Minutes for the
Basic Energy Sciences Advisory Committee Meeting
February 25-26, 2003
Doubletree Hotel, Rockville, Maryland

BESAC members present:

Nora Berrah
Collin Broholm
Philip Bucksbaum
George Flynn
Laura Greene
John Hemminger
Eric Isaacs
Anthony Johnson
Walter Kohn
Gabrielle Long
Bradley Moore, Vice Chair
Martin Moskovits
Ward Plummer
John Richards
Geraldine Richmond, Chair
Richard Smalley
Joachim Stohr
Samuel Stupp
Kathleen Taylor
Rudolf Tromp
Mary Wirth

BESAC members absent:

Patricia Dove
Mostafa El-Sayed
D. Wayne Goodman
Anne Mayes
William McCurdy, Jr.
Daniel Morse
Cherry Murray
Stanley Williams

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

Tuesday, February 25, 2003

The meeting was called to order at 8:27 a.m. by the chair, **Geraldine Richmond**. She welcomed the attendees and asked each committee member to introduce himself or herself. Richmond reviewed the agenda and introduced **Raymond Orbach**, Director, Office of Science (SC), U.S. Department of Energy (DOE). He pointed out that the 20-year roadmap is very important. It is needed so SC and its Office of Basic Energy Sciences (BES) can figure out where the frontiers are and what the important and exciting science will be. The plan should not give generalizations but specifics regarding facilities and the nature of SC. The United States does not have a Department of Science. It provides a great diversity of support for science, and the complementarity makes the country strong, but duplication must be avoided. Thus, SC's role must be identified. Some themes are emerging from the strategic planning effort:

1. Convergent science, where life science meets computer science. This area involves high-risk, high-payback research, which sets SC apart from much of the rest of the research funded by the federal government.
2. High-end computation is going to be involved in the progress of science. It is the third pillar of research, along with theory and experiment. DOE must invest in hardware and software to provide this important aspect of research.
3. Recognition that SC builds and operates world-class facilities for the use by all. Each of the Office Associate Directors was asked to look out 20 years to see what facilities will be

needed. This effort provided an estimate of what SC will want to fund and thus an estimate of the needed budget in the future. The Associate Directors put forward 53 proposals. This number fits within the envelope between the operating costs and the likely funding of SC during the next 15 to 20 years. Now community input is needed on whether these proposed programs and facilities are the right ones. Each advisory committee has been asked to weigh all these capital project proposals and to comment on them and rank them by March 2003.

As of now, SC is down about $9 million from the President's proposed budget, and another $15 million may be cut in the SC budget, a budget for an organization that has really contributed to the health and welfare of our country.

The FY04 budget request by program (which was just released) was compared against the FY03 request that was just funded. The comparison showed an increase of 1.4% in FY04, which does not fit the growth curve expected. The hope is that the Energy authorization bill will be passed and will include funding for research. However, a rampdown in construction spending allows an increase of about 4.5% in actual research funds in the FY04 budget. DOE is now working on the FY05 request.

The top three research priorities in the FY04 budget request are:

< $12 million for the International Thermonuclear Experimental Reactor (ITER) negotiations and supporting R&D in an effort to develop a burning plasma and to bring fusion power online in 35 years. The fusion process is essentially a materials problem. The British plan to replace their current nuclear-power and natural gas burning plants with fusion plants in 35 to 50 years and thus meet their responsibilities under the Kyoto Protocol while expanding the availability of electric power.

< $15 million (an increase of $7 million) for next-generation computing architecture. The computing capabilities of the United States have not kept up to the science that uses them. A sustained 25 to 50 teraflops are needed to simulate and solve science problems. DOE needs to think about ultrascale computers the way it thinks about light sources now.

< $196 million (an increase of $64 million) for nanoscale science, engineering, and technology. This effort is being backed to this extent because of its promise and its extant accomplishments.

Richmond said that the process of the 20-year prospect report was invigorating and extensive.

Kohn said that he was surprised that the British are counting on fusion for such a large contribution to the energy supply. The projection is worrisome. He questioned whether the United States should follow that way of thinking or be more conservative. Orbach responded that there has been progress. In the United Kingdom, about 6% of the energy supply comes from renewable resources. About 25% of their capacity will be lost when nuclear plants reach their design lifetimes; they are not building any more nuclear power plants. Their North Sea gas resources will also run out in 20 years. The Joint European Torus (JET) and other experiments show that a sustained, stable fusion process is likely possible. Nothing is guaranteed. Fusion offers a path to meet the energy demand of the world. Simulations indicate that the 35-year horizon is realistic.

Richmond then introduced **Patricia Dehmer** to report on the activities of BES. She reviewed the FY03 appropriations. This budget included funds for nanoscience centers in New Mexico and at Brookhaven National Laboratory (BNL). The overall budget was reduced 6.5% to account for the effects of the FY02 continuation resolutions.

The FY04 budget request was very favorable to BES. The Spallation Neutron Source (SNS)

would get a rolloff (an increase in the budget), as would the SPEAR 3 upgrade of the Stanford Positron Electron Accelerating Ring (SPEAR) at the Stanford Synchrotron Radiation Laboratory (SSRL) and the nanoscience center at Oak Ridge National Laboratory (ORNL).

The Department is preparing a strategic plan with a 20-year time horizon. The draft is still undergoing revisions; the plan will be printed in May.

