will move forward, and we should try to maintain that momentum. He said that he was not a political person and does not know how these things work.

El-Sayed asked who are the leaders that members of the scientific community should write to. Orbach replied that he did not know; the names of the 60 PACE sponsors will be supplied to the Committee members. SC leadership will be talking with the budget analyst of the AAAS and will emphasize that this is a unique opportunity. El-Sayed asked when the outcome will be known. Orbach replied that no one can predict when Congress will do anything.

Isaacs asked about workforce development for this doubling of the budget. Orbach noted that the PACE Bill talks about this subject directly. It calls for increased science and mathematics education. The question will be raised time and again. Discovery is the way to get young people into science. Physics needs to be brought back home so U.S. graduate students can go into the laboratory and work on experiments.

DiSalvo noted that most education dollars are at the state and local levels. Orbach replied that DOE can try to leverage state and local funding through scholarships and teacher training. There is also an important effect from the president and other visible leaders' talking about this subject.

Hemminger asked, if there were an Undersecretary of Science, how that would affect the structure of BES. Orbach said that he would like to defer answering that question and thanked the Committee for its tributes to Rick Smalley; his death was a great loss.

Hemminger opened the floor to public comment.

Robert Marianelli noted that a dear-colleague letter written in 1978 identified the two areas of biomass production and hydrogen storage as critical. Two of the three Nobel prize recipients in chemistry were Americans who looked at homogeneous catalysis under BES support. One has to invest for the long-term. The Combustion Research Facility has done some things that were commercially significant. There are many other success stories. If one wants cooperation across disciplinary boundaries, one has to put it in people's performance measures. One prevents earmarking by telling what you will achieve with the funding you will get. NIH does not get hit with earmarks; everything is peer-reviewed. DOE programs are not seen as so defensible.

Hemminger adjourned the meeting for the day at 5:34 p.m.

Friday, February 17, 2006

Chairman Hemminger called the meeting to order at 9:06 a.m. He reviewed the charge of a year ago from Ray Orbach to consider the grand challenges in science. He displayed the charge letter. It calls for a workshop on "How atomic assembly governs the world we live in: Key scientific questions for the basic energy sciences." Hemminger wanted to come up with about three to a dozen major scientific questions facing energy sciences. The importance of those questions and the resources needed to address them also need to be identified. He asked Dehmer to give her thoughts on the matter.

Dehmer suggested the model of the NAS of convening a blue-ribbon panel of about 20 people to identify a dozen or so grand challenges through a process of holding hearings and writing issue papers. The panel might want to hold a workshop to bring about convergence of the ideas brought forward by the panel, its advisers, and its issue papers.

Hemminger asked what BESAC's role would be in this process. Specifically, is this a process BESAC would endorse? Would BESAC members want to be participants? Would the panel come back to BESAC to have its final report accepted? He asked the Committee if this is a reasonable way to proceed.

Berrah said that this is an excellent idea. Some of the panel members should come from other parts of the world. Hemminger said that that was a good point; BESAC members will be asked for nominations to the panel.

Spence suggested changing the title to "How atomic assembly and processes (or mechanisms) govern the world ... . As written, it sounds as though one is not interested in structure. Something like prediction of thermodynamic pathways at the atomic level would be very relevant.

Kohn noted that, on the theoretical side, not much progress has been made. Transitions between eigenstates are talked about, but this is not what happens in very fast processes. Not much progress has been made beyond Hartree-Fock theory, which is quite primitive. What should be addressed are the "major gaps" in theory, and that is not captured by the term "atomic assemblage."

DiSalvo noted that the charge seems to be to look at all science. Dehmer replied that it does not include astrophysics and many other areas. DiSalvo said that the panel might think broadly about materials science. Hemminger said that the audience is SC, but this Committee represents and reflects BES. The subjects of the Office of Basic Energy Sciences are what the effort should be restricted to.

Moskovits said that Orbach could be asked what he had in mind. He believed that Orbach wants to know the most sublime questions that prevent advances in energy sciences (but not high-energy physics and other areas outside the BES portfolio). What this Committee considers those questions to be should be given to the panel as examples to guide it in its task.

El-Sayed was of the opinion that Orbach wants to go down to the fundamentals in each area of energy production.

Richards said that it would be good if the panel understood how BES differs from the Office of High-Energy Physics (HEP) and the Office Of Biological and Environmental Research (BER). Dehmer replied that, if the panel came up with suggestions outside the expertise of BES, those suggestions would just get chopped out.

Long suggested that a multiscale model of basic energy production processes would be a good starting point.

Cummings said that fluctuation at the nanoscale is an area that is ripe for understanding.

