

**BESAC Subcommittee Workshop Report
on
20-Year Basic Energy Sciences
Facilities Roadmap**

Co-Chaired by:

**Geraldine Richmond, BESAC Chair
University of Oregon**

and

**Sunil Sinha
University of California, San Diego**

February 22-24, 2003

Doubletree Hotel and Executive Meeting Center
1750 Rockville Pike
Rockville, MD 20852



UNIVERSITY OF OREGON

6 March 2003

Dr. Ray Orbach
Director
Office of Science
U.S. Department of Energy
19901 Germantown Road
Germantown, Maryland 20874-1290

Dear Dr. Orbach,

On behalf of the Basic Energy Sciences Advisory Committee I am forwarding to you the report that you had requested in your December 2002 charge letter. This report, the 20-Year Basic Energy Sciences Facilities Roadmap, and is the result of a BESAC Subcommittee that met at a workshop in February to address your charge. Dr. Sunhil Sinha and I co-chaired this Subcommittee.

The recommendations of the Subcommittee and the contents of this report were unanimously accepted by the members of BESAC at our February 2003 meeting.

We want to thank you for the opportunity to involve BESAC in this very important planning process. Those of us that participated in the study found it to be a rewarding opportunity to look towards the future and envision the important new science and discoveries that these facilities will enable in the future.

Sincerely,

Geraldine L. Richmond
Chair
Basic Energy Sciences Advisory Committee

cc: Sunhil Sinha, UC San Diego
Pat Dehmer
Sharon Long

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Workshop Participants

Subcommittee:

Geri Richmond, U of Oregon (Co-Chair)

Sunil Sinha, UCSD (Co-Chair)

Nora Berrah, Western Michigan U. (BESAC)

Joe Bisognano, Synchrotron Radiation Center, Wisc.

Collin Broholm, Johns Hopkins (BESAC)

Phil Bucksbaum, U. of Michigan (BESAC)

Jack Crow, National Magnetic Lab, Florida

Pascal Elleaume, European Synchrotron Rad. Fac., France

Eric Isaacs, Bell Labs/Lucent (BESAC)

Gabrielle Long, NIST (BESAC)

Gerhard Materlik, Diamond Light Source Ltd.

Les Price, ORO

Kathy Taylor, Retired GM (BESAC)

Laboratory Technical Representatives:

ANL-- Robert Kustom

BNL-- Jim Murphy

LBNL-- Howard Padmore

ORNL-- Norbert Holtkamp

PNNL-- Ray Doug

SLAC-- Max Cornacchia

TJNAF-- Swapan Chattopadhyay

Workshop Agenda

Saturday, February 22, 2003		
7:30am - 8:00am	Continental Breakfast	
8:00am - 8:15am	Introduction from Subcommittee Co-Chairs	Geri Richmond (U. of Oregon) Sunil Sinha (U. of CA San Diego)
8:15am - 8:30am	Introduction from BES	Pat Dehmer, Basic Energy Sciences
8:30am - 9:30am	Linac Coherent Light Source	John Galayda, SLAC
9:30am - 10:30am	SNS Power Upgrade	Thom Mason, ORNL
10:30am - 11:00am	Break	
11:00am - 12:00pm	Transmission Electron Aberration Microscope	Ulrich Dahmen, LBNL
12:00pm - 1:30pm	Lunch	
1:30pm - 2:30pm	SNS Long Wavelength Target Station	Thom Mason, ORNL
2:30pm - 3:30pm	High Flux Isotope Reactor Target Station II	Jim Roberto, ORNL
3:30pm - 4:00pm	Break	
4:00pm - 5:00pm	Linac-based Ultrafast X-ray Source	Steve Leone and John Corlett, LBNL
5:00pm - 6:00pm	National Synchrotron Light Source Upgrade/Energy Recovery Linac	Steve Dierker, BNL
7:00pm	Dinner	
Sunday, February 23, 2003		
8:00am - 8:30am	Continental Breakfast	
8:30am - 9:30am	Linac Coherent Light Source Upgrade	Jerry Hastings, SLAC
9:30am - 10:30am	Green-Field Free Electron Laser (SLAC, ANL, and BNL)	Kwang-Je Kim, ANL
10:30am - 11:00am	Break	
11:00am - 12:00pm	Advanced Photon Source Upgrade	Murray Gibson, ANL
12:00pm - 1:30pm	Lunch	
1:30pm - 2:30pm	Keeping the Advanced Light Source at the Cutting Edge	Neville Smith and Michael Martin, LBNL
2:30pm - 4:00pm	Additional Submissions/Presentations Complex Interfacial Catalysis Facility Energy Recovering Free Electron Laser Scientific User Facility The Ames Plant Metabolomics Resource Facility Accelerator Based Continuous Neutron Source	Dave Dixon and Chuck Peden, PNNL Gwyn Williams, TJLAB Ed Yeung and Basil Nikolau, AMES Steve Shapiro, BNL
7:00pm	Dinner	
4:00pm - 10:00pm	Report writing, with break for dinner	Subcommittee Members and Technical Assessment Team
Monday, February 24, 2003		
8:00am - 12:00pm	Report writing	Subcommittee Members
12:00pm - 1:30pm	Lunch	
1:00pm - 5:00pm	Preparation of Report for BESAC Meeting	Geri, Sunny and Subcommittee