She pointed out where the various budget processes (FY03, FY04, and FY05) currently stand. For the FY03 budget, allocations of appropriation are being worked out. For the FY04 budget, testimony is being given before Congress. And for the FY05 budget, the BES request is being prepared.

She turned her attention to the Subcommittee to Assess the 20-Year BES Facilities Plan and started with the background that led to the empaneling of that subcommittee.

< In the summer of 2002, Orbach requested that each Associate Director of SC develop a 20-year plan for facilities, using input from advisory committees, National Research Council (NRC) studies, community workshops, etc.
< In November 2002, the five SC Associate Directors presented a list of 53 upgrades and new facilities to Orbach.
< In December 2002, Orbach charged each advisory committee with assessing these plans by March 2003.
< In December 2002, a BESAC subcommittee was formed, co-chaired by Geraldine Richmond and Sunil Sinha.

That subcommittee met February 22-24, 2003, and considered 11 new or upgraded facilities:

Neutron-scattering facilities:
- A power upgrade for the SNS
- A second target station for the SNS
- A second guide hall for the High-Flux Isotope Reactor (HFIR)

Photon-scattering facilities:
- Linac Coherent Light Source (LCLS)
- An upgrade for the LCLS
- A linac-based femtosecond source
- An upgrade for the National Synchrotron Light Source (NSLS)
- An upgrade for the Advanced Photon Source (APS)
- An upgrade for the Advanced Light Source (ALS)
- A greenfield XFEL facility

Electron-scattering facility:
- TEAM (transmission electron aberration-corrected microscope)

In addition, four additional proposals were received from representatives from DOE/SC laboratories.

< A catalysis facility at Pacific Northwest National Laboratory (PNNL)
< A plant metabolomics facility at Ames Laboratory (AMES)
< An energy-recovering free-electron laser FEL at Thomas Jefferson National Accelerator Facility (TJNAF)
< An accelerator-based continuous neutron source at Brookhaven National Laboratory (BNL)

The workshop was one of the best technical workshops she had ever seen, with a lot of high-level give and take. Together with the Energy Security workshop, the 20-year plan workshop will rank very high in importance and will have a very long effective lifetime.

Richmond pointed out to the Committee that the two workshop reports had been supplied to

them and asked that each member to provide input on each. She declared a break at 9:32 a.m.

Richmond called the meeting back to order at 9:52 a.m. She asked **Sunil Sinha** to report on the Workshop on the 20-Year Basic Energy Sciences Facilities Roadmap. At the workshop, a series of proposals was presented, each of which was assessed according to two principles. The first was the importance of the science: the extent to which the proposed facility would answer the most important scientific questions; whether there are other ways or other facilities that would be able to answer these questions; whether the facility would contribute to many or few areas of research; whether construction of the facility would create new synergies within a field or among fields of research; and what level of demand for the facility exists within the scientific community. The second was the readiness of the facility: whether the concept of the facility has been formally studied in any way; the level of confidence that the technical challenges involved in building the facility can be met; the sufficiency of R&D performed to-date to assure technical feasibility of the facility; and the extent to which the cost to build and operate the facility is understood. This latter task could not be carried out uniformly among all the proposed facilities.

Kohn asked about the compatibility of the proposed facility with the DOE mission. Sinha responded that that topic was considered in most cases.

The projects proposed were organized into facility types and crosscutting issues. Three light sources presented requests for an upgrade initiative: the ALS, APS, and NSLS. Proposals were also received for new facilities: the Linac Coherent Light Source (LCLS), LCLS II (an upgrade of the LCLS), a greenfield XFEL, a linac-based ultrafast X-ray source (LUX), the Thomas Jefferson National Accelerator Facility Infrared FEL, the Coherent-Infrared Center (CIRCE) at the ALS, an APS super storage ring for synchrotron radiation, and an NSLS third-generation ring.

The Subcommittee believed that the four DOE light sources are central to our nation's research enterprise and that urgent upgrades are required to optimize scientific productivity and to maintain competitiveness. All of these upgrades are important, and increases in capital funds and operating funds will be needed. The Subcommittee recommended that DOE aggressively pursue an upgrade initiative, which should be coordinated among the four light sources.

Flynn asked what the total cost might be. Sinha responded, about $300 to 400 million over 20 years. He pointed out that the Subcommittee was asked not to focus on the dollar amounts but on the science. It was also asked not to set priorities.

The LCLS is essential for exploring future science using intense femtosecond coherent X-ray beams. DOE Critical Decision 0 and Critical Decision 1 have been approved; the LCLS is scientifically exciting and important. The Subcommittee recommended continued strong support.

The NSLS is one of the world's most scientifically productive x-ray sources with about 4000 users. It has the world record for producing scientific publications. It is still important to the U.S. scientific enterprise. The NSLS proposed a third-generation ring, a superconducting linac, the addition of an high-gain harmonic generation (HGHG) FEL, and an upgraded vacuum ultraviolet (VUV) ring. The Subcommittee recognized the continued need for third-generation X-ray sources and recommended that NSLS and BES formulate a plan for a third-generation ring. It asserted that BNL should focus on a third-generation ring. Richmond added that the Subcommittee considered at length such aspects as regional access to light sources.

The APS is one of the world's premier hard X-ray sources. Its beamlines need to keep up with improvements in instrumentation. The APS, therefore, proposed Phase I and II upgrades as being essential to optimize scientific output and to maintain international competitiveness with

tailor-made undulators for each experiment. Unique undulators can optimize the source and beamlines. In Phase III and Phase IV, a "super storage ring" and advanced instrumentation would be introduced. Although these latter phases are important, they are a consideration for the long term. The Subcommittee strongly supports the upgrade of facility beamlines and source optimization (Phases I and II) and supports long-term development of Phases III and IV.

There is no question that XFEL represents an important, new way to use synchrotron radiation. Therefore, the 20-year vision includes full-fledged XFEL-based user facilities. The technical challenges that exist include the e-gun, detector, and controlling spatial and temporal stability. Progress towards XFEL feasibility by the LCLS is critical. The Subcommittee recommended that R&D on XFEL must proceed with an emphasis on elucidating future scientific opportunities before going forward with greenfield XFELs.

Johnson asked him to define "greenfield." Sinha said that the Subcommittee took it to mean something built from scratch that does not use nor is not tied to any existing facility.

Two terahertz radiation facilities were proposed, the TJNAF terahertz FEL/ERL [energy-recovery linac] and the Coherent IR CEnter (CIRCE) at ALS. The Subcommittee concluded the following:

1. low-energy-excitation spectroscopy is critical to understanding collective dynamics
2. a potentially large user community exists
3. the national scientific agenda and user needs should be better developed before a recommendation is formulated.

Another innovative proposal came out of LBNL: a LUX facility. Such an ultra-fast VUV/X-ray facility would offer exciting new scientific opportunities to a huge community in chemistry and physics. Going to higher frequencies and intensities may provide new capabilities. The technical challenges include the HGHG cascades essential for VUV production. The Subcommittee recommended the development of a national scientific community of potential users as well as R&D to address the technical challenges.

In neutron scattering, the Subcommittee considered an SNS power upgrade, an SNS long-wavelength target station, a second cold source for the HFIR, and an accelerator-based continuous neutron source proposed by BNL.

The Subcommittee is convinced of the importance of neutron scattering to materials science and other disciplines. The SNS will be the world's premier neutron source. A 10% additional investment would increase scientific productivity by a factor of 2 to 3. The technical challenges include target modifications, which are ready for an initial critical decision (CD-0). The Subcommittee strongly recommended DOE support for this project.

The long-wavelength (20 vs 60 Hz) target station would be used to investigate small-angle neutron scattering, soft condensed matter, magnetism, nanomaterials, etc. It would increase the SNS user community by a factor of 3. No technical challenges were foreseen; the facility would use existing infrastructure. The Subcommittee recommended that initial planning begin.

The subcommittee concluded that the ORNL proposal for a cold waveguide for HFIR should be looked at in more detail and that the national neutron scattering community should get together and formulate the need for the accelerator-based continuous neutron source proposed by BNL.

Other facilities considered by the Subcommittee were the TEAM proposed by LBNL, a Plant Metabolomics Resource Facility proposed by Ames Laboratory, and a Complex Interfacial Catalysis Facility proposed by PNNL.

The TEAM concept would link a network of electron microscopes capable of atomic-

resolution 3D imaging. The microscopes would cost about $25 million apiece, and the first one would be at LBNL. Aberration-corrected microscopes have the advantage of a large focal length, the technology has been demonstrated, and the technology is considered central to the DOE mission. The Subcommittee recommended that this project be funded and that the principals work closely with the supplier/instrument community for development and construction.

Metabolomics is an interesting and important area of science. The leading researchers in the field are located at Ames Laboratory and important science is occurring there. The Subcommittee concluded that the research should be supported but that it is premature to view this as a national facility.

The Complex Interfacial Catalysis Facility was proposed as a user facility for catalysis research, which is a key piece of DOE's portfolio and an important research field for the nation. Given that BESAC has another subcommittee looking at this topic, the Subcommittee recommended that any decision on a catalysis facility such as this needs to be reviewed in the context of competing proposals.

In terms of crosscutting issues, detectors and other instrumentation are required, especially 2D ultrafast detectors. Electron-gun development to provide high brightness will be critical to the success of several projects. Superconducting short-period undulators will be needed. And the ERL is a possible, new way of producing synchrotron radiation. However, R&D is needed in all of these areas.

The Subcommittee will

< continue to gather input to complete the assessment of BES facilities,
< finalize the evaluations and summary,
< distribute final draft information to all BESAC members by March 4, and
< finalize the report and submit it to Orbach by March 10.

Moore asked about the timeframe and the materials to be provided to BESAC members. Richmond said that the Executive Summary would be done by the next day. Summaries of each proposal would be ready by the end of the week.

Kohn noted that Orbach had said to put the science first, but the Committee had not heard much about the science associated with each of these proposed projects. He said that he would appreciate a succinct presentation of the scientific objectives. Sinha responded that each of the presenters touched on the science but it is difficult to summarize that science. Richmond added that, in some cases, the Subcommittee did not believe there was a clear-enough statement of the science; in those cases it recommended that the community get together and delve into the subject.

Moskovits asked, given uncertainty, how one makes plans for 20 years out. How do you triage among proposals and existing facilities? Dehmer said that one way is to make a conservative decision to make a small facility with the ability to be upgraded. Another strategy is to pull together representatives of the community and ask them to pool their intellectual resources. It is hard to end an existing facility, but it has to be done, and it *is* done by all scientific agencies.