Kohn called attention to the fact that this charge overlooks the energy crisis that the world faces. One must not exclude a strong commitment to make contributions to the provision of the world's energy needs. Hemminger agreed that BES's focus needs to be on energy supply, but the Committee is being asked here to look at the broad support of science in the next 10 to 20 years.

McCurdy asked how old this charge was. Hemminger responded, about a year. McCurdy noted that, when the Committee first saw this charge, it was talking about how to increase funding for BES. Now things have changed. Dehmer said that an important consideration is how science is going to be integrated into the Department of Energy and into the technology. The goals of basic research in the Department are two-fold. One is to advance the energy mission in all the basic-research-needs workshops that we hold. The other is to advance the frontiers of science for future transformational changes that we may not even see. It is extremely important that the Office of Science not lose sight of this second part of basic research. The new Undersecretary of Science will integrate the science of nuclear energy, waste management, waste cleanup, etc. One wants to make sure that basic science is not overlooked and that BES does not become an arm of the technology offices. That assertion should be stressed now in response to this charge letter.

Moskovits suggested that such an assertion could be made at the beginning of the report to by saying something like: "Whereas we are in a state of transition ... ." Also, one needs to ask what the future of energy science is, such as the integration of hard and soft materials. One challenge is where the boundaries of energy science are; any areas of overlap should be looked at as opportunities for partnering. One does not want to restrict what people can think about and imagine. Rather, their best thoughts are wanted. The Committee can always reject the findings.

Ceyer noted that the big breakthroughs may not be foreseeable by any panel of experts.

El-Sayed said that how photosynthesis works to produce, gather, and store energy is important. One should not shy away from something because it is biology.

DiSalvo suggested seeking such statements as "wouldn't it be great if we could ...?" This is more like what should be sought here, and it is a continuing conversation. Identifying panel members who can do that will be very difficult.

Gates cautioned that one needs to be specific about the time horizon that is being addressed. "Grand challenge" is not what one should be looking for; rather, one should be looking for grounds for conceptual breakthroughs.

Taylor noted that the scientific community has an opportunity to pull things together using new tools in an organized way. What needs to be done it is a "human genome of materials." The topic needs to be addressed from a high level and articulated so that the money and people to do it will be guaranteed.

Kohn noted that Smalley went in a very definite direction. He did not know what the end of point would be. Theory can bring about new technologies. It might be good to assume quantum computing actually works and see what would be needed to do it.

Isaacs said that what is wanted is to identify exciting concepts that might emerge in 10 to 20 years, but quantifiable research goals also have to be identified. The results have to be realistic but also must be imaginative.

Berrah said that the panel should come up with some great new concepts. Years ago, people dreamed about manipulating data at the atomic level; now we can do it.

Greene said that such effort will need to show some historical context and to show how one would go from the laboratory to the marketplace. This is a good time for putting forward a template for funding.

Spence noted that surprise cannot be planned, but institutions need plans. One needs experimental tools to limit theoretical possibilities.

DiSalvo asked what type of people one would want to have on such a panel. Both science and nonscientists should be present, including such people as Peter Edwards or Bill Brinkman or Freeman Dyson.

Hemminger commented that it is important for the Committee to help BES not become an applied science shop. BES is very good at putting together targeted workshops. BES needs to support at a fundamental level all the sciences that make BES what it is.

Isaacs said that this is not a one-time thing but should be a living document. This document should be owned by BESAC, not by a transient panel, and it should be continuously revisited.

McCurdy said that this document will define the scope of energy science for the future. This is the time to elbow our way out a little bit, suggesting that some things could become technologies.

Cummings noted that DOE is now in a competition with NSF and NIST for funding.

Richards asked if Hemminger wanted the Committee to submit some names for this panel. Hemminger replied, yes, and in the short term.

DiSalvo suggested putting together a huge, very broad list of names that can then be pared back. It should include CEOs, technologists, nonscientists, scientists, and young scholars.

El-Sayed suggested holding a preliminary workshop to identify experiments that need to be done, the instruments needed, and theoretical questions that need to be addressed in order to guide the panel.

Hemminger proposed that each member prepare a list of useful people during the next week and to send it to him by e-mail.

Greene asked that a copy of the charge letter be sent to each Committee member.

Berrah asked what the timeline was for the first meeting of the panelists. Hemminger replied that a summer BESAC meeting was being planned, so the panel should have some preliminary meetings before that.

Richards noted that one of the Committee of Visitors (COV) recommendations was increasing the size of awards. That increase should be made if BES's funding is increased. The way this money is leveraged makes it very important money. Also, there is an 83% increase in funding for heavy-element chemistry in BES; someone did a great job in getting the funding that was recommended by the COV.

Hemminger stated that the next COV will be convened in April and its results will be reported at the summer BESAC meeting. He called for public comment. There being none, he adjourned meeting at 10:20 a.m.