20-Year BES Facilities Roadmap Workshop Report

Executive Summary

The Department of Energy's Office of Science has historically played a key role in the creation and support of world-class scientific research user facilities. Basic Energy Sciences has been a central player in this effort, particularly in envisioning, designing and advancing facilities that are critically needed in areas such as biology, chemistry, physics, materials science, optics and catalysis. Stewardship of these facilities requires vigilant evaluation of the existing facilities as well as a visionary foresight into what new facilities will support the research needs and enable the discoveries of the future. This Subcommittee of the Basic Energy Sciences Advisory Committee has completed this study as a mechanism for assisting in the planning process for Basic Energy Sciences and the Office of Science.

The task of the subcommittee has been to conduct a review of received proposals, originating predominately from the DOE National Laboratories, that propose what facilities may be needed in the next 20 years. The review sought to identify the projects in those proposals with the highest potential for producing world-class research tools. In our deliberations the subcommittee considered both the importance of the science as well as the readiness of the facility for construction, criteria outlined in the charge given to BESAC by Dr. Ray Orbach, Director of the Office of Science.

Recommendations for Proposed Projects:

Proposed projects were organized into several categories for consideration: (1) photon based facilities, (2) neutron based facilities, (3) other facilities and (4) cross cutting issues that are key to successful advances in a number of the future facilities. The subcommittee found the most exciting science and the immediate need for action in the following areas:

Light Source Facilities

The four DOE light sources are an important component to our nation's scientific and technological enterprise. As we look towards the future, DOE has the dual responsibility of developing unique new facilities to address future scientific needs while also maintaining and upgrading its current world class facilities in areas where these facilities continue to respond to the critical scientific needs of the nation. The BESAC Subcommittee strongly believes that it is essential that timely investment in upgrades of the four DOE light sources be made. These facilities are heavily used by over 7000 scientists across the country and are the envy of many around the world. To continue to

produce cutting-edge science, upgrades at these facilities are needed. Furthermore, the upgrades must be done in the near future so that the facilities remain at the forefront in light source activities. The BESAC Subcommittee urges DOE to aggressively pursue a Light Source Facilities Initiative that involves a coordinated effort among the four light sources. Based on presentations to the BESAC Subcommittee we recommend:

- The National Synchrotron Light Source (NSLS) is one of the world's most scientifically productive user facilities. We recommend that NSLS and BES formulate a plan for construction of a 3rd generation ring at NSLS.
- The Advanced Photon Source (APS) is one of the world's premier hard X-ray sources. It has proposed a Phase I and II upgrade that we strongly support through the Light Source Facilities Initiative called for above.
- The Advanced Light Source (ALS) is the nation's 3rd generation ultra-violet and X-ray ring. The BESAC Subcommittee recommends support of their upgrade proposal to go to full energy injection and higher current, as well as to replace obsolescent insertion devices (IDs) and beamlines with state-of-the-art IDs and new beamlines.

We are pleased to note that the Stanford Synchrotron Radiation Laboratory (SSRL) is currently undergoing an upgrade that will make it a 3rd generation X-ray source, and thus it is not mentioned further in this context.

Looking toward the immediate future, one proposal that ranked very highly in both quality of proposed science and facility readiness is the Linear Coherent Light Source. This Free Electron Laser (FEL) facility is essential for exploring future science using intense femtosecond coherent X-ray beams. The knowledge gained from operation of this facility is critical for providing preliminary assessments of many science drivers for these new intense coherent fast X-ray sources and providing critical guidance to the planning and ultimate success of several future proposed X-ray FEL sources that offer exciting new prospects for future scientific endeavors in BES. The BESAC Subcommittee enthusiastically supports this project.

Neutron Source Facilities

Neutron facilities are another essential component in the nation's science and technology infrastructure for addressing a broad range of important issues in modern materials. The newest neutron facility, the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, will be the centerpiece of the DOE effort in the application of neutrons and is positioned to become the world's premier neutron source. We support the proposal from the SNS to undergo a power upgrade from 1.4 MW to 3 MW that will significantly enhance the scientific productivity of this facility with only a modest additional 10% investment. This upgrade would open unique scientific opportunities in areas previously inaccessible to measurement science, and it would substantially increase throughput in the portfolio of experiments already on line. The power upgrade proposal

is an integral part of a well-developed longer-term plan exploring avenues to further capitalize on the major investment in the SNS. The project is ready for CD-0. The SNS facility can significantly broaden its scientific impact especially in the central areas of nano- and bio-sciences through construction of a long wavelength target station. The committee strongly endorses this project and recommends planning for CD-0 before 2010.

Transmission Electron Aberration-corrected Microscope (TEAM)

The transmission electron aberration-corrected microscope proposal would develop a remarkable new class of electron imaging, down to atomic resolution, which can provide new capabilities including an *in-situ* experimental stage. The projected improvement in the spatial resolution, contrast, sensitivity and flexibility of design of electron optical instruments will provide an unprecedented opportunity to observe directly the atomic-scale order, electronic structure and dynamics of individual nanoscale structures. With remote access capabilities, this “distributed facility” will also serve as a future model for how to optimize both accessibility and utilization of the instruments. The project has central importance and the BESAC Subcommittee strongly recommends it go forward. The TEAM instrument will serve as a platform for multiple aberration corrected instruments optimized for different purposes such as wide-gap *in-situ* experimentation, ultimate spectroscopy, ultra-fast high resolution imaging, synthesis, field-free high resolution magnetic imaging, electron diffraction and spectroscopy under a variety of extremes of temporal, spectral, spatial or sample environmental conditions. The development team is strongly urged to carefully explore collaborations with the private sector that helps advance their vision and will lead to a broader impact of the investment on future instrumentation.

Cross Cutting Issues

As scientists across the nation utilize US facilities, they currently experience an urgent need for optimized instrumentation to make best use of the intense X-ray and neutron beams available there. While the 1996 Facility Instrumentation Initiative significantly strengthened the facilities and enabled important advances in science, a large subset of instruments remain inadequate for utilizing the bright beams that are now available. It is therefore time for a new instrumentation initiative to enable advances in detector performance and other advanced instrumentation that will allow scientific breakthroughs. The BESAC Subcommittee recommends that development in the following areas be a priority: electron gun technology, detector technologies, cutting edge end stations, automation, robotics, energy recovery linacs (ERLs) and superconducting short period undulators. Training of personnel in development of a broad range of scientific instrumentation, and particularly in accelerator design, is an important cross cutting issue that must be effectively addressed.

Additional Important Recommendations:

Workforce for the Future

Looking to the future of DOE facility design, implementation and operation, a highly educated scientific and technological workforce is critical. We recommend that every effort be made to retain our current workforce and to recruit and train the next generation of the best minds to build and exploit the capabilities of these world-class facilities. This includes the training of accelerator physicists. The success of these facilities is determined by the quality of the scientists and engineers that design, operate, and use these facilities. It is imperative that DOE address workforce infrastructure issues on the same level of priority that they address construction and operation issues in order to realize the full range of outstanding opportunities that these future facilities offer.

General Recommendation for the Future

We urge that facilities road-mapping not be limited to one workshop, but become a regular part of the BES strategic planning process, with 20-year facilities roadmaps conducted every five years. Furthermore, we suggest additional periodic long-range evaluations of the science program needs of BES, so that large facilities can be considered in the context of the overall BES science mission. This is the best way to ensure that the large facilities of the future will continue to effectively serve the BES program.

I. Charge to BESAC and the Subcommittee

The charge from the Director of the Office of Science to the BES 20 Year Facilities Roadmap Subcommittee was to evaluate the scientific merit and technical readiness of proposals for future facilities and upgrades. (Appendix I) Only requests in excess of \$50 M were reviewed, and nearly all requests came from BES laboratories. Our subcommittee was asked not to rank-order the facilities, and not to consider their overall budgetary impact. We did consolidate some proposals to underscore important cross-cutting issues, as discussed below. In some cases we also took the liberty of separating parts of multi-component proposals and evaluated these parts separately.

This report focuses on large user facilities, such as X-ray light sources and neutron sources, and is obviously limited to those needs that can be articulated now. Proposals were solicited from DOE laboratories and existing facilities such as the National Synchrotron Light Source (NSLS), the Advanced Photon Source (APS), the Advanced Light Source (ALS), the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR). We were not charged and did not consider a far broader range of potential future facilities beyond those presented to the subcommittee that might become crucial to the 20-year BES mission, such as facilities specializing in nanofabrication, or catalysis, or high energy lasers. Finally, this is not a comprehensive review of the science program needs of BES over the next 20 years, much of which does not involve large facilities.

II. Evaluation and Recommendations

A. Light Sources:

1. Light Source Facilities Initiative

The four DOE light sources are absolutely central for the advancement of the nation's scientific research and technology. Each light source has unique characteristics and is successful in its performance and service to the scientific users. They produce forefront research and serve more than 7000 scientists across the nation. However, each of the light sources requires urgent upgrades to respond to the scientific challenges in the future and for the scientific output to remain internationally competitive. It is crucial that the DOE provide adequate upgrade support funds in a timely manner. We strongly recommend that DOE aggressively pursue a funding initiative, in coordination with all four light source facilities, which will address the needed upgrades and best serve the

user community. Based on the presentations to the BESAC Subcommittee, these include, but are not limited to, the following:

Advanced Light Source (ALS) Upgrade

The ALS is a VUV-X-ray 3rd-generation light source that has been operating successfully for almost a decade and is generating forefront science over broad areas of research. However, the ALS was the first 3rd generation machine to be commissioned, and its performance will soon be outstripped by the new light sources in Europe (Swiss, British, and French light sources). For the science to remain competitive in a variety of research areas that require the highest possible source brightness, such as high-spatial-resolution soft X-ray microscopy, high-resolution spectroscopy, and coherent scattering and imaging, the ALS needs to be upgraded. The scientific programs are clearly pushing against the limits of current ALS capabilities.

The upgrade of this VUV-X-Ray light source consists of implementing full energy injection and higher current, as well as replacing obsolescent insertion devices (IDs) and beamlines with state-of-the-art IDs and new beamlines that will ensure groundbreaking research. A substantial and sustained increase in their accelerator improvement project (AIP) funding over the next five years would enable this upgrade in an effective and timely manner.

Advanced Photon Source (APS) Upgrade

The Advanced Photon Source is one of the world's leading hard X-ray synchrotron sources. As the country's only high energy 3rd generation source, it plays a critical role in serving the nation's hard X-ray scientific community. The APS must remain in this leadership role by continuing to develop and implement new accelerator design and state-of-the-art instrumentation so that its performance and scientific output continue at the leading edge. The APS upgrade proposal is divided into four phases. The first two phases are described below:

Phase I: Complete the installation of the remaining beamlines and optimize the earlier beamlines.

Phase II: Optimize the source by means of innovative insertion devices and accelerator development.

The proposed Phases I and II are an effective path to maintain APS leadership through growth of its scientific community and scientific output. The appropriate mechanisms for achieving these goals are through increased and sustained AIP support and through a scientific facilities instrumentation initiative.

National Synchrotron Light Source (NSLS) Upgrade.

The NSLS is one of the world's most productive synchrotron facilities. Having led the way for dedicated X-ray sources, it continues to be a world leader in the output of synchrotron-based science with an impressive 650 publications per year. It is critical that the NSLS continue to deliver the highest quality synchrotron radiation and support its scientifically diverse user community, which is predominantly in the northeastern sector of the nation. To maintain their prodigious scientific output in the near future will require continued beamline innovation and development, and, for instance, instrumentation for higher energy and spatial resolution. These enhancements will best be achieved through increased and sustained AIP support.

2. New Light Source Facilities

Near Term:

Linac Coherent Light Source (LCLS)

The Linac Coherent Light Source (LCLS) proposal is the only proposal among those considered by the 20-Year BES Facilities Roadmap Subcommittee that has already passed CD-0 and CD-1. Although currently not a traditional user facility, this project is critical for the planning of science and ultimately needed to validate many aspects of the science driving the entire class of future X-ray free electron lasers (XFEL) that were proposed. The LCLS will provide both scientific and technical benchmarks for further developments in this field. The scientific case for the LCLS, which had earlier been demonstrated continues to grow. Evidence of this comes from recent successful experiments at the TESLA Test Facility at DESY in Hamburg, and the rapid growth of interest within the potential user community. The BESAC Subcommittee gives this project its highest recommendation for strong continued support.

Longer Term:

National Synchrotron Light Source (NSLS) Third Generation Ring

With the implementation of third generation facilities around the world, including the APS, the European Synchrotron Radiation Facility (ESRF) and the Diamond rings, the NSLS is at a critical juncture. Recognizing the importance of meeting the future needs of its user community, NSLS has proposed an NSLS II facility upgrade. The proposed upgrade includes the construction of a 3 GeV, 500 mA, highly optimized third generation storage ring with top-off injection, a self-seeded SASE FEL, a high gain harmonic generation FEL, and a superconducting RF linac for both top-off injection of the storage ring and to drive the FELs. Furthermore, the current X-ray ring would be refurbished into an enhanced VUV/IR storage ring.

The NSLS II project is an ambitious plan that embraces the needs of its scientific community and beyond by including elements of fourth generation light sources. However, the committee believes that the scope of this proposal is too broad and does not take into account DOE's national facilities portfolio. The committee believes that it is critical that NSLS focus on the elements of their proposal that fosters growth in the strongest and most productive sectors of their user community. The BESAC Subcommittee recommends that NSLS place their attention on the design and construction of a third generation storage ring that includes an injector facility optimized for top-off. The BESAC Subcommittee also recognizes the importance of VUV/IR production and encourages the NSLS to consider accommodating VUV/IR science within the concept of a third generation ring.

Additional BESAC Subcommittee concerns include the following:

- There is a fundamental incompatibility of linac sources in dual use for FEL and top-off injection. The latter requires a fixed parameter set for stability while the former, by its very nature, requires flexibility. For top-off injection, a superconducting linac is overkill and a costly option. The electron-gun requirements for FEL and top-off are also different.
- Cost estimates for various elements of the proposal appear unrealistic or inadequate.

Advanced Photon Source (APS) Super Storage Ring

The APS proposal to the BESAC Subcommittee details their vision for the Future APS Super Storage Ring as Phase III and Phase IV as described below:

Phase III is an upgrade of the whole instrument suite to next-generation capabilities. This includes improving efficiency and performance through advanced detectors, automation, and robotics.

Phase IV involves a major upgrade of the synchrotron facility to develop a super photon ring.

The BESAC Subcommittee believes that the proposed Phase III is an effective path to maintain APS leadership and growth of its user scientific community and scientific output. Increased and sustained AIP support and funding from a scientific facilities instrumentation initiative should be used to achieve this goal.

While the APS focuses on carrying out its mission to provide the U.S. with a high brightness source of X rays for the next ten years, it is also important that APS maintain its leadership role into the next decade by utilizing its strengths in accelerator design and instrumentation. Phase IV is a Super Storage Ring, which would provide a factor of 100 increase in brilliance over the existing APS machine. This is the ultimate storage ring; however, it is premature to commit to such a design before it is clear that many of the

technical hurdles have been cleared. We believe that the Phase III upgrade to the facilities beamlines should be a component of Phase IV to optimize the new next generation facility concept. The linac injector for the FEL source should be considered as a separate proposal in the context of a “Greenfield FEL”. Meanwhile, an injector optimized for the super-ring concept should be considered as part of Phase IV.

X-Ray Free Electron Lasers (XFELs): Linac Coherent Light Source II (LCLS II) and Greenfield Free Electron Laser

These proposals are in the earliest stages of development.

The LCLS II proposal shows that the Stanford Linear Accelerator Center (SLAC) site could accommodate a future user facility based on XFELs, with multiple undulators, end stations, and full use of the SLAC linac. The proposal suggests several possible improvements to XFEL technology, such as improved gun emittance and higher energy injectors, that might be implemented in future machines. One very important element of the LCLS II proposal is that SLAC would incorporate the increased use of the linac for future XFEL operations. We feel that the LCLS project is in a unique position to evaluate critical technologies that will enable future XFELs.

Looking ahead 20 years, and assuming that the predicted successes of LCLS are realized, the community will demand a full-scale, state-of-the-art, fully coherent, super-bright, multiplexed, diffraction limited facility, the so called “Greenfield” XFEL. The committee feels that the appropriate research and development that could enable this facility must go forward. Critical areas that need improvement include gun technology, detector optimization, and electron beam stability, as well as continued advances in the scientific case. Within five years, experience with XFEL science and technology should mature to the point that a decision can be made on the scope of any future Greenfield facility.

Far Infrared (Terahertz) Light Source Facilities

There is considerable scientific interest in high power, short-pulse radiation in the terahertz and far infrared region. This range is important for studying collective excitations in solids, molecular librations and rotations, protein conformational dynamics, superconductor bandgaps, and electronic and magnetic scattering. A facility that provides short pulsed and high average power radiation in this spectral region offers exciting opportunities for probing fast and ultra-fast chemical, physical and biological processes.

Two proposals for facilities that would produce terahertz and far infrared coherent synchrotron radiation in this region were presented. Lawrence Berkeley National Laboratory proposed a Coherent Infrared Center (CIRCE) at the ALS. Thomas Jefferson Laboratory proposed an IR/UV FEL user facility.

While each of these two groups has identified an exciting new potential user community, it is not yet clear whether the scientific communities that might use these facilities have embraced this new technology. The BESAC Subcommittee encourages the DOE to organize national workshops to explore the scientific advantages of research with terahertz radiation at user facilities. Further the BESAC Subcommittee notes that some of the parameters of these coherent synchrotron machines are only comparable to available table-top sources: the energy per pulse, full dc to terahertz coherence, and pulse durations are not much different. However, there are opportunities for significantly higher stability and average power in these machines. Some significant technical hurdles need to be explored more fully. The BESAC Subcommittee noted that trials at BESSY have explored coherent synchrotron radiation (CSR) instabilities in storage rings, but have not yet addressed the issue fully. Research to resolve this issue, as well as to develop the energy recovery technology needed for linac-based sources, must precede any full-scale commitment to a new facility.

The cost of these new light sources should be relatively modest, partly because the level of hazard and the amount of shielding required in this wavelength range is far less than with present sources. Therefore, it should be possible to develop these sources without the kind of full-scale new facilities requests needed for X-ray or neutron facilities. The BESAC Subcommittee recommends that issues related to instrument development and sample environment be more carefully examined to enhance the likelihood of success in this area. It is also important to more completely document the science demand for such a national user facility dedicated to this frequency range and to have the national community assist in deciding the type of facility that best serves its needs.

Linac-based Ultra-fast X-ray (LUX) Facility at Lawrence Berkeley National Laboratory (LBNL)

This is an innovative proposal for an ultrafast X-ray and VUV facility. It consists of a recirculating superconducting linac employing a novel bunch compression scheme and x-ray compression capable of a few tens of femtoseconds, combined with a novel high-gain harmonic-generation (HGFG) capability, and a novel clock derived from an optical ultrafast laser to ensure a high precision synchronization for pump-probe experiments. This facility is appropriate for weak probe experiments for the most part, and as such it does not compete with XFEL or VUV FEL sources. The proposed site is adjacent to the Advanced Light Source.

The proposal presents a strong scientific case, based on a large community involved in femtosecond chemistry and physics who could take advantage of this source to do pump-probe experiments with short wavelength probes. The location will allow a high degree of synergy with existing ALS users and infrastructure, as well as connections to the LBNL materials groups, and the Molecular Foundry Nanoscience center. The

machine is open to future upgrade to utilize energy recovery when this technology becomes available.

This proposal is for a new facility, not an upgrade, and the planning is in the very earliest stages. The proposal is not yet ready to proceed to CD-0. The BESAC Subcommittee applauds this group for its vision and innovation and suggests that they organize national reviews of the science case, which are necessary before a national competition for such a new facility. The BESAC Subcommittee notes that local reviews (e.g., the Napa conference in 2002) were very positive. Important weaknesses that need to be addressed in a future proposal are: the relatively high cost of the machine, its low average power, and the lack of demonstrated HGHG cascades on which the VUV portion depends.

Spallation Neutron Source (SNS) Power Upgrade

The Spallation Neutron Source is the centerpiece of the DOE effort in the application of neutrons to science and technology. Because neutron scattering generally remains flux-limited technique, a central specification for the SNS is the peak power of the proton beam that creates neutrons through spallation. The proton accelerator in the baseline SNS project will provide 1.4 MW protons in 700 ns pulses at a 60 Hz repetition rate.

Throughout the design, the SNS project has retained the option for substantial future upgrades of neutron production capabilities. This proposal seeks to realize the potential by (1) upgrading the proton accelerator system to 3 MW with a potential of going to 5 MW (2) upgrading the power handling capabilities of the target to that same power, and (3) developing new neutron scattering detector systems to handle the increased neutron flux. These enhancements could be completed in 2009 if initiated as proposed in 2006. This enhancement of the original facility would double the capabilities of SNS for an added investment of perhaps 10% of the original facility cost.

Because neutron scattering is generally flux limited, the upgrade to the neutron flux would substantially increase throughput and open unique new science opportunities. While this impact is not contingent on realization of the second target station, the project does prepare the facility for such an upgrade.

Technically this proposal is part of a well-developed long-term plan for upgrading the SNS. The accelerator upgrades are considered as relatively simple extrapolations of existing technologies. The target upgrade is probably more challenging but within the limits that are considered to be realistic in the spallation target community. Inclusion of investments in detector technology is crucial and prudent. The timing of the project ensures that the accelerator and target expertise will be available to carry out the upgrade

in the most efficient fashion. In addition, the upgrade can be accomplished with minimal disruption to the early operating schedule of the facility.

The BESAC Subcommittee considers the potential science impact of the proposed upgrade to the SNS facility to be excellent and the project to be ready for CD-0.

Spallation Neutron Source (SNS) Long Wavelength Target Station (LWTS)

The construction of a long-wavelength second target station for SNS operated at 20 Hz compared with the 60 Hz for the primary target station will enable SNS to be optimized for experiments such as small-angle neutron scattering, reflectivity, and high-resolution inelastic neutron scattering and diffraction. For these types of experiments, an intensity gain of a factor of 3 will be realized with a concomitant increase in the efficiency and throughput of experiments geared to the study of soft condensed matter, magnetism, and nanomaterials. These are the areas of the highest demand from the scientific and technical community. Thus, the scientific need for this facility is well justified. The scientific case and technical planning for this facility has been done comprehensively by SNS. The subcommittee strongly endorses this project and recommends planning for CD-0 before 2010.

Accelerator-based Continuous-Neutron Source (ACNS)- Brookhaven National Laboratory

This proposal calls for the development of an accelerator-based continuous-neutron source (ACNS). The proposed accelerator is a ~200 m long, 1.25 GeV superconducting proton linac operating at 8 mA producing 10 MW of average beam power and a thermal neutron flux of $> 10^{15}$ n/cm²-sec. The flux from this proposed ACNS would be comparable to the two highest flux reactors in the world today, the High Flux Isotope Reactor (HFIR) and the Institut Laue Langevin (ILL).

The ACNS proposal addresses neutron scattering in the US 10-20 years from now. At that time the SNS will be fully operational and with the proposed upgrades mentioned elsewhere in this report, it should be a formidable short pulsed neutron scattering facility. However, the nation's fission neutron sources will be close to the end of their useful lives. It is suggested that their capabilities could be replaced by an ACNS.

The complementary aspects of continuous and pulsed sources have been highlighted in many previous studies. However, a continuous beam plays a special role mainly for fission based sources. Given the proposed use of a proton accelerator to produce neutrons at the ACNS, it is by no means clear that the choice is between μ s pulses at ~60 Hz and a continuous beam. As experience is gained with state of the art short pulsed spallation sources and as present fission neutron sources approach the end of

their useful lives, the US neutron community will have to determine the need and the best approach, to complement the capabilities of the SNS. Given the long term nature of the proposal, the ACNS project does not sufficiently push the envelope to produce exciting new capabilities for science. Specifically, the documentation indicates that the neutron flux at the proposed ACNS would only be on a par with that which has been available at the HFIR and the ILL since the mid sixties.

The BESAC Subcommittee recommends that the scientific need and the best technology and time structure for a neutron source to complement the SNS continues to be explored. Finally, if an ACNS or quasi-ACNS becomes a serious option for the future, then site selection should be opened to competition.

HB-2 Cold Neutron Facility at the High Flux Isotope Reactor (HFIR)- Oak Ridge National Laboratory

This project calls for the construction of a new 40,000 sq. ft. guide hall at the HFIR with