Flynn noted that the Subcommittee had inadvertently prioritized the proposals. He asserted that BESAC should recognize several classes: (1) needs more thought; (2) needs to be funded; (3) should be done if funds are available. In addition, the way that the number of users is calculated has to be standardized. Dehmer commented that the numbers presented are the unique users that visit the facility each year. She noted that grouping the proposals as Flynn had suggested is an excellent way to proceed.

Tromp commented that most of the proposals offered are business-as-usual. There is a lack of any consideration for biosciences, proteomics, etc. Dehmer responded that the divisions of SC devoted to those topics had their own workshop and the needs for facilities of those divisions will be communicated to BES. Isaacs injected that a lot of such sciences were presented and considered at the workshop. Broholm observed that the biological sciences will use neutrons to perform protein crystallography, an important area in medical science. High-temperature superconductivity is being elucidated by neutron scattering. Getting to the bottom of some of these questions is inordinately complicated and no clear-cut answers are available. Berrah added that the Subcommittee had heard scientific cases made for each of the facilities proposed. Many of the beamlines at synchrotrons are already being used by crystallographers. Long noted that a lot of fresh, new information had been presented at the workshop and that, perhaps, summaries of those scientific presentations should be prepared for BESAC members so that they can recognize the science involved.

Greene commented that such a roadmap has to be rewritten periodically. The Committee should ask Orbach if this roadmap can be regularly updated.

Plummer noted that Orbach had stressed the training of accelerator-based personnel and stated that the Subcommittee should stress the need to maintain the facilities that train such workers. Isaacs said that the greenfield XFEL proposal offered such exciting science that it would draw people into this field.

Stupp asked why the development of complex-probe techniques was not being discussed. Not everything in bioscience is solvable by crystallography. Great science is to be done in other fields, also. Maybe BES should reach out to a broader community. Sinha responded that the Subcommittee was charged to look at only big (>$50-million) facilities and centers. Stupp asserted that there are a lot of opportunities where new imaging and other techniques are being developed. In these fields, DOE needs to be more proactive.

Stohr commented that great excitement was elicited by the science proposals, coupling closely with nanoscience and other fields, as they did. That science was very strong. The time available to the presenters was very short. Many could have used more time to expand and interpret their proposals. He was glad that the Subcommittee recognized the needs that can be filled by the proposed facilities despite the loop not being completely closed.

Bucksbaum commented that the Subcommittee was not charged to look at the entire scientific portfolio of SC. It did hear from a broad spectrum of users served by BES. Those 20-year visions need not be limited to what Orbach requested. The Committee could also periodically look over the needs of science in general.

Richards observed that magnetic resonance does not use neutrons but could easily use $50 million. The laboratories do not pursue electromagnetic technologies and science. Sinha pointed out that the proposal from Ames Laboratory was based heavily on magnetic resonance imaging (MRI) and nuclear magnetic resonance (NMR) imaging.

Johnson asked if the discussion of each facility included a consideration of workforce issues, noting that the demographics of the scientific community are going to be quite different in 20 years. Sinha conceded that the topic was not significantly addressed. Richmond said that the topic should be added to the crosscutting issues.

Tromp noted that the workshop had asked the existing facilities what they would like to do in the next 20 years. It could also have asked what science opportunities (e.g., biological) existed and then decided if a fundamentally new type of facility should be built to address that opportunity.

Johnson noted that today one can get to 30 to 40 THz with a tabletop laser. Bucksbaum commented that the interesting thing about large facilities is that they can achieve three orders of magnitude higher power with stability. However, they are limited to 1 THz. R&D might push back that barrier.

Taylor noted that increasing productivity does not just consist of pushing additional users through a facility but of doing new science there.

Crow stated that NMR and other topics did not fall on this table because of the scope of the charge. These topics have traditionally been discussed elsewhere. Important issues still exist to be discussed, however, and the table should be kept open to accommodate surprises. Periodic reviews may be very useful.

Broholm commented that these X-ray and neutron facilities address a very broad range of topics. Small science is occurring on a very broad carpet. This breadth is the strength of these facilities. A very broad range of science was discussed at the workshop.

Kohn noted that attosecond science had not been discussed. Sinha said that several presentations touched fundamentally on very short X-ray pulses, many of them being pulse-probe problems.

Bucksbaum stated that there is a well-vetted path to get there, and it was represented at the workshop. The present systems are facilities in the range of $1 million to $2 million, but this area can only be studied by multibody-dynamics simulations.

Smalley commented that the distributed facilities in NMR are similar to the situation in nanoscience. He asked if BESAC had looked at the concept of distributed facilities, where DOE would provide instrumentation and staffing at 20 to 30 locations across the country. The big - facility approach leaves a lot of science unaddressed. Crow said that one proposal presented on electron microscopies took a regional-facility approach. The National Science Foundation (NSF) has supported such facilities, and the National Institutes of Health (NIH) is funding a little of that now. The NMR instrument is only one part of such a facility, but the probes are an important component.

Richards noted that NSF and NIH often fund a series of facilities and then go away, leaving the centers to wither and die. Crow said that the dynamic is driven by what the commercial market does. One does not know what will happen in the area of, say, 900 Ghz and what the market will do if something interesting occurs there.

Hemminger stated that the way this process is being carried out just propagates what is being done now. He asked if the Subcommittee devoted time to consider what is missing in the national laboratories' research portfolio. For example, no national laboratory has a world-class program in making stuff. Great ideas are coming forward, but the Subcommittee should also consider what is missing.

Richards agreed that BESAC should address that concern and stated that this topic should be on the July agenda. She asked **Michael Lubell** from the American Physical Society to give a monetary reality check on these proposals. He stated that the budget requests for FY02 and FY03 are flat. The outlook for discretionary spending is not optimistic. There have to be increases in the SC budget. Costs of doing research go up faster than the consumer price index. The higher-education cost index is probably a better measure of the cost of doing research. There is legislation (HR 34) pending to authorize greater funding. The importance of physical science needs to be impressed on people. Also, workforce issues and the necessity of employing foreign nationals needs to be addressed. The will is there (such an increase in funding has been achieved for NIH), but the case must be made. The scientific community has to get involved locally. Each

member of Congress and senator looks to his or her own constituency. Only about 2% of APS members speak out to their elected representatives. That does not carry much weight; many advocacy groups do a much better job than that.

Richmond asked each member to consider the report of the Subcommittee, to point out any show-stoppers, and to comment on whether they approve of what they have heard so far (which could include saying that not enough information has been provided).

Kohn said that, given the Subcommittee's time constraint, they did an excellent job and that he was willing to accept their report.

Moskovits seconded that opinion.

Taylor said that this material is so fresh that the Subcommittee has not had a chance to step back from it and assess it objectively. Some of the topics brought up today should be added.

Long seconded what Taylor had just said.

Isaacs likewise ascribed to Taylor's statements. He noted that the Subcommittee should also acknowledge the presenters and convey coherently the science content of the presentations.

Greene added that the report must state that roadmapping is a continuing process.

Bucksbaum pointed out that it should include technical-workforce issues and that BES should periodically look at what research it wants to do.

Wirth suggested that the long-term goals of DOE should be included with the science.

Hemminger said that he would be happy to endorse the recommendations included in the report with the addition of the discussion of science and workforce issues.

Stohr said that he would accept the recommendations and that he had found the workshop exciting.

Moore stated that the Subcommittee had done an excellent job.

Johnson said that, with the suggested additions, he would accept the report.

Broholm noted that the report has the ability to incorporate feedback and stated that he fully supported it.

Berrah noted that she would totally support the report with the addition of a discussion of workforce issues. BESAC should also review facilities periodically to make sure they do not deteriorate.

Plummer stated that he would like to see more before making a decision.

Richards suggested that some scientific research should be put in as sidebars as well as adding workforce issues and "overlooked" science.

Tromp said that he was not concerned about the science. This facility roadmap should not be the BES roadmap. There is more to science than facilities.

Stupp said that he had not read the report yet, but he believed that something should be added about novel facilities that do not currently exist.

Smalley echoed that sentiment.

Richmond said that she was relieved to see that the Subcommittee had not said, "Do it all, and do it now." That lends to the credibility of the Subcommittee and its report. The draft summary will be distributed this coming weekend, and feedback from the Committee will be sought.

Plummer asked how the intrinsic ranking of proposals is going to be dealt with. Richmond responded that the Subcommittee had assessed and graded each proposal in terms of science and readiness. The Subcommittee had not ranked them relative to one another.

Hemminger called attention to the fact that Flynn had previously noted that the continuing programs of BES should not be hurt by these additional research facilities. That goal should be

stated in the Executive Summary. Bucksbaum said that, if such a sentiment can be carefully stated in a positively manner, including it in the Executive Summary would be fine.
The meeting was adjourned for lunch at 12:14 p.m.

Tuesday Afternoon

Richmond called the meeting back to order at 2:06 p.m. and called upon **John Stringer** to report on the Workshop on Basic Research Needs to Assure a Secure Energy Future. He listed the Subcommittee members and staff assistants, reviewed the charge to the Subcommittee, and quoted Sec. Abraham's assertion that, "if we ever hope to leapfrog today's energy challenges we must look to basic research."

The reasons for the concern about energy security are the increase in the world's population, the increase in individual expectation for energy worldwide, the current (worldwide) dependency on fossil fuels, the finite resources of fossil fuels, the need to extend the time to the peaking in the use of current energy sources, and the need to develop new alternatives in order to lower CO_2 emissions (although the Subcommittee did not address the issue of global warming explicitly).

An input-output analysis of U.S. energy use indicated that the country imports almost the same amount of energy as it uses for transportation.

Energy use and gross domestic product are linked. Below 10^3 dollars of annual gross domestic product (GDP) per capita and 10^2 kilowatt-hours of annual energy use per capita, only the basic survival needs (food, water, shelter, and minimal health services) can be supported. Between 10^3 and 10^4 dollars (10^2 and 10^3 kWh), a basic quality of life (literacy, sanitation, life expectancy, and physical and social security) can be sustained. Between 10^4 and 10^5 dollars (10^3 and 10^4 kWh), amenities (education, recreation, clean environment, and intergenerational investment) can be afforded. And above 10^5 dollars (10^4 kWh), international collaboration (global investment, peace, and technology) can occur.

Currently, the world as a whole is lagging about 50 years behind the United States in per capita energy use, and the developing countries are lagging even further behind. World population is growing at a very high rate. As a result, the global demand for energy is going to get very large. Even with conservative growth, current energy sources are not going to last past 2100.

The mission of BES is to "deliver the scientific knowledge and discoveries for DOE's applied missions; advance the frontiers of the physical sciences and areas of the biological, environmental, and computational sciences; and provide world-class research facilities and essential scientific human capital to the Nation's overall science enterprise." Restated for the purposes of the workshop, this mission translates into discovering what needs to be done to make the jump to the next stage of energy supply and use.

The path chosen to attain the objectives of the workshop called for the participation of stakeholders; the representation of as wide a constituency as possible; the focusing of discussions to a limited number of proposals; the desire to support, not duplicate, applied-mission offices of DOE; and an understanding of the time scale of the objectives.

The stakeholders in the workshop were the DOE applied missions offices (8% of the workshop attendees), academia (27%), the national laboratories (39%), industry (16%), and SC (10%).

The workshop leaders defined nine topical areas:

< Fossil energy;

- Distributed generation;
- Nuclear energy;
- Industrial, residential, and commercial;
- Transportation;
- Renewable energy;
- Fusion energy;
- Energy biosciences; and
- Crosscutting research

After the initial workshop, the energy biosciences were recognized as having been under represented, so a small workshop on that topic was subsequently conducted, and its results were integrated with those from the initial workshop. The products of the two workshops consisted of four items:

- A set of proposed research directions (PRDs). Altogether, 37 were produced.
- Supporting statements for each PRD, each in the form of a one-page executive summary and three pages of detailed information.
- A list of 10 general research areas derived from the PRDs.
- The "Factual Document," summarizing the status of energy supply and use.

The final condensation produced a list of ten basic research directions to be expanded upon and pursued:

- Materials research to transcend energy barriers (which topic turned up in half of the 37 PRDs)
- Energy biosciences
- Research toward the hydrogen economy
- Energy storage
- Novel membrane assemblies
- Heterogeneous catalysis
- Energy conversion
- Energy utilization efficiency
- Nuclear fuel cycles and actinide chemistry
- Geosciences

Many of the technological barriers related to energy hinge on improved materials. Fields of work that look promising for overcoming those barriers include nanomaterials (including materials with nanomaterials dispersed in them), materials degradation, composite materials, materials fabrication issues, and advanced materials and new materials opportunities.

The topic of energy biosciences came up because of solar energy. How does one store the energy (besides in biomass)? Promising avenues of research include biomimetic approaches to solar energy capture and generation of fuels and chemicals, using emerging knowledge in functional genomics and molecular technology to develop plants optimized to produce fuels and chemicals, and the development of biocatalysts.

In research towards the hydrogen economy, hydrogen production is the key. It can be accomplished by (1) high-temperature splitting of water, (2) thermochemical splitting, or (3) harnessing light for photovoltaic splitting. In addition, an atomistic understanding of hydrogen conductors for fuel cells and new hydrogen storage concepts are needed.

Energy storage is of great importance for the development of "transient" renewable resources, such as wind or solar energy. Two pathways forward in this area include (1) photoconversion of renewable substrates to liquid or gaseous fuels and (2) phase transitions in

materials for energy storage (an area in which R&D could lead to great improvements).

Heterogeneous catalysis underlies a number of the concepts proposed for new directions in energy production and utilization.

In energy conversion, basic research is needed to support advances in diagnostic tools to advance combustion science and lead to predictive models for design and real-time operation control. Multiphase fluid flow and heat transfer would benefit from study as would the understanding of the effect of nanophase dispersions in materials. R&D could decrease the efficiency losses in solar devices caused by the rapid decay of photogenerated carriers. Fuel cells could be developed for transportation and distributed power. And significant improvements could be made in thermoelectric materials.

Basic research could significantly improve energy utilization/efficiency, especially in lighting. New light-emitting materials are possible and research is needed on biomass energy.

If fuel reprocessing is not allowed, the nuclear option will be available for only another 65 years.

Geosciences underpin the discovery of new fossil fuel resources. Research in subsurface imaging would allow one to look at in situ alteration of fluid/rock interactions.

In summary, there is no single solution to the problem of ensuring a secure energy future for the United States. Problems that must be addressed are truly interdisciplinary. This means that research will require the *coordinated* participation of investigators with different skill sets. Basic science skills have to be complemented by awareness of the overall nature of the problem, and with knowledge of the engineering, design, and control issues in an eventual solution. It is necessary to find ways in which this can be done while still preserving the ability to do first-class basic science. The traditional structure of research, with specific disciplinary groupings, will not be sufficient. This situation presents great challenges and also great opportunities.

The recommendations that came out of the workshop were not a laundry list of research projects but a set of guidelines and principles for progress. They are:

< A major program should be funded to conduct a multidisciplinary research program to address the underlying fundamental knowledge that must be developed to handle the issues involved in providing a secure energy future for the United States.
< This program must be ensured of a long-term stability.
< DOE's BES is well-positioned to support this initiative by the enhancement of its already world-class scientific research programs and user facilities.

Ensuring energy security will not be possible without experimentation, the development of predictive models, the extension of computational skills, the optimization of solutions, and the validation through high-quality experimental data.

Richmond thanked Stringer and Linda Horton for their work. Greene pointed out that this is not in consilience with what Orbach had said in the morning session. It points out that the country cannot put all of its eggs in one basket.

Stupp asked if any research directions had been brought up at the workshop that are absent from the DOE research portfolio. Stringer said that not many things were brought up that are not already present. Smalley noted that geothermal energy had been missed but is in there now. Perhaps there should have been a PRD on space-based solar energy. The report has not been reviewed to identify first steps or the most productive areas.

Stringer noted that one important issue is how to predict the future. It is easier to predict the present; that is to say, to go back 20 years and see if you can predict current conditions. Predictions of world population from decades ago are drastically different from what we see

now. That is because population was expected to be resource-restrained and the predictions did not take into consideration the changes in food production that the world has seen. Something unexpected may always happen.

Taylor added that the technology pipeline is not orderly. She was pleased to see input from the mission agency at the beginning. That input needs to be cycled because the problems may change.

Moskovits asked if BES has a role in conservation and efficiency and whether policy considerations enter into the determination of the extent of nuclear resources. He noted that, when crises loom, people look into possibilities that had been rejected before. Stringer said that the Subcommittee did not look at the nuclear future in detail because it is being looked at by the Gen-IV initiative. All of the possibilities they are looking at may extend the nuclear option. A graph of the energy intensity used per 10^3 dollars of annual GDP per capita (a measure of energy-use efficiency) shows an improvement of about 30% from 1950 to 1990 and is projected to improve significantly through 2050. That projection is based on no fuel recycling, the pursuit of which was terminated out of concern for proliferation.

Richards asked how the British got it so wrong about fusion. Stringer replied that, if it worked, it would make everything fine. But there are a lot of R&D gaps along the way. The materials challenges are still very great. (But the payoff would be very great, too.) He could not say that it will work, but he could not say that it will not work, either.

Richards asked if superconducting electrical transmission was factored in. Stringer responded, yes, it was. The average IR [current-resistance (I^2R heating)] losses are about 7%.

Richards observed that, as per capita energy consumption goes up, the birth rate goes down and expressed hope that, as conditions in the third world improve, the birth rate will decrease. Stringer said that he had been told that this phenomenon is being seen in China. However, even if the population stayed the same and energy usage was brought up to the current U.S. energy usage, the energy consumption would still skyrocket.

Kohn asked if the problem can be characterized as follows. Eventually the Earth will run out of nonrenewables. How much would humanity need from new technologies? What population could be sustained by renewables at current U.S. consumption rates, and what level could be sustained at current technological capabilities? Stringer replied that solar energy is able to sustain our current population. The current U.S. energy demand could be met by paving one or two counties in Arizona with solar converters. One of the terrifying ideas is convincing the Chinese that everybody should have personal vehicles and roads should be installed throughout the country. Horton added that <10% of energy worldwide is currently supplied by renewables. That would indicate that the standard of living would fall dramatically if nonrenewable sources were no longer available. Stringer continued, the energy needs of the world could be supplied by solar energy at current levels of usage but at great cost.

Tromp noted that the recommendation to support a research program in energy security is vague. Stringer agreed, but it is not different from what has been done in the past in nature or scope. The Subcommittee's suggestion is to support that nature and scope, which is substantial. Tromp said that, basically, he did not understand the recommendation. Stringer interpreted it to mean that the R&D needs cannot be met by tweaking the current programs. A large, sustained, focused effort is needed. Horton added that the Executive Summary states that the report is talking about a national initiative with the infusion of resources. Tromp said that the recommendation needs to be radically rewritten. Stringer agreed. Richmond asked if others felt the same way. Stohr said that he certainly did. The current expression is a motherhood statement.

It needs to say what it really means.

Hemminger noted that, in the presentation, not much appeared about radical solutions. He was also disappointed that there was not much underlining of the term "basic science." Horton replied that all the authors are cognizant that BES does basic research. The research community must be aware of the needs. This is not an applied research report. The report calls for basic and interdisciplinary research. Hemminger agreed that, if someone reads the report as a whole, they will get that impression, but they will not get it from the Executive Summary. Horton said that the reader will find it in the first 15 pages of the report.

Smalley agreed that solving the energy problem is an applied-engineering problem. He pointed out that each of these PRDs was tested to ensure that they dealt with basic R&D. If it was known how to get to energy security, the workshop would not have been needed. But it is not know how to solve the problem with current technology and at manageable cost. New, now-unknown technologies are needed. So the writers of the report are driven to such a motherhood statement; they almost need to say, " We need a miracle." A statement about the need for basic research in the Executive Summary is probably called for. Hemminger said that that would certainly address some of his concerns. What needs to be said is that the R&D must be done to take advantage of new breakthroughs.

Moskovits noted that simply bulleting a number of areas discussed does not give the flavor of the needed research. The document is full of specific notions. It would be helpful to have those specifics mentioned in the Executive Summary. The substance of the workshop should be reflected in the Executive Summary. The reason this group was put together was to come up with options, and those options do not come across in the current Executive Summary.

Richmond said that the organization and recommendation has to be a lot clearer on what the report is about because this report will be read by a lot of people who are not scientists. She suggested including in the Executive Summary the statement, "We recommend that DOE aggressively pursue a basic research program for a secure energy future. This initiative would focus on multidisciplinary, basic research to address the underlying, fundamental problems."

Tromp attempted to paraphrase the Committee's sentiment: The current funding level is not adequate to meet the challenges in energy security, and a new initiative needs to be launched. But that is a much bigger fish than BESAC can handle. BES needs the buy-in from many other DOE offices and other agencies. The report needs to admit that what needs to be done is bigger than what BES alone can do. Dehmer pointed out that there are several presidential initiatives on climate-change technology. A lot of what has been described in this report fills in the blanks in the Climate Change Technology Initiative (CCTI). This report outlines what needs to be done at the basic research level to accomplish what the CCTI calls for. Saying that a new initiative needs to be started indicates that the Subcommittee failed to recognize the context in which the task was undertaken. The detailed backup material provides the direction that needs to be taken. Richards asked if that could be stated explicitly in the Executive Summary.

Tromp pointed out that, as currently stated, the Executive Summary and recommendations do not say what will be done with this science; all they say is that a bigger program is needed.

Richards said that there are good words on p. 15 of the draft report. What is said there is more specific and passionate than what is in the Executive Summary.

Tromp stated that this report needs to say in clear language what is called for.

Richmond pointed out that most BESAC reports are not specific about dollars or levels of effort. She suggested that the BESAC members get together during the coming evening and suggest better language for the Executive Summary. Moskovits stated that the Executive

Summary simply needs to lay out some specific options. It should reflect the intelligent recommendations stated in the report and to do justice to the report. Richmond commented that the report is a tremendous resource and should be used as a guide.

Kohn said that he wanted to understand better the element of cost involved because some topics were not being considered because the cost would be too great. Dehmer said that it would be a mistake to talk about the cost of delivered systems because things change so quickly.

Richmond noted that, if this proposal is characterized as a new initiative, it would raise the question of what was being done with the current funding. Smalley suggested saying that: current research directions are not leading to the desired results and that this report lists 37 suggestions of new pathways. Revolutionary breakthroughs are needed (for example) to make photovoltaics "as cheap as paint." The magnitude of the problem needs to be stated in the Executive Summary and in the recommendations. Plummer said that what is needed is Rick Smalley's passion and Linda Horton's down-to-earth recommendations in the Executive Summary. Richmond added, along with John Stringer's sense of humor.

Broholm said that he was impressed by the report. Some thought needs to go into how to distribute it to excite the students of today. It places BES as the link between the doomsday scenario and the solution of the problems.

Long pointed out that BES must also be sensitive to the sensibilities of the other DOE offices.

Richmond asked the Subcommittee to recraft the Executive Summary overnight for reconsideration the next morning. She opened the floor to public comment.

Helen Farrell asked if methane hydrates had been considered in the assessment of energy technologies. Nick Woodward replied that that topic was not discussed at the workshop but the Office of Fossil Energy has a program on that topic.

Tina Kaarsberg said that she was intrigued that BES had $38 million in the Climate Change Technology Program (CCTP) of DOE and wondered where it was. Dehmer replied that could not tell without looking at the crosscut. Kaarsberg noted that Undersecretary Card had said that the CCTP strategic plan would be completed by this summer and suggested that this Committee should use the Energy Security Report to inform the strategic-planning process. Dehmer responded that that was a good idea.

Kurt Schoenberg pointed out that an enabling difference will require a large fiscal commitment. One reason fusion is constantly 50 years in the future is the lack of fiscal commitment. To make a real difference in energy security will require a large investment and a significant redirection of resources.

Richmond adjourned the meeting for the day at 5:17 p.m.

Wednesday Morning

Richmond called the meeting to order at 8:36 a.m., reviewed the agenda for the day, and asked **Linda Horton** and **John Stringer** to review the changes that had been made in the Energy Security report. They projected the revised text of the Executive Summary on the screen and explained that the language had been changed to reflect that

- several options are available and many or all of them must be pursued;
- the opportunity exists for major new discoveries, virtually all of which are interdisciplinary in character; and
- BES should review its current research portfolio to assess how it measures up to the research

charge proposed by this study.

In response to concerns about the costs involved in the expansion of energy use worldwide, Springer pointed out that electricity plants cost about $1000 per installed kilowatt. To build generation capacity to provide power worldwide at the energy intensity currently observed in the United States would be a massive investment, in the billions of dollars. However, the required annual rate of investment would be slightly less than what the world currently spends on cigarettes. When the cost is stated, it looks like a large amount. But when you compare that cost with the amount of money that is available for things that we do not think too much about, it is not so large.

Kohn asserted that the problem of electricity supply will never be entirely solved. What the world is faced with now is making a transition from an energy economy based on fossil fuels to one with a more sustainable base.

After extensive word smithing of the Executive Summary by the Subcommittee members as well as the other BESAC members, Richards moved the acceptance of the report. Stupp (inter alia) seconded, and the report was accepted unanimously.

Richmond asked for a report on the Biomolecular Materials Workshop. **Samuel Stupp** presented the final version of the report, which had been previously distributed to the members of BESAC. John Richards moved to accept the report. Smalley seconded, and the report was unanimously accepted.

Richmond called for discussion of the report on Opportunities for Catalysis in the 21st Century. **John Hemminger** presented the revised version of the report, which had been previously distributed to the members of BESAC, and formally thanked John Bercaw and Jens Norskov for their help in the writing and revision of the report. Richmond said she would send each of them a letter of thanks. Richards moved to accept the report. Smalley seconded, and the report was accepted unanimously.

Richmond opened the floor for public comment. There was none. She reviewed upcoming events (specifically, the rollout of the Nanoscience Research Centers, which was to occur on the following two days) and adjourned the meeting at 9:32 a.m.

Submitted March 7, 2003
Frederick M. O'Hara, Jr.
Recording Secretary