Minutes for the
Basic Energy Sciences Advisory Committee Meeting
June 6-7, 2005
Omni Shoreham Hotel, Washington, D.C.

BESAC members present:

- Sue Clarke
- Peter Cummings
- Mostafa El-Sayed
- George Flynn
- Laura Greene
- Bruce Gates
- John Hemminger, Chairman
- Eric Isaacs
- Anthony Johnson
- Kate Kirby
- Walter Kohn
- Gabrielle Long
- William McCurdy, Jr.
- Daniel Morse
- Martin Moskovits
- John Richards
- Kathleen Taylor
- Ward Plummer
- Samuel Stupp

BESAC members absent:

- Nora Berrah
- Philip Bucksbaum
- Richard Smalley
- Stanley Williams
- Mary Wirth

Also participating:

- Paul Alivisatos, Director, Molecular Foundry, Lawrence Berkeley National Laboratory
- Gordon Brown, School of Earth Sciences, Stanford University
- Patricia Dehmer, Associate Director of Science for Basic Energy Sciences, USDOE
- Richard Hilderbrandt, Program Manager, Basic Energy Sciences, USDOE
- Keith Hodgson, Deputy Director, Stanford Linear Accelerator Center, Stanford University
- Linda Horton, Director, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
- Robert Hwang, Director, Center for Functional Nanomaterials, Brookhaven National Laboratory
- Harriet Kung, Office of Basic Energy Sciences, USDOE
- Nathan Lewis, Division of Chemistry and Chemical Engineering, California Institute of Technology
- Derrick Mancini, Project Manager, Center for Nanoscale Materials, Argonne National Laboratory
- Frederick M. O'Hara, Jr., BESAC Recording Secretary
- Raymond Orbach, Director, Office of Science, USDOE
- Joel Parriott, Program Examiner, Office of Management and Budget
- Julie Phillips, Director, Center for Integrated Nanotechnologies, Sandia National Laboratories
- Leslie Shapard, Oak Ridge Institute of Science and Education
- Walter Stevens, Office of Basic Energy Sciences, USDOE

Karen Talamini, Office of Basic Energy Sciences, USDOE
Toni Taylor, Associate Director, Center for Integrated Nanotechnologies, Los Alamos National Laboratory

About 130 others were in attendance in the course of the two-day meeting.

Chairman Hemminger called the meeting to order at 8:18 a.m. **Leslie Shapard** made administrative, safety, and convenience announcements. Hemminger had the Committee members introduce themselves and announced a luncheon talk about the bureaucracy of the Committee. He asked **Patricia Dehmer** to update the Committee on the activities of the Office of Basic Energy Sciences (BES).

She apologized for the cancellation of the meeting scheduled in March and thanked the Committee for its frank and incisive comments to the General Counsel about the constitution of advisory committees.

At this point, the Federal Government is closing out FY05; Congress is working on the FY06 budget request; the House has completed its markup of that request; and the Senate is preparing its markup. Initiatives are being formulated for FY07.

The lead slide used by Ray Orbach in the FY06 Office of Science (SC) budget rollout presentation was a quote from the publication *U.S. Competitiveness 2001* by the Council on Competitiveness: "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."

The budget is forcing the nation to make tough choices. SC's prioritization provides for a strong and healthy future for U.S. science, consistent with the 20-year facilities outlook. SC is going to maintain world leadership in science. In the SC FY06 budget request, BES's request is 3.75% greater than its FY05 appropriation, and the House markup adds another $200 million. All facilities are in the Materials Sciences and Engineering and the Chemical Sciences, Geosciences, and Energy BioSciences sections of the budget request.

The House provided an additional $19,737,000 to maintain operating time on the BES user facilities at FY05 levels and an additional $7,395,000 to restore university grants for core research in the basic energy sciences. This will bring levels of operation up to those of FY04. Also included within this account is $7,280,000 for university grants under the Experimental Program to Stimulate Competitive Research (EPSCoR).

Construction is fully funded. SC and DOE gave extremely high priority to the completion of the Spallation Neutron Source (SNS), Center for Nanophase Materials Sciences at Oak Ridge National Laboratory (ORNL), and the Linac Coherent Light Source at the Stanford Linear Accelerator Center (SLAC). These facilities are to produce world leadership in science.

The operating facilities in SC's Division of Scientific User Facilities were flat funded at FY04 levels, a decrease of 6.26% from FY05 to FY06. As a result, some operations will be cut back, and isotope production at ORNL will be eliminated. $30 million was provided to BES in FY06 for the support of the SLAC linear accelerator. This $30 million begins the transition of ownership of that facility from High Energy Physics (HEP) to BES. This addition alone accounts for 2.72% on the 3.75% increase in the BES budget. The change to the core research activities in the Division of Materials Sciences and Engineering is –8.84% and in the Division of Chemical Sciences, Geosciences, and BioSciences is –8.29%.

The Senate markup is expected soon, and indications are hopeful.

Virtually all of the FY05 out-year projections are trending downward, generally by 7% over 5 years; this amounts to a 20% decrease over the 5 years when inflation is factored in. Such a decrease would lead to large layoffs. One might ask what the scientific community should do. The answer is to be aggressive; everyone (even the school lunch program) is facing similar funding projections.

The BESAC report *Basic Research Needs to Assure a Secure Energy Future* said, "Considering the urgency of the energy problem, the magnitude of the needed scientific breakthroughs, and the historic rate of scientific discovery, current efforts will likely be too little, too late. Accordingly, BESAC believes that a new national energy research program is essential and must be initiated with the intensity and commitment of the Manhattan Project, and sustained until this problem is solved." This recommendation was carefully crafted, and BES has worked hard to build this case.

In that report, energy was considered very broadly, allowing one to ask where energy research can make an impact. Two workshops have subsequently been conducted, one on hydrogen and one on solar energy. A report summarizing the Hydrogen Production, Storage, and Use Workshop that was held 2 years ago resulted in $20 million being added to the BES Hydrogen Initiative.

Two solicitations for the Basic Research for Hydrogen Fuel Initiative were issued in April 2004. By July 15, 2004, 668 qualified preproposals were received; and by January 4, 2005, 227 full proposals were received. Reviewers selected 70 hydrogen research projects. Universities received 55% of the support.

The timeline of activities shows that a lot of work was done in a short time: the hydrogen workshop was held; the report was released; follow-on activities like presentations at universities, on television news shows, etc. were conducted; and funding was obtained with projections out to FY08. In addition, the solar-energy workshop was held, and some coordination is already going on.

The next steps toward a secure energy future must be very carefully picked. Only the BES research community can provide insights into the choices that must be made. Ideally, 8 to 12 focused activities will be pursued, partnering together at substantial funding levels.

BES has a roadmap that covers three areas: energy security, fundamental science, and major scientific user facilities and special instruments.

She left the Committee with the notion that tremendous opportunities are coming at very difficult budget times. The Committee and the community it represents have a compelling case to make.

Kohn asked how the U.S. outlook compared with that of our global competitors? Dehmer responded that the United States was not keeping up. Europe and China are very aggressively pursuing nanotechnology. The United States could soon be behind Japan in light sources. One has to look at international benchmarks to assess the United State's position vis à vis its international competitors.

Hemminger introduced **Gordon Brown** to review the Committee of Visitors (COV) assessment of the Division of Chemical Sciences, Geosciences, and Biosciences Division (CSGB) and thanked Brown and his Committee for an outstanding job. Brown listed the members of the Committee and its six subpanels that reviewed the Computational and Theoretical Chemistry, Geosciences Research, Plant Sciences, and Biochemistry and Biophysics groups.

The charge to the COV was to assess (1) the efficacy and quality of processes used to solicit, review, and document proposal actions and to monitor active projects and programs; (2) how the award process has affected the breadth and depth of portfolio elements; and (3) each program's contribution to progress in achieving the long-term BES goals:

A. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, and biomaterials and (more particularly at the nanoscale) for energy-related applications.
B. By 2015, 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.
C. By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 BESAC workshop report.
D. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Four possible ratings were available to characterize progress toward these goals: excellent, effective, insufficient, and not applicable.

The six subpanels reviewed about a dozen representative jackets for each program containing a proposal, mail reviews, written summaries of panel reviews, anonymous mail reviews, correspondence between program managers and principal investigators (PIs), recommendation of the Program Manager, response of the CSGB Division Director, and summary of actions taken. Each subpanel conducted a "first-read" assessment of the jackets. Then the subpanels were reorganized for a second reading in which the jackets were reassessed at a more general level. The opinions of the first- and second-read subpanels were merged, and each program was rated on its progress in achieving the long-term BES goals.

The major findings of the COV are that

- The CSGB Division is very well managed and in generally excellent shape, with an opportunity to better integrate the Energy Biosciences program with several other programs in the Division.
- The proposal solicitation, review, and action process works well.
- However, the lack of an integrated SC-wide or BES-wide computer database and lack of standardized database software is viewed as a major shortcoming that should be fixed as soon as possible.
- Program managers have too few opportunities to visit grantees at national laboratories and academic institutions or to meet with them informally at scientific conferences. The primary limitation appears to be the low travel budget available to program managers.

- The quality of science, depth and breadth of portfolio elements, and national and international standing of these elements are very good to excellent in all nine programs reviewed, with unique results of high impact in many cases.
- Many of the PIs are world-leading in their research, with a number of Nobel Laureates, National Academy of Science members, and major award winners.
- The level of diversity in BES programs appears to be low in terms of career stage, race, and gender.
- Research funded by the CSGB Division is world-leading in a large number of areas.

The key COV recommendations are:

- The establishment of a BES-wide database and standardized database software is seen by the COV as *mandatory* to the effective management of a program as diverse and complex as the BES research portfolio. BES should take the lead in this much needed effort.
- The annual travel budget of program managers should be increased by 40 to 50%.
- The BES practice of providing long-term support to very high-quality research programs that address the DOE mission and long-term BES goals should be continued.
- The CSGB Division should consider implementing a young-investigator program.
- Portfolio elements in the Energy Biosciences program with the Photochemistry and Radiation Research, Catalysis and Chemical Transformation, and Geosciences programs should be better integrated.
- The Energy Biosciences program should be reevaluated and, if needed, refocused to improve alignment with the overall directions and mission priorities of BES and the Division.
- Maintain and if possible expand funding in the Heavy Element Chemistry program and in other areas of particular importance to the DOE mission, especially for those programs with no other realistic funding sources.
- DOE should design appropriate methods to monitor diversity.

The ratings assigned by the COV are

Program	Goal A	Goal B	Goal C	Goal D
AMO Science	Excellent	Excellent	Excellent	Excellent
Chemical Physics	Excellent	Excellent	N.A.	Excellent
Photochemistry and Radiation Research	Excellent	Excellent/Effective	Excellent	N.A.
Catalysis and Chemical Transformation	Excellent	Excellent	Effective	Excellent
Chemical Energy and Chemical Engineering/Separations and Analysis/Heavy Element Chemistry	Excellent	Excellent	Excellent	Effective
Energy Biosciences	Excellent	Excellent	Excellent	N.A.
Geosciences	N.A.	Excellent	Excellent	Excellent

In general, the CSGB Division is remarkably responsive to the long-term goals of BES and is making excellent progress toward meeting those goals. Improvements are needed in 3 of 24 applicable categories in 3 of 9 programs.

El-Sayed asked if there should there be an initiative to encourage students to enter some of these areas. Brown replied that it is unlikely that DOE funding would alter university hiring practices. Clark commented that DOE funding does occasionally influence academic infrastructure that feeds into the national laboratories (through postdocs and graduate students).

Taylor commented that sitting in the room and talking about the proposals draws out the expertise of the proposers. Proposal-review panels should not be anonymous. Brown agreed but noted that the Committee is saying that the initial proposals from universities, national laboratories, and industry should be anonymously reviewed.

Moskovits noted that there is little one can do to influence universities, but changes in academia are necessary. Critical long-term questions have to be posed, and the universities and other elements of society have to address those questions. One needs to know what is in the future; and, in some areas, DOE is the only remaining player (such as in heavy elements). Brown agreed; one of the issues for universities is safety; this issue is important in doing research with high-level radioactive materials; universities are not set up to carry out such research. Clark noted that academia looks to partnerships between national laboratories and universities in such a case.

Richards commented that one should not forget that DOE started the Human Genome Project; DOE is a wonderful place; BES is doing a lot of important work that no one else is even considering. Brown responded that the report says that Energy Biosciences should stay within the Division.

Morse noted that nothing is said about energy bioscience. That failure pulls the teeth from the ratings of excellence given elsewhere. Brown rejoined that the research being done in BES is excellent by any standards. The Committee does not want to change that rating.

Richards offered that there should now be a different program with a different focus.

Cummings called attention to the young investigators, and asked if the Committee was able to find any data on good people who did not get into the program. Brown replied, yes! The standards for young investigators' proposals, though, would have to be lower than for those for experienced PIs' proposals. Stevens said that to institute something like this would require a set-aside, which BES does not do. One could also compete renewals against new proposals.

Plummer stated that the findings have serious problems. The Committee might want to reconsider its assessments of excellence. Brown responded that the assessments are in terms of progress toward the long-range goals; they do not focus on the problematic areas. There are a few exceptions. Hemminger observed that the full report points out in terms of the Office of Management and Budget (OMB) rating scheme why ratings of excellence are called for.

Moskovits moved to accept the report; El-Sayed seconded. The vote was unanimous in favor of the motion.

A break was declared at 9:59 a.m. Hemminger called the meeting back into session at 10:15 a.m. and introduced **Raymond Orbach** to update the Committee on the activities of the Office of Science. Orbach apologized for the cancellation of the March meeting, which occurred because the Department is moving to a new method of managing advisory committees.

The committee structure in the House has changed, and the Senate went along with the House. As a result, the entire DOE budget is now considered by a single appropriations subcommittee in the House, along with the budgets for NASA and NSF. It will be interesting to watch for the consequences of this new structure.

SC is now preparing its presentations to the Secretary of Energy for the FY07 budget request. He will put together the Department's requirements that will go to OMB, which will pass it back around Thanksgiving. After modification, the President's request will go to Congress at the beginning of the next calendar year.

There are some misconceptions on how the FY06 budget was put together. The President has commitments, among which is to halve the deficit. Everyone wants to see the deficit reduced.

The statement on U.S. competitiveness cited earlier by Dehmer is still true. If the United States is to do science, it should be the best in the world. The FY06 budget request has been put together to guarantee that world pre-eminence.

SC is the primary source of support for the physical sciences. It provides 42% of all federal support to the physical sciences. Its support is roughly twice the size of the Department of Defense's research funding and three times the support of the NSF for physical science. SC manages long-term, high-risk, high-payoff, multidisciplinary science programs to support DOE missions, and it directly supports (in FY05) the research of about 23,500 PhDs, postdocs, and graduate students.

SC constructs and operates large scientific facilities used by more than 19,000 researchers every year. The SNS will add 2000 more users. Construction is being started on the Linac Coherent Light Source (LCLS), which will be 10 billion times brighter, in the hard x-ray range, than any other light source in the world, giving the United States more than a decade lead on any competitor.

SC has benefited enormously from being in a mission agency. It deals with the mission of energy security with additional roles in the environment and the future of science. The very best science programs need to be carried out here in United States to get young people to study and work here.

This is a difficult budget year. The Energy Authorization Bill, H.R. 6, has passed the House. The Senate is moving a companion bill through committee, and it may be out during the week of this meeting. That bill is terribly important to SC because it contains SC's authorization.

It is useful to look at the funding history of SC. If the Superconducting Super Collider (SSC) had been built, it would be producing data now. Instead, the United States is borrowing instruments at CERN [Conseil Européen pour la Recherche Nucléaire]. The future of high-energy physics in the United States is at risk. One cannot write off a field of science. SC's budget did not go up when the SSC was eliminated; it went down. SC has to recover from that dropoff. The FY05 budget was the highest ever for SC. The FY06 budget request reduces funding for SC to the FY04 plateau, although the House and Senate may increase that funding. Currently, BES is slated for a 3.7% increase in funding from FY05 to FY06, an augmentation of $41 million. However, the total SC budget is slated for a 3.8% decrease, a 1.6% reduction, excluding earmarks.

The issue is world leadership with the nanoscience centers, the LCLS, leadership-class computation, etc. The consequences of these advances are uniform reductions of 10% in core-research categories. That tradeoff was made to give U.S. scientists the best facilities in the world to work with. Some consequences of that tradeoff are that, from FY04 to FY05 to FY06, the percentage of the SC budget supporting operations and construction increases from 40 to 42 to 42%, respectively. At the same time, the percentage supporting research declines from 49 to 48 to 45%. This decrease in research support is worrisome and needs attention. If one looks at the amount of carbon-neutral energy that the United States will need to supply by the end of this century, it equals the amount of energy the United States now consumes. Fusion energy has a good shot at supplying some of that new energy in a carbon-neutral fashion, so the United States is contributing to the International Thermonuclear Experimental Reactor (ITER) program. SC will put two 20-Tflop machines on the floor in Oak Ridge and will open these machines up to the whole country through the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Program. SC now has all the available architecture needed by the scientific community. For the first time, there is a discovery-oriented computational opportunity available in this country. These machines will be protected for high-end computation. This computational capability will have a tremendous influence on materials science and fusion energy.

In FY06, the SNS will begin operation at ORNL, and four of five Nanoscale Science Research Centers will begin operations. Construction of the Linac Coherent Light Source at SLAC will be started; it will be able to see chemical bonding in real time. In high-energy physics, the United States is in a race with CERN to observe the Higgs and supersymmetry. Fermilab is running flat out to win this race. In 2007 or 2008, one should see if anything will be found in 2010. It is hoped to make the discoveries here in the United States before CERN's Large Hadron Collider (LHC) is turned on. String theory is coming of age with the perfect-liquid findings at the Relativistic Heavy Ion Collider (RHIC).

Following the BESAC report *Basic Research Needs to Assure a Secure Energy Future* and two follow-on workshops, the solicitation on hydrogen production, storage, and use garnered 800+ proposals with good quality. Other areas of focus are solar-energy conversion, materials for extreme energy environments, nanostructured materials, the control of chemical pathways, and complex systems science. The intellectual rewards that these areas hold need to be mined.

Hemminger asked if there were anything that could be done about the shrinkage of core research. Orbach replied that this Committee and its members can do what they want. At the American Association for the Advancement of Science (AAAS), he [Orbach] laid out what he thinks the science community can do. The issue is whether science is treated in an average manner or is treated as a part of the protected budget. The discretionary part of the budget will be reduced to reduce the deficit. Each person should express his or her views.

Kohn said that the solar energy meeting was excellent. In solar electricity, Japan controls more than half the world market. Like small cars, the United States is taking a long time to catch up. ITER is to demonstrate the feasibility of fusion energy. One has no idea whether it will work at all. Orbach said that producing 1/2 GW for 500 seconds is the goal for demonstration. An operating power plant will require a q of about 30, where *q* equals the energy out/energy ratio of a power plant. The only machine operating today has a *q* of 0.7. It is believed that ITER with a *q* of 10 to 20 will convince industry that fusion energy will work. The United States is only 10% of the ITER effort. A lot of other countries are investing in this effort. Kohn responded that he was happy the United States is supporting that research progress.

Stupp stated that there is a misalignment in the FY06 budget: there is not an alignment between energy security and funding; and asked how that alignment can be moved. Orbach replied that energy is a major part of the investment. The last page of the budget presentation lists opportunities fueled by the major investments like the SNS and nanocenters. He said that Stupp was right. The Office's major investments may need to be reoriented in the future.

Hemminger noted that, in decreasing funding, administrative costs are going up. Orbach said that, ironically, that is the Committee's own fault. The COVs are recommending increased staffing. SC is staffed at only 25% the levels of other agencies.

Hemminger introduced **Nathan Lewis** to present his personal view of the global energy situation and then to report on the Solar Energy Workshop. Lewis started with a global perspective on the role of solar energy as a primary energy source.

Global energy consumption in 1998 was 13 trillion watts worldwide, with the United States consuming one-quarter of that energy. In terms of heat content, oil dominated that consumption, exceeding coal and gas consumption by 50% each. The consumption of these fuels dwarfed the consumption of biomass, nuclear energy, hydropower, and renewable energy. The energy from renewable sources was dominated by hydropower with biomass following close behind. Succeeding rates of generation were by geothermal energy, wind, low-thermal solar, solar thermal, marine power, and solar photovoltaics.

The production costs of electricity today in the United States are 1 to 4 cents for coal, 2.3 to 5.0 cents for gas, 6 to 8 cents for oil, 5 to 7 cents for wind, 6 to 7 cents for nuclear, and 25 to 50 cents for solar without storage. But most of our energy is used to heat houses, run cars, etc., not using electricity. In terms of heat content, the cost of electricity is almost eight times that of coal and five times that of oil.

At the 1998 rate of consumption, the world has 40 to 78 years of proven oil reserves, 68 to 176 years of gas reserves, and 224 years of coal reserves. What is more important, however, is the resource base, which would give the world 51 to 151 years of oil, 207 to 590 years of gas, and 2160 years of coal. (We could convert coal to oil.)

Conclusions to be drawn are that the world has an abundant, inexpensive resource base of fossil fuels. Renewables will not play a large role in primary power generation unless technological and cost breakthroughs are achieved or unpriced externalities are introduced (e.g., environmentally driven carbon taxes).

To calculate energy demand, one needs to know (1) population growth, (2) per capita gross domestic product (GDP) growth, and (3) energy consumption per unit of GDP. In the next century, population growth is expected to increase to about 11 billion people; per capita GDP is expected to grow at 1.6% per year; and energy consumption per unit of GDP is expected to decline 1% per year. Energy consumption vs. GDP varies widely between the developed and underdeveloped countries. The target average energy consumption per capita is 1/5 the current energy usage in the United States.

Between 1890 and 2000, the energy mix (the fuels used to produce the world's energy) steadily decreased in carbon intensity. Under a business-as-usual scenario, one would expect decarbonization to continue; but one cannot continue that trend much beyond 2060, even in a purely gas economy.

As carbon emissions to the atmosphere mount, one eventually can get to a point where the effects will be irreversible. Under extreme scenarios, carbon emissions can be driven to zero; but to meet this criterion, one would need to eliminate carbon fuel use forever. Under the most optimistic scenario, nuclear and renewable energy could meet world energy demand, but the amount of renewable energy consumed would equal all the energy used today. If such large amounts of carbon-free power are needed, current pricing is not the issue for year-2050 primary energy supply. The issue is, where do the physics of the planet allow one to get such large amounts of energy? There are three sources of carbon-free power: (1) nuclear (this is the only proven technology that could scale to the requisite need of 10 TW, but a new reactor would have to be constructed every other day somewhere in the world for the next 50 years, consuming all the uranium in the world with a once-through fuel cycle in the next 50 years), (2) carbon sequestration, and (3) renewables. In theory, carbon sequestration is an option and could buy some time, but the question is whether it will leak. The CO_2 would have to be sequestered for 100,000 years. This question should be investigated.

The total hydroelectric power potential of the world is 4.6 TW; it is technically feasible to exploit 1.6 TW of this power; it is economically feasible to exploit 0.9 TW; the current installed capacity is 0.6 TW. One must conclude that there is nowhere to grow with hydropower.

Geothermal energy produces a mean flux at the surface of the Earth of 0.057 W/m^2; the continental total potential is 11.6 TW.

Wind allows 4% utilization at Class-3 locations and above, allowing a total production of 2 to 3 TW.

The world's solar energy potential is 1.2×10^5 TW; the practical limit is between 600 and 1000 TW. The energy from the Sun striking the Earth in 1 hour of sunlight is more than all the energy consumed by the world. This is the only big number in the mix besides nuclear energy. To produce 3 TW, one would need to cover everybody's roofs 10 times over; one would need a collecting area a little smaller than the state of Kansas for each continent.

Photosynthesis works well, but is extremely inefficient. Photosynthesis converts about 90 TW of energy per year. Photovoltaics do the same job but do it much more efficiently. Biomass energy potential requires large areas because it is inefficient; to meet energy demand by biomass would require 31% of the total land area to produce 20 TW if one could water all those plants. At 8.5 to 15 oven-dry tonnes per hectare per year and 20 GJ higher heating value per dry tonne, the energy potential is 7 to 12 TW.

From 1950 to 2000, the efficiency of photovoltaic devices has increased from near 0 to 25%. At current costs and efficiencies, photovoltaic devices would have to collect 10% for 10 years to produce a cost of 35 cents/kW. One must raise the efficiency and/or lower the costs. The cost has to be less than ten times the current cost for painting a surface.

Science must learn to develop disruptive solar technology (solar paint), to develop grain boundary passivation by taking many individual crystals and glueing them together so they act as a single crystal, and to produce interpenetrating networks while minimizing recombination losses. What is needed is a way to make fuel directly from the sunlight; one can do that now with reverse hydropower. However it is hard to envision scaling up that technology. A system is needed that borrows hard from what nature teaches. Catalysts, integrated processes, and "artificial plants" are needed.

In summary, that the world is going to need to additional primary energy is apparent. Options are needed. The options are: hope fusion works in time, build thousands of nuclear power plants, provide disruptive solar technology, and devise inexpensive conversion systems and effective storage/distribution systems.

There are four securities: energy security, national security, environmental security, and economic security. One can meet all of them only with solar, but one needs R&D to get there. Others have already said this: President's Committee of Advisors on Science and Technology (PCAST), BESAC (*Secure Energy Future*), DOE Hydrogen, National Research Council/National Academy of Sciences (NRC/NAS), Chu, Smalley, Kohn, and Heeger. The questions are: Will there be the needed commitment? Is failure an option? An interesting observation is that we now spend more money at the pump in 10 minutes than we spend on solar energy R&D in a year.

Lewis then turned his attention to the results of the BESAC solar-energy workshop.

There are three ways to capture solar energy: solar fuels made by plants or machines, solar electricity, and solar thermal-to-electricity. Plants and solar cells absorb only part of the solar spectrum. The rest is dissipated as heat or not absorbed, limiting efficiency to 35%. At the lower end of that spectrum, the band gaps are too large; and at the upper end, they are too small.

Efficiency can be improved by using photons to boost one valence electron up to the conduction band and to use quantum structures to boost another electron to the second quantum-dot energy level and then collect both electrons at once. Another strategy is to design molecular photovoltaic materials and structures to extract the maximum energy from solar photons and make lots of them at very low cost. New materials are approaching the needed low costs.

Another way to improve efficiency would be to use tandem cells (with different absorbance characteristics) to absorb more of the spectrum, as does color film.

One can also increase efficiency by using two interpenetrating nanostructures to increase the interfacial area density and shorten the pathways that produced/collected electrons have to follow. An extreme way to do the same thing would be to use a randomly structured material, but not enough is known about the dynamics involved to allow one to change something randomly and have it work better.

In 1977, a monolithic photoelectrochemical cell was discovered that directly converted solar energy to fuel through ultraviolet (UV) photoelectrolysis. Materials that will absorb and convert visible light need to be found and controlled.

Nature has developed catalytic pathways for water splitting (in photosynthesis). Models of these natural systems should be studied to see if a functional, hydrogenase can be built to electrolyze water to produce hydrogen for fuel. Can one take the key pieces of the natural systems and analyze and replicate them?

Another path of discovery is to improve plants and microbes to increase their ability to produce solar-energy-dependent biofuels. These approaches would require mining biological diversity to improve catalysts for biofuel production, capturing the high efficiency of the early steps of photosynthesis, and understanding and modifying bioprocesses. After all, global photosynthesis makes 90 TW of stored energy. However, science does not have good processes and materials to split water at 1700 K and produce solar thermochemical fuel efficiently. Gen-IV nuclear reactors will need similar materials. Science needs to develop experimental and theoretical methods to design, identify, and synthesize solar energy conversion materials with targeted properties for (1) thermoelectrics, (2) thermophotovoltaics (TPV), (3) solar heating, and (4) concentrated solar power (CSP) for use in solar concentration, thermoelectric energy conversion, and increased intensity on TPV emitters. To accomplish these goals, science also needs to be able to put together pieces by self-assembly on many length scales from the molecular scale to the nanoscale to the manufacturing scale.

One more challenge is that these devices need to last for 30 years, probably achieving this longevity through self-repair and defect tolerance.

One can also use dimensionality to control the flow of energy with nanotechnology and nanodevices through enhanced photon management. After all, the absorption length of energy is in the micron-to-nano scale. Nanostructure could help move the electrons to where they are wanted. Such management can be achieved by control of carrier excitation, charge transport, and energy migration and by manipulating the interface science of photo-driven systems.

Kohn stated that the perspective that Lewis provided should always be kept in mind, but another perspective should be kept in mind, as well: energy for those off the grid. Providing off-the-grid electricity could revolutionize the continent of Africa, a large fraction of which is off the grid. There are also population perspectives and conservation perspectives and others that can be employed in assessing energy paths. Alluding to a recent book by Tom Friedman of the *New York Times*, he pointed out that Europe affords $4/gal gasoline, and they still eat! Lewis agreed that producing off-the-grid electricity could be the biggest business in the world for the United States.

McCurdy pointed out that this talk by Lewis was disconnected from the budget talks, where the funding of the core research is declining. The needs expressed here are for exactly those core research activities, not facilities. Dehmer commented that an Energy Security Plan has to be on the scale of a major facility or program. In planning for the out-year budgets, one has to support and protect what one thinks will produce the great discoveries.

Hemminger declared a break for lunch at 12:19 p.m. He called the meeting back into session at 1:44 p.m. and asked **Joel Parriott** to provide an overview of science funding from an OMB perspective.

OMB is but one office in the Executive Office of the President, but its 530 employees make it the largest. OMB assists the President and has a hand in the development and resolution of all budget, policy, legislative, regulatory, procurement, e-government, and management issues. Its director, Joshua Bolten, is a Presidential Cabinet member. The program associate directors (or PADs) are political appointees but are not confirmed by Congress. The speaker is a program examiner.

The President's FY06 budget is meeting the priorities of the nation while achieving spending restraint. The priorities of the President are to defend the homeland from attack, transform the military and support our troops in the global war on terror, help to spread freedom throughout the world, promote high standards in our schools, and tax reform. In the current budget request, R&D makes up 15% of discretionary spending. Future discretionary spending (2005 to 2009) for nondefense budget items is planned to be flat at about $480 billion. This figure is what is driving the out-year planning. The four PADs oversee programs in natural resources, human resources, general government, and national security, respectively. In natural-resource programs, the competition is among DOE, NSF, National Aeronautics and Space Administration (NASA), U.S. Department of Agriculture (USDA), U.S. Geological Survey (USGS), Environmental Protection Agency (EPA), and the Smithsonian Institution. This grouping is different from that used by Congress. The natural-resources PAD has the highest percentage of funding devoted to R&D. At the same time, it has the smallest amount of funding to administer ($135 billion).

The Administration's R&D priorities map onto the SC portfolio as follows:

Program	**DOE Offices**
ITER	Fusion Energy Sciences (FES)
Hydrogen	BES [and Biological and Environmental Research (BER)]
Nano	BES
Supercomputing	Advanced Scientific Computing Research (ASCR)
Climate change	BER [and BES]
Systems biology	BER [and BES]
Physical sciences (those that have broad societal impact are priorities)	BES, HEP, and Nuclear Physics (NP)

BES has a large presence on this map.

Each fall, each PAD is presented with *n* dollars and is asked to take care of the President's priorities (ITER and the hydrogen initiative), take care of other Administration priorities (nanoscience, climate change, and supercomputing), be cognizant of Congressional priorities (especially where they might be at odds with the above), fix other miscellaneous problems (e.g., stewardship of disciplines and national laboratories), and present a recommended program that clearly identifies where problems remain.

Questions that will be asked while addressing the lingering problems are

- What are the consequences of not addressing this problem?
- What is the political landscape, if one exists?
- Are there nonmoney solutions available?
- Is more money really the only viable solution?
- Why were not funds from lower-priority efforts used within the account?
- Is this account optimizing the use of the funds it does have? (This is where COV results come in.)
- What is the compelling policy argument for the proposed solution?

The perceived communication breakdown is between what the agencies think they are providing to OMB and what OMB sees as coming from the agencies. One can usually make a better case. Typically, what the scientific and technical community says to OMB is

- Basic research is critical to the long-term interests of the United States.
- More research money is always good; less is always bad.

- Producing the next generation of scientists is of paramount importance.
- The Administration must not understand (or perhaps is hostile to) our compelling arguments, or else they would follow our recommendations.
- We are smart, so you should listen and send us more dollars, and we will do good things … trust us.

Typically, what the OMB staff says to the scientific and technical community is

- Large, sustained budget deficits should be avoided if possible.
- Basic research is a good thing, and support is typically a clear federal role, but it is difficult or impossible to know when investment is subcritical, and generational timescales add to the complexity of the analysis.
- The appetite of the community for more dollars is boundless; everyone claims to be doing compelling, ripe-for-great-advance work.
- It is difficult to impossible for most of the scientific and technical community to set priorities.
- Universities are good; national laboratories are unique but uncontrollable entities.
- The Federal Government needs to spend tax dollars more wisely and efficiently.

To make a better case, agencies should work to put themselves in OMB's shoes, asking how to realistically implement one's own recommendations within a fixed budget envelope and using the framework of the R&D Investment Criteria to drive arguments. They should improve their consensus reports. Most advisory-committee reports would not pass peer review; anecdotes drive the arguments rather than data; a better job should be done on executive summaries and navigational elements; the assumptions and context should be revealed; admit limitations. Workforce arguments are typically weak ones. Let the science drive the case; then one gets the people for free at the end of the argument. Well-grounded constructive criticism adds to one's credibility. Strong participation by outsiders adds to a report's credibility. Many decisions are political at their core, so the community needs to be more politically astute, but partisanship should be avoided.

The R&D Investment Criteria are quality, relevance, and performance. Quality is bolstered by using a good award mechanism (e.g., peer review) and by expert reviews of successes and failures. Relevance is improved by planning and prioritization.

The argument of BES with particle physics about ownership of "fundamental" research is not important to outsiders. But, identifying intellectual grand challenges would be a useful product. Materials/chemistry has the easiest case to make within SC, so it should be embraced. Relevance to the energy security mission of the Department should also be embraced, but not overstated or over-promised.

Gates asked Parriott how he perceived energy security now and what the outfall of this situation might be. Parriott replied that he was at the bottom of the food chain and did not have a sense of that. The energy policy was set out by the energy conference in 2000/2001, and perspectives vary district by district.

Johnson asked what role world leadership of science plays. Parriott responded that the NAS cited quality, relevance, and leadership as the goals of science. The administration replaced performance for leadership.

Kohn observed that the war in Iraq has no termination date and is a large part of the budget. Consequently, it impacts every other part of the budget. Parriott answered that the President's second priority is to transform the military and support our troops in the global war on terror.

Moscovitz pointed out that the scientific community is just a lobby group. Every lobbyist says the same thing. He asked what the best the way for science to communicate would be. Parriott responded that, if there were a clear way to do it, people would be doing it already. One of the unique aspects of the hydrogen report is that everything is tied to the real world, especially in calling for additional basic research. Advisory committee reports all sound the same. Recommendations have to be concrete and justified with demonstrable facts.

Cummings stated that, when an advisory committee is tasked to write these reports, it is asked to make them understandable by an educated layman. Parriott said that they should not use the same language as a peer-reviewed publication but should use the same logic. Often, the assumptions are not put down on paper.

Stupp asked if OMB is aware how other countries fund their R&D. Parriott replied affirmatively. A lot of international information comes through the Office of Science and Technology Policy (OSTP) and is called to OMB's attention by them. OMB's budget-setting process has a lot of history, and it is aware about what other countries are doing in science and technology.

Morse noted that other administrations have placed a lot of leadership in OSTP but that that is not how OSTP's role would be characterized now. He asked if OSTP is involved in the shaping of the science component of the budget. Parriott answered that Dr. Marberger is in the room during OMB's budget deliberations. All offices of the Executive Office of the President (EOP) are supposed to be involved in the budget discussions.

McCurdy observed that advisory committees tend to write to a broader audience than just to OMB, they tend to include DOE program managers. He mused that perhaps advisory committees should reconsider who their audience is. The similarities from report to report become deafening. Currently, BESAC has some issues with the core research program. He asked if BES is at a disadvantage trying to sell research and whether it is easier to sell facilities. Parriott said that he was concerned about that issue. Many other players are on the roster. It is tempting to say, "BES builds great facilities; let's let them keep doing that and put our R&D funding elsewhere." There is a way to take care of the research program, but one has to put forward more compelling arguments than just "we need to do more research."

Hemminger noted that Parriott had distinguished between leadership and performance. The United States has been in a leadership position in many areas of science. That is changing now. HEP in the United States is becoming secondary to that in Europe and Japan. ITER is going to be based in Europe or Japan. Japan is leading in nanoscience, also. He asked if the people at the upper levels of OMB can be educated about how serious the scientific community thinks that problem is. Parriott said that, to the degree that one can supply data, one would be better off. If one wants science to advance, advances by other countries should be celebrated.

Morse asked if he meant to say that ownership as well as leadership is not a priority. Parriott replied that, if the nation makes an investment, it should not be for something that duplicates what is being done elsewhere. The leadership has not been presented with the problem as you perceive it.

Hemminger called for presentations from the nanoscience centers and introduced **Robert Hwang** to speak about the Center for Functional Nanomaterials (CFN) at

Brookhaven National Laboratory (BNL). The project is split into building the facility, developing the user base, and transitioning to operations.

These centers are really dispersed laboratories for getting people from various disciplines working together. The CFN site is located close to the National Synchrotron Light Source (NSLS) and was dedicated on April 15, 2005. Bids on construction are due July 1, 2005; award of the construction contract will be made July 31, 2005; notice to proceed will be issued August 21, 2005; construction will start September 2, 2005; beneficial occupancy will begin February 28, 2007; construction will be complete March 30, 2007; CD-4a (initial operations) will commence April 30, 2007; and CD-4b (full operations) will begin April 30, 2008.

The building will contain facilities for nanopatterning (including lithography and complementary capabilities), proximal probes, electron microscopy, theory and computation, ultrafast optical sources, and materials synthesis. The scientific themes of the Center are nanostructured catalysts, electronic nanomaterials, and bio/soft nanomaterials and interfaces.

The Scientific Advisory Committee (SAC) has met once and meets again this summer. It advises the Center on how to develop its major equipment, focusing on spatial analysis, temporal analysis, energy (composition), fabrication, and function.

With the low-energy electron microscope/photoelectron emission microscope (LEEM/PEEM) at the NSLS, electrons interact very strongly with the sample and do not penetrate very deeply into it, and one can do real-time surface imaging of heating and gas dosing. Coupling with NSLS photons allows one to conduct structural-information and other studies.

As part of its jumpstart and user-outreach activities, the Center is holding a series of workshops. A May 2004 user meeting held jointly with the NSLS attracted 300 attendees. A topical workshop on Opportunities in Nanocatalysis will be held in Tarrytown, New York, on October 19-21, 2005, to see what CFN can do to support the scientific community in energy security.

The jumpstart activity received 139 proposals, of which 91 were accepted and 65 have been completed. Of those proposals, electron microscopy made up 50, materials synthesis 12, nanopatterning 32, proximal probes 10, NSLS 30, computation and theory 2, and ultrafast optical sources 2. (There were some overlaps.) A Proposal Review Panel has been established and is operating.

The CFN organizational structure is becoming more defined. Groups are going to be clustered around laboratory facilities and scientific themes. The goal is to foster an integration between the facility and the science people. Staffing is ramping up. The Center has hired user interactions/administrative support personnel (a Technical Outreach Coordinator, User Administrator, and CFN User Safety Officer) and new science/technical staff for the transmission electron microscopy facility (one staff, one technician, and two postdocs), the scanning-probe microscopy facility (leader, one technician, and one postdoc), and soft-materials synthesis (one staff and two postdocs). It has also continued to leverage BNL's existing staff.

El-Sayed asked if BNL was taking proposals now. Hwang answered that they were using existing equipment now and will have electron beam lithography and other capabilities later.

Plummer stated that these nanocenters have to be built on core-research personnel at the host institutions. He put forward three questions for each of the nanocenters to answer: How many full-time equivalents (FTEs) from the core-research program will be transferred? How will damage to the core-research program be avoided? And what independent research will new hires be allowed to do? Hwang replied that BNL had moved the whole microscopy group (ten people) into the center. More of that may happen. The total staff will be about 70 people. New people will also be brought in to do new things. He did not see this as competition but a synergy with the core-research programs. New hires will bring in new research because they will develop new techniques or capabilities and are natural collaborators.

Hemminger observed that one needs to be careful how one blends new staff into these facilities so as not to deplete the core-research staff. One needs dedicated people and not unified loyalties. Hwang responded that there will be people reporting to the directors in charge of the user program. The number of new people will be a large fraction of the total staff. Hemminger asked what the jumpstart funding is. Hwang replied, $1.5 million per year from BES.

Hemminger asked **Paul Alivisatos** to report on the Molecular Foundry at LBL. Alivisatos commented that the premise of the previous questions is not correct. The obligation on the Foundry staff is that they conduct basic research that comes back to serve the user community. A method to make hollow nanoparticles was discovered at LBL. Researchers at Lawrence Livermore National Laboratory (LLNL) picked up on this capability, and the Foundry developed a means to mass produce hollow noble-metal nanoparticles from which a “spectroscopic ruler” was developed. Loops of interactions like this are expected from the ongoing research programs.

The mission of the Molecular Foundry is to provide a national facility to enable interdisciplinary nanoscale science and engineering by fostering, developing, and disseminating methods and knowledge for the patterning and control of matter on the nanometer scale.

The Foundry has six user facilities (types of fabrication): imaging and manipulation, nanofabrication, theory, inorganic structures, biological structures, and organic structures. The group leaders of these facilities will provide the primary intellectual direction along with their associate group leaders. Each group will have a lead scientist, scientists, and technicians. It also has an advisory board. There will also be postdocs, graduate students, and undergraduate students. A Foundry Fellows Program will start soon. The Biological Nanostructures Group plans to have mammalian, plant, and microbial cell culture; ribonucleic acid (RNA) preparation; etc. and will hire a staff scientist, senior technicians, and a staff scientist/cell biologist. The Organic Nanostructures Group will conduct the synthesis of building blocks, small libraries, electroactive polymers, and light-harvesting materials. The Imaging/Manipulation Group will primarily focus on scanning probes (atomic-force microscopy, AFM) for studies in air and controlled atmospheres, electron microscopy with in situ manipulators and electrical probes, and new optical systems for imaging and fluorescence studies at the single-molecule level. The Nanofabrication Group will perform advanced lithography (e-beam lithography and soft lithography) and process integration; the Foundry will hire specialists in these areas. The Inorganic Nanostructures Group will study nanotube synthesis, nanowire synthesis, and colloidal nanocrystal growth; it has advertised for some of these positions already. The Theory Group has a variety of capabilities it wants to bring forward.

Foundry proposals have been received from across the country. Of the 54 proposals received, 36 were approved, 14 were rejected, and 4 are still under review.
The Foundry has also forged some strategic partnerships. Intel has sent three scientists to the Foundry already. That company would like to keep some scientists there on a permanent basis. Five strategic partners are expected at the Foundry eventually. Currently, 66% of the user affiliations are with universities, 20% with government laboratories, and 15% with industrial organizations. The accepted proposals also included requests for use of the ALS (5), the National Center for Electron Microscopy (NCEM) (14), National Energy Research Scientific Computing Center (NERSC) (4), and affiliated laboratories (16).

The Foundry has also been conducting Nano*High on Saturdays with 350 to 400 high school students attending.

Johnson asked if there was support for tenure-track professors to come to the Foundry. Alivisatos replied that the facilities are there for them to use, but the Foundry does not fund them.

Gates asked who coordinates the use of the various facilities at LBL. Alivisatos answered that one proposal goes to all facilities. If it is approved, then access to all the needed facilities are made available. Gates asked how one moves samples around to avoid contamination. Alivisatos said that there was no global policy.

Stupp asked what motivates the user to use the Foundry's capabilities. Alivisatos replied that a successful project is one in which a capability is developed at LBL and someone comes in from the outside to use that technique or process. Users are motivated to use existing capabilities at the Foundry to save the time of developing the capability on their own. One develops a lot of capabilities, and some of them actually work.

Hemminger declared a break at 3:49 p.m. and called the members back into session at 4:04 p.m. to hear **Julie Phillips** and **Toni Taylor** describe the progress of the Center for Integrated Nanotechnologies (CINT), which is located at Sandia National Laboratories (SNL) in Albuquerque and at Los Alamos National Laboratory (LANL). Phillips began the presentation.

Phillips began the presentation. At the CINT at Sandia, about half the personnel will be new hires. At LANL, the portion of new hires will be lower. It is expected that several capabilities of the core program will be moved into CINT. The research portfolio of new hires will include collaboration with the users.

CINT is a unique partnership between two national laboratories, SNL and LANL, that makes extensive use of videoconferencing. The Memorandum of Agreement calls for management teams to be split between the two laboratories. It has a Proposal Review Committee and a Scientific Advisory Committee (SAC). It has a Core Facility through which users will enter and gateways to SNL and LANL. Sandia is interested in using the Microelectronics Laboratory and Microsystems and Engineering Sciences Applications (MESA), and LANL is interested in biosciences, the National High Magnetic Field Laboratory, and the Lujan Neutron Scattering Center. Both laboratories have capabilities in synthesis, characterization, and theory.

Thrust areas include nanoelectronics and nanophotonics, complex functional nanomaterials, nano-bio-micro interfaces, nanomechanics (understanding the mechanical behavior of nanostructured materials, and theory and simulation (which crosscuts everything else).

The Core Facility in Albuquerque will have 95,200 ft^2 on 20 acres just off Kirtland Air Force Base. It will host 150 occupants with synthesis laboratories, low-vibration characterization laboratories, and a Class-1000 clean room. It is being built in stages and is about 50% complete. The Sandia Gateway uses an existing building. The Los Alamos Gateway building is under construction. It will have 36,500 ft^2 and house 50 occupants. It will have synthesis and characterization labs, a computational graphics room, and a computer laboratory. Buildings are on schedule for completion in November 2005. Operations will begin in April 2006. Construction will be complete in June 2007.

A lot of special equipment will support the research at these facilities. The Sandia Gateway will have atom-tracking scanning tunneling microscopy (AT-STM), interfacial force microscopy (IFM), chemical preparation of oxides, Langmuir-Blodgett film, and microfluidics. The Los Alamos Gateway will have near-field scanning optical microscopy (NSOM), AFM, scanning electron microscopy (SEM), a nano-indenter, an ultrafast laser, and a computer cluster. For the 37 items of special equipment costing $11.5 million, 7 contracts have been placed, and 11 contracts are being drawn up.

For the Core Facility, the building was 54% complete at the end of April, it is on schedule, and the schedule float prior to CD-4a is 12 weeks. For the gateways, the building was 43% complete at the end April, it is on schedule, and the schedule float prior to CD-4a is 12 weeks. For the special equipment, 49% of the procurements are committed, and procurement is ahead of schedule. The overall project is 53% complete, and the overall contingency is more than 20%. Facility completion is defined in extensive commissioning plans, and operations will not start until the life and safety systems are approved.

The laboratory-by-laboratory commissioning process includes

- A subject-matter expert (SME) being identified for each laboratory;
- Procurement and acceptance of special equipment (lab SME interfaces with equipment SME);
- Temporary integrated work document (IWD) generation (LANL) or Preliminary Hazard Analysis (PHA) (SNL);
- Building commissioning;
- Installation of all necessary administrative and engineering controls for safety considerations;
- Installation of the special equipment including lab furniture, utilities, training, acceptance, or other special considerations;
- Completion of the Management Self Assessment (for LANL);
- Completion of the Readiness Assessment for both laboratories; and
- Acceptance for operation by the CINT Project Director; DOE; laboratory environment, safety, and health (ES&H); facility management; and line management.

Toni Taylor took the floor. The promised operational laboratories at CD-4a in April 2006 are

- At the Core Facility, two chemistry laboratories; a chemical diagnostics laboratory with Fourier transfer infrared (FTIR) analysis, ellipsometer, and UV-visible; and a scanning-probe laboratory with AFM.

- At the Los Alamos Gateway, a spectroscopy/novel optical scanning probe laboratory with an ultrafast laser system and a thin-films laboratory with a spectroscopic ellipsometer.

Hazards to be addressed include Class-4 lasers and chemical operations in hoods. There will be a phased commissioning of laboratories after CD-4a.

In terms of CINT staffing, management estimates there being 30 staff and technologists and 10 postdocs. It is in the process of identifying CINT scientists to work in the three facilities and expects to have a combination of dedicated and matrixed scientific staff.

At LANL, CINT resides in the Strategic Research Directorate and reports to the Materials Science and Technology Division leadership. At Sandia, CINT is located in the Science and Technology Division and reports to the director of the Energy Science Division and then to the director of the Physics, Chemistry, and Nano Sciences Center.

At CD-4a, CINT staffing consists of the management team (Director, Associate Director, Chief Scientist, and User Program Manager), additional support (user administrators, building managers, ES&H personnel, and secretarial support), thrust leaders and alternates, assigned SMEs, and two postdocs. It is expected that approximately 75% of the CINT scientific staff will be identified before the start of normal operations.

Sandia is currently hiring externally in specific areas: a TEM expert, an integration laboratory coordinator, and microelectronics integration. LANL is hiring for positions at the Core Facility; the strategy is to hire current postdocs working in nanoscience into staff positions so that there is a real connection to LANL.

CINT has had two rounds of successful jumpstart projects (in 12/03 and 12/04). 188 proposals were submitted, and 65 projects were supported from 40 institutions in 22 states and 3 foreign countries. The selection process was based on an external review committee; the first round was judged by the SAC, and the second round by current users. Proposal success was limited by resource availability. For the third (and final) jumpstart round, 70 proposals were received on May 2, 2005, and the review process is under way.

To engage users in the jumpstart process, three workshops were held. The first had 200 attendees and focused on construction and special equipment planning and included science-thrust discussions. The second had 194 attendees and focused on nanoscience integration challenges and outreach and included a Jumpstart Capability Expo. The third had 218 attendees and focused on user science talks and Discovery Platforms™ and included a Jumpstart Capability Expo.

CINT also provides access to national user facilities, such as the Los Alamos Neutron Science Center, National High Magnetic Field Laboratory, Combustion Research Facility, MicroElectroMechanical Systems, Ion-Beam Materials Laboratory, and Scanning-Probe Microscopy Facility.

One of the CINT Discovery Platforms™ is the modular microlabs for nanoscience, leveraging capabilities at SNL and LANL in mechanics, optics, electronics, and fluidics.

In the user program in normal operations CINT will implement lessons learned from the jumpstart experience, explore multiyear user projects, address integrated-training at SNL/LANL and improving foreign national access, develop focused calls for user access, and promote its Discovery Platforms™.

So, CINT is becoming a reality! The project is on budget and on schedule for a CD-4a in April 2006. The management team is in place. It has a user program that was launched by a strong jumpstart program. A transitions-to-operations plan and scientific staffing are under way.

Hemminger asked where the thrust leaders came from. Toni Taylor replied that half came from Sandia, and half from LANL. Normal operations have not started, so postdocs are still being brought into the Center. This is the transition period. The Center will be their home when they have made the transition, and they will form a group at the Center.

Flynn asked about the flow of scientific effort and whether new people will be hired into the old positions that are vacated by those moving into CINT. Toni Taylor answered that they will leverage their expertise into the Center. Sometimes their old positions will be filled by new hires and at other times, they will not. Flynn asked about the long-range plan. Toni Taylor responded that it will vary case by case. Sometimes they will move over entirely. Sometimes they will be part-time in the Center.

Kathleen Taylor asked if this nanoscience integration unique was to CINT. Phillips answered, yes. The Center is doing what Sandia does in microelectronics and is bringing it down another three orders of magnitude.

Hemminger introduced **Derrick Mancini** to describe the Center for Nanoscale Materials (CNM) at Argonne National Laboratory (ANL).

The CNM is to provide the nation with a state-of-the-art user facility for the development and dissemination of techniques for the design, synthesis, characterization, and theory of materials at the nanoscale; bridging the materials; chemical, biological, and computational sciences; and advanced characterization tools.

The CNM will have six major themes: bionanocomposites, electronic and magnetic materials and devices, nanophotonics, theory and simulation, lithography and nanopatterning, and X-ray nanoprobe.

The existing scientific theme leaders are all current ANL employees, except one; all are dedicated to and involved with the Center.

The highlight of the CNM is the production and development of energy-related nanomaterials for light harvesting, friction and wear reduction, ultrastrong magnets, ultrafast information processing, and advanced catalysis.

It is a partnership with the State of Illinois, which gave funds for construction of the building. The CNM building will be complete in the winter of 2006; the facility will be complete in the fall of 2007. It will have 85,000 ft^2 of laboratory and office space integrated with the Advanced Photon Source (APS). Construction is more than 50% complete, and the building will be ready for occupancy in March 2006.

One unique piece of equipment is the hard X-ray nanoprobe at the APS. Collocating the instrument with the APS will be a major advantage for the CNM. X-ray imaging will be able to be done by three modes: scanning probe, coherent diffraction, and full-field imaging.

The Nanoprobe Beamline saw its first light on March 15, 2005.

The wide range of tools at the CNM will enable science through nanosynthesis, nanopatterning, and nanocharacterization as well as theory and simulation.

Long-lead-time items (e-beam lithography and near-field scanning optical microscope) have been ordered and acquired.

All the people involved in the Center are currently matrixed and will make a transition to the Center when it opens. The CNM reports to the ANL Associate Director for Physical, Biological, and Computing Sciences. The building is on track for acceptance in April 2006, and the CD-4b will be determined by the critical path being completed by July 2007.

The CNM user mission is to provide a new type of DOE facility for the design, synthesis, characterization, and theory of new nanomaterials and novel nanodevices with open access for all users.

The jumpstart user program's goal is to build a scientifically vibrant, productive, and growing user community by the time the CNM becomes fully operational in the fall of 2007. Implementation is being carried out by using Argonne scientists' studying nanoscience accepting CNM users into their laboratories. Jumpstart funds were used to hire nine CNM postdoctoral fellows.

The Early Access User Program has registered 149 users, 66 for the CNM only and 83 for the CNM and other ANL facilities; there is a great deal of synergy between CNM and ANL. Fifty proposals were accepted, and 25 of those have been executed. These proposals represent 34 universities, 5 industrial companies, and 3 government laboratories. Proposals were received from 15 states and 11 foreign countries.

The criteria for success for the CNM are high-impact science and user service and satisfaction. The challenge is to balance programmatic research at the Center with user support. The CNM has a directorate structure with six functional groups. The group leaders' responsibilities are to ensure user productivity and satisfaction in a safe environment; execute innovative, internationally recognized research in the area of bionanocomposites and nanoscience; and develop and implement world-class instrumentation for nanoscience.

The projected staffing includes 8 leaders, 8 administrators, 6 lead scientists, 12 staff scientists, 20 technical staff, 15 postdocs, and 2 visiting fellows. Some (though not most) scientific staff may have joint appointments with divisions and regional universities.

Recruiting plans call for every position to be competed; a hiring committee to make recommendations to the CNM Director; positions to be based on a bottom-up exercise for technical staffing needs; and advertising for positions to be started this summer, looking for world-class science candidates as well as outstanding technical candidates. The first hires will be full-time ES&H, clean room manager, and computer support personnel.

In the transition to operations, equipment will be made available to users as quickly as possible. The project plans a phased-readiness approach. A Transition-to-Operations Team (TOT) will be responsible for verifying that the CNM building has been constructed and the Nanoprobe Beamline and technical equipment has been installed so that they fulfill all requirements and specifications. The CNM will be ready for start of full operations when the criteria for CD-4b are met:

- All technical equipment accepted for operation and equipment successfully tested for planned modes of operation.
- All required building utilities needed for operation of the technical equipment are in the final configuration.
- Required safety systems are fully operational.
- Training for CNM staff to operate and maintain the equipment is completed.
- All required documentation has been provided.

To that will be added the Integrated Facilities Model at Argonne, providing one-stop user access to all facilities at Argonne. As a result, will CNM provide a new kind of DOE facility for materials.

Plummer noted that the presentation had mentioned 16 or 20 theme leaders and 8 group leaders and asked how they differed. Mancini replied that the theme leaders are group leaders. Plummer asked how they were going to compete positions that are already filled. Mancini answered that some personnel might take on other responsibilities, like lead scientists.

El-Sayed asked how the proposals were selected. Mancini responded that it was done competitively. El-Sayed asked what areas were needed. Mancini replied that there are not enough data yet to answer that question.

Moskovits stated that he counted about 120 new hires in the field and asked if anyone had thought about coordinating this hiring. Moskovits said that the different nanoscience directors have discussed this. The CNM is also competing with other centers and industry. Moskovits asked what would happen if one could not find the proper expertise. Mancini said that they were confident that they could find the proper personnel. A hiring plan has been developed with the APS, but an eye will have to be kept on the availability of expertise.

Hemminger introduced **Linda Horton** to discuss the progress of the Center for Nanophase Materials Science (CNMS) at ORNL. It is located on the SNS campus at ORNL and is physically connected to that facility.

The Center for Nanophase Materials Sciences building is on the SNS campus. CNMS is going to integrate nanoscale science with three synergistic research needs: neutron science (offering an opportunity to assume world leadership using the unique capabilities of neutron scattering to understand nanoscale materials and processes), synthesis science, and theory/modeling/simulation (to stimulate U.S. leadership in using theory, modeling, and simulation to design new nanomaterials).

CNMS research is organized under seven scientific themes that address grand challenges in nanotechnology: Macromolecular Complex Systems; Functional Nanomaterials; Nanoscale Magnetism and Transport; Catalysis and Nano-Building Blocks; Nanomaterials Theory Institute: Theory, Modeling, Simulation; Nanofabrication Research Laboratory; and Nanoscale Imaging, Characterization, and Manipulation.

The CNMS conducted a peer review of the initial proposal in the summer of 2001. Beneficial occupancy and CD-4a occurred on April 27, 2005, and the CNMS Inaugural User Meeting was held on May 23-25, 2005. User research will begin in the CNMS building in October 2005. Completion of the project (CD-4b), including installation of all equipment, will be completed in September 2006.

The Center has a four-story laboratory/office building and a clean room. Each floor of the CNMS has a technical focus. The ground floor has the clean room and sensitive instrumentation. Level 1 has the laser laboratories and other heavy equipment. Level 2 hosts catalysis, soft material characterization, and theory offices. Level 3 has wet chemistry laboratories and more theory offices. The laboratories are in the back of the building, and offices are in the front; bridges have interaction space.

The CNMS clean room has Class-1000, Class-100, and Class-100,000 rooms and an electromagnetic-, vibration-, and acoustic-sensitive area.

The direct-write electron-beam lithography (DWEBL) system is in the country in air-conditioned storage awaiting completion of construction. The focused ion beam/scanning electron microscope (FIB/SEM, a dual-beam system) has been delivered.

The calls for proposals elicited an enthusiastic response. About 135 proposals were received from 24 states. These included proposals from 96 universities, 8 from industrial organizations, 5 from other government laboratories, and 7 from foreign countries. In FY04, 41 proposals were selected on the basis of external peer review; in FY05, 32 proposals were selected.

The Nanomaterials Theory Institute (NTI) is sponsoring Computational Nanoscience Focused User Laboratories (NanoFocULs). The first NanoFocULs were conducted in mid-August 2004 in conjunction with ORNL’s Center for Computational Sciences (CCS) and its Joint Institute for Computational Sciences (JICS). These NanoFocULs provide access by user application for up to a year.

Polymer and carbon nanotube synthesis and characterization were a major component of the jumpstart program. Research projects used shared user equipment at ORNL. A downloadable proposal form has been developed. Proposals are peer-reviewed by an entirely external Proposal Review Committee with 17 members who are experts in each research area. Successful proposals are coordinated with other user facilities at ORNL.

At the inaugural CNMS user meeting, held May 23-25, 2005, more than 280 attendees represented about 50 universities and nearly 20 industrial participants. A lot of one-on-one interaction occurred on modes of access, and the Users Executive Committee was seeded. Proposals are due July 22, 2005, for the current call for proposals.

During the past few months, the Center has seen expanded integration activities with the SNS and High-Flux Isotope Reactor (HFIR) and the broader neutron-scattering community. The goal is to take advantage of opportunities to apply neutron scattering to nanoscience R&D. White papers are being prepared that will be the basis for strategic planning that will focus on synergies of collocation with other key laboratory user facilities. The week after this BESAC meeting, it will hold a National Nanotechnology Initiative (NNI) workshop on X-rays and Neutrons: Essential Tools for Nanoscience Research.

In anticipation of FY06 operations, the SAC has been expanded. As part of the transition to operations, CNMS has been established as an ORNL division within the Physical Sciences Directorate. The management team has been announced, a finance officer has been appointed, and the Operations Manager position has been advertised. National advertising, interviewing, and hiring are under way for positions for the research staff and postdocs (10 initial positions were advertised and hired under the jumpstart program). The Center has been integrated with other ORNL divisions since the beginning. A Coordination Committee is in place that will ensure integration of equipment and staff.

The management council will avoid harm to the core research program. One cannot hire research postdocs without expecting them to do research. Staff development is critical. The employees have to have a career path. Part of the CNMS salaries goes toward postdocs’ individual research. Divided loyalties and stovepipes have to be balanced. About half the staff will be new people. CNMS will be ready to welcome users to the new facility in October 2005. The building is completed, and installation of equipment is under way. Staff moves begin in June. Hiring is under way, and national searches are being conducted for staff and postdoctoral fellows. The jumpstart user program has established both the application and the review processes. A User Executive Committee has been seeded. An expanded SAC is in place, as is the management and scientific leadership team. Integration and synergies with ORNL divisions that are the home of the basic materials and chemical sciences research is critical, and those relationships will continue to be nurtured.

Stupp stated that everybody had done a great job on presenting the progress of the centers and commented that the centers look much more similar than was expected. He asked if there were a need for an intercenter organization that looks at coordination and overlap. Hemminger said that the center directors get together regularly and discuss such issues. Dehmer commented that (1) each is collocated with a unique facility and (2) the facilities generally will not voluntarily coordinate; some external urging will be necessary to get them to coordinate their strategic plans; that will evolve during the next several years.

Morse commented that the draw of the jumpstart programs seemed to be largely regional. Horton suggested that the regional aspects of the light sources probably drove that situation.

Hemminger commented that, if a new-hire spends only 40% of the time on his or her research, the research will not get done. Horton observed that most of the new hires have leveraged their work with users to a good publication history and gotten good leads and letters of recommendation for jobs elsewhere.

El-Sayed noted that all of the centers have to house some basic instruments, but the people and research interests will have different emphases. Hemminger called for public comment. There being none, he adjourned the meeting for the day at 5:48 p.m.

Tuesday, June 7, 2005

Chairman Hemminger called the meeting to order at 8:31 a.m. and reviewed the agenda. He introduced **Richard Hilderbrandt** to present the response of the Chemical Sciences, Geosciences, and Biosciences Division to the BESAC report *Opportunities for Discovery: Theory and Computation in Basic Energy Sciences.*

That report recommends increased support for theory and computation to enhance and complement the substantial BES investments in experimental science and facilities and additional investment to capitalize on recent investments in tabletop science and laboratory facilities (such as the ALS, APS, SNS) and nanotechnology centers. It points out that theory and computation are essential to provide a fundamental understanding of the exciting new frontiers that are emerging in nanoscience, ultrafast science, quantum control and information, biomimetics, and other areas. In addition, DOE is about to embark on ultrascale computing that will enable many new advances. A number of areas of opportunity were identified, producing a list that was not exhaustive but included exciting areas for support.

The Subcommittee recommended that BES should become strongly engaged with ASCR to ensure that large amounts of time on terascale capacity facilities are available to the BES scientific community. BES should consider supporting some of this capacity with local institutional computing, while ensuring that demand at the higher end of computing power is supplied by larger facilities. BES has started to work with the ASCR program. However, at NERSC alone, the Division's requests for advanced scientific computing have increased from 3.5 million to 6.5 million cycles. At the present time, the availability of DOE computing resources is seriously impeding the progress of research. The current demand exceeds the supply of available resources by factors of 3 to 5. There is good cooperation between BES program managers and ASCR on the issue of computing resources. BES is already supporting clusters in conjunction with laboratory and academic research programs, investments that have been made over the years.

The Subcommittee also recommended that BES should support the development and maintenance of scientific codes in the disciplines in its portfolio, just as it now funds the development of shared beamlines at its experimental facilities, thereby creating new scientific capabilities for the nation. Such investments will also be critical in allowing BES researchers to take full advantage of the capabilities of DOE's leadership-class computing facilities. The questions that arise include: Will BES researchers be ready for leadership-class computing facilities? There are two parts to this question:

- Has the community identified the grand-challenge applications?
- And what kinds of software can use these machines?

Two projects were a good start: SciDAC [Scientific Discovery Through Advanced Computing] and TMS [Theory, Modeling, and Simulation] in Nanoscience. They focused on the development of software tools. The community now needs to identify for DOE what the strategic needs are. DOE also needs to know what the correct support model is. Is it similar to beamlines and endstations? Is it finite-duration development projects with milestones and deliverables? Is it the Computational Material Science Network for porting to other users? Or is it a model similar to the U.K. Collaborative Computational Projects (CCPs)?

Other issues that will need to be considered in responding to this report are

- What is the proper balance between single-PI funding and large-scale collaborative research projects?
- What is the proper balance between investments in university research vs. national laboratory research?
- What is the proper balance between support of basic research and investments in research infrastructure (software development)?

Within the current budget constraints, it is unlikely that DOE can afford to issue a solicitation in this area.

In 2004, Bill Lester of LBL was given 1 million hours of NERSC time to investigate photosynthesis. In 2005, Jacqueline Chen was awarded 2.5 million hours of NERSC time to develop a 3-D simulation code of turbulent combustion, from which was learned a great deal about the temperature effect on inhomogeneities under homogeneous charge compression ignition (HCCI) conditions.

In FY05, the Division set aside $1 million to fund new starts in theory and computation. With that reserve, seven new theory and computing starts were funded between the Chemical Physics and the AMOS programs. Within Chemical Physics, 36% of the funds are spent on theory and computation; in AMOS, it is 22% of the funds. The Division will set aside a $1 million reserve again in FY06 for the same purpose. The Division will be guided in its future support of theory and computing by the recommendations in this subcommittee report.

McCurdy called attention to the fact that the Subcommittee concluded that most work comes from between a few hundred and a thousand processors, which is larger than the usual cluster. If there are only going to be 6 or 10 large projects on the large machines at Oak Ridge, to what degree does that address the needs of scientists? The connection of theory with experimental facilities was not mentioned. There is a particular urgency associated with such facilities as the LCLS and the other ultrafast experimental capabilities. Hilderbrandt agreed; it comes down to where the funds are and how much is available.

Hemminger asked what the breakdown was between universities and national laboratories in the seven new starts. Hildebrandt replied, one national laboratory and six universities. Hemminger asked what his thinking was about that distribution. Hildebrandt responded that these seven came about from proposal pressure to support theory. A lot of proposals were reviewed, and those seven emerged from that pack. One does not want to arouse expectations that one cannot meet, but one needs to recognize the demand that exists. Some planning should be done to see how those people fit in. He did not know who should do that planning. Stevens observed that proposals in theory development have not had a difficult time getting funding. This report brought home that there is an infrastructure issue that needs to be addressed. Some individual or group needs to push for the infrastructure needs to be addressed. The future support of computational science at the facilities would be looked on favorably.

McCurdy stated that, if one wants this process to be proposal driven, one will have to find theoreticians who are willing to collaborate with experimentalists. Stevens said that the Department cannot issue a solicitation without money in the bank. In the future, theoretical and computational science will play a big role, and there will be solicitations. Dehmer pointed out that the nanocenters are built on a theoretical/experimental interaction model. That is not the model that the light sources started with. These institutions will have to move to a culture where the owner of a facility fosters such cooperation. That is a major culture shift. BES is struggling to optimize what funds it has. Hemminger asked if the LCLS were getting encouragement to foster such interaction. Dehmer responded, yes.

Kirby said that she appreciated that the hours for BES were doubled but encouraged BES to keep up the pressure to further increase that allocation.

Cummings asked if these new starts would compensate for the budget cuts and phase-out of the Chemical Engineering Program that had several computer science grants. That program was forward-funded as much as possible to buy the PIs time to make a transition and provide continuity. Substantial cuts across the board should not be imposed.

Kohn said that to say that there is a factor of 3 to 5 excess demand for computing resources does not say very much. This argument is about *theory* and computation. For BES, the most valuable use of high-end facilities is to develop exciting, new concepts (e.g., the development of the renormalization group, the Carr-Parrinello method, and the development of quantum Monte Carlo). Once new concepts are developed, there are codes, and you can run large projects. They are brilliant conceptual advances with very useful applications. When you choose between proposals, there should be a bias toward proposals that include some conceptual innovation rather than proposals that just work out something practical with well-set concepts. There are some very important experimental regimes: highly excited states, time-dependent phenomena, and high intensities of radiation. These regimes require a new conceptual framework and the connection between theory and experimentation that McCurdy referred to. These good insights have to be turned into algorithms that can be used to investigate problems.

Hemminger asked **Harriet Kung** to present the response from the Materials Science and Engineering Division.

Dramatic progress has been made in theory and modeling, including density functional theory (DFT), ab initio molecular dynamics, quantum Monte Carlo, dynamical mean field theory, etc.

Materials science needs large-scale computing to make advances. The new frontiers are the ultrasmall and ultrafast sciences, quantum-level control of matter and information, and infusion of biological approaches and techniques. New structures allow the manipulation of matter at the nanoscale, which will enable revolutionary advances and provide unprecedented information about structure and properties. In addition, new computational capabilities enable 1-million-atom studies.

The Division's current portfolio has four parts: (1) electronic structure, (2) a strong emphasis on new materials (nano and other low-dimensional structures, self assembly, and pattern formation are hot topics), (3) surfaces and interfaces (especially patterns of crystal growth and defects in solids), and (4) a strong emphasis on the development of computational techniques.

There is a strong correlation between this portfolio and the recommendations of the report (*Opportunities for Discovery: Theory and Computation in Basic Energy Sciences*) in such areas as nanoscale science, biomimetic materials and energy processes, correlated electrons in solids, excited electronic states, magnetic spin systems and single-electron devices, defects in solids, etc.

Some examples of what the Division already supports include

- Simulations of self assembly of gold nanoparticles, in which simulations have explored the formation of nanocrystals composed of passivated 3-D gold clusters, which are building blocks for constructing nanomachines.
- Studies of theoretical strength and deformation in nanostructured metals to determine how nanomaterials achieve their strength, where atomistic simulations are being used to gain insight on the unit processes involved in deformation.
- Theory and computation that have helped gain new ideas that underlie experimental interpretations.

A goal of the Division is to advance frontiers in computational materials science through strong coupling of table-top experimental efforts and bigger BES user facilities to benchmark theoretical models and to guide experimental designs. The bridge is theory and computation.

The Computational Materials Science Network (CMCN) is a cooperative research team designed to advance frontiers in computational materials science by assembling diverse sets of researchers committed to working together to solve relevant materials problems that require cooperation across organizational and disciplinary boundaries. Currently, the Division supports several such teams, and a new team on multiscale studies of formation and stability of surface-based nanostructures is starting up. These teams of disparate researchers produce a great multidisciplinary synergy.

The Division is also supporting

- A visitors program designed to attract leading scientists with expertise that complements that available at the host institutions;

- The growth and expansion of theoretical science by catalyzing interdisciplinary interactions and collaborations with experimentalists as well as theorists at the host institution; and
- The enabling of mobile, well-focused, and highly interactive research through workshops and other mechanisms.

The Division recognizes many outstanding materials sciences issues could benefit considerably from high-end computing, such as access to high-end computer resources and reliability in time allocation over a period of several years. The Division is pursuing options to seek further resource allocations within SC/ASCR, leverage resources at other computer centers (e.g., NSF centers), expand DOE centers, and provide additional clusters. BESAC could help allocate resources effectively in several endeavors.

The Division has a good history in supporting software as a shared research infrastructure, as evidenced by some current efforts in algorithm and technique development: hyperdynamics and other multiple-time-scale techniques, the Geometric Cluster Algorithm for complex fluids simulation, and the routine Linear Expansion of Geometric Objects (LEGO). There will be compelling future needs to develop new algorithms and codes for general use at DOE's leadership-class computing facilities in the Division's research portfolio.

New avenues to computation need to be supported, such as spintronics (dissipationless spin currents) and quantum computing (magnetic molecules and entangled states).

To summarize, in theory and computation, the Division needs to

- increase support for investigators at universities and national laboratories, particularly in nanoscience, correlated electrons systems, defects in solids, and electronically excited states;
- provide additional computer clusters;
- continue to encourage theorists and computer scientists to work with facility users and other experimental efforts;
- expand collaborative efforts;
- enhance usage of high-end computers;
- support the development of new algorithms and codes for general use; and
- support research in new forms of computing.

A bright spot is that the Division FY06 budget includes an increase of $3 million for theory and computation in nanoscience.

The challenges in theory and computation are to build a "properly balanced" program under resource constraints and maintain a coherent basic unity of theory, computation, and experimental activities. The investment strategies in theory and computation are to seek close coupling with nanoscience, influence BES user facilities to enhance support for theory and computation, expand efforts through new funding opportunities (e.g., the Hydrogen Fuel Initiative), and contribute to and take advantage of BES strategic growth areas (i.e., ultrafast science and energy-security research).

She thanked the Subcommittee that produced the report for a document that will guide theory and computation activities for years to come.

Hemminger said that SC is missing the boat in not taking advantage of National Nuclear Security Administration (NNSA) computational resources. The people at those laboratories seem welcoming. He asked if she had looked at this issue. Kung replied, no, although LLNL is trying to separate the domains of access. The Division will pursue such opportunities as they present themselves. Hemminger encouraged BES to do that.

El-Sayed suggested having a special program on surface properties. Kung agreed with the importance of the theory of surface properties and effects and said that it should be a core interest.

Kohn noted that one can also turn it around. There is a lot of work done on rough surfaces and those with defects. Nanoparticles provide an opportunity to understand these properties and effects.

Kirby asked how the search for additional computational resources is going. Kung said that BES's requests are being heard, but one cannot let up on the pressure. Kirby said that access to leadership-scale computing seems to be closed. Kung said that BES is working on that access. One way would be to define "grand challenges" differently and to diversify the types of computing resources used.

Cummings asked if Materials Science is planning to participate in the next round of SciDAC activities. Kung replied that the Division is ready to participate in any new SciDAC activities.

Kohn pointed out that excited states can be (1) one or two electrons or (2) many electrons. The two situations are very different, and the spectroscopic way of looking at the problem becomes useless with many electrons.

Hemminger initiated a discussion of the new charge to the Committee to conduct a Grand Challenges Workshop. Plummer said that the greatest challenge is saving Planet Earth from the ravages of the human race. Kathleen Taylor suggested adding "through BES."

Stupp noted that this charge was written by a physicist and it overlooks life sciences issues and perspectives.

Moskovits said that people tend to extrapolate into the future without knowing all the derivatives. He said that he would like to hear people muse about

- the interface between the inanimate world and life (it has something to do with energy),
- what can be computed with confidence and what cannot,
- genetic modification in the service of energy, and
- improving on 1 billion years of evolution.

El-Sayed worried that producing a report (that will be interpreted as guiding DOE funding) in a short time is disturbing. Hemminger said that he hoped that the report would be prescriptive. El-Sayed observed that the answers received will depend on who is invited; the report will reflect the participants.

Richards noted that weak forces are what make biology work and produce self-assembly. The biological and the medical worlds can be transformed by the simulation and understanding of weak forces.

McCurdy stated that Orbach seems frustrated in stating with conviction what the big questions are. Advisory committees tend to make lists, not put together the whole mosaic that would allow one to understand the big picture. Dehmer noted that other fields are thinking about the big questions because they have had difficulty explaining why they need funding [e.g., the International Linear Collider (ILC)]. BES has an analogous problem: thousands of PIs, each of whom is working on a piece of the puzzle, not the whole puzzle. The Grand Challenge questions are grander than what is dark matter or dark energy. If one is too successful in selling, say, energy security, someone may say "take the money you now have and apply it to energy security." One cannot abandon fundamental science.

Kohn commented that he would like to relate the charge letter to his experiences at Bell Laboratories. The grand challenge to Bell Labs was to make the telephone system better. Bell Labs carried out its mission successfully, largely because it had such a depth of talent and interest. The term "energy security" does not occur in this charge letter, and the nation cannot afford to ignore energy security.

Hemminger suggested that the Committee should not take this letter literally but should place it in context.

Morse stated that Kohn had just articulated the challenge needed: to articulate the overarching concerns that drive all BES science.

Greene stated that this report offers a great opportunity. Superconductivity should be in here. It also has to address the basic science needed to save the planet from humanity.

Gates said that society has lots of energy resources and the temptation to use them is great. What will get society off that path? We as a society ought to be able to do better. Biology shows we can. We should be able to control molecules with such subtlety that we can make fuels and eliminate pollutants. The question is, "With what molecular assemblages?"

Stupp noted that many of the great ideas are from biology. How do you do replication? This would be a way to make highly sophisticated structures to do the tasks that need to be done. Dynamic self-assembly is an unknown world and leads to great functionality. He suggested that science needs to think about how these networks evolve. BES might tap into the people who have thought about these networks. This workshop needs a lot of homework and needs to focus on fewer problems to be useful.

Moskovits said that BESAC should go forward with this workshop but that the Committee members do not need to think up all the themes here. A committee is needed to do that.

Cummings suggested "how to understand nature's energies" as an overarching theme.

Hemminger said that an appropriate method may be to put together a small (10 or so members) subcommittee to draw up a plan forward; these members do not necessarily need to be BESAC members. He asked for suggestions for people to be on such a subcommittee.

The Committee's members will be polled in the near future for possible dates in early September for the next meeting.

Hemminger opened the floor to public discussion. Hodgson commented that the Biological and Environmental Research Advisory Committee (BERAC) used the term "to life" in a title and found that that term should have been avoided.

There being no other public input, Hemminger adjourned the meeting at 10:48 a.m.

Respectfully submitted,
Frederick M. O'Hara, Jr.
July 15, 2005
Revised August 8, 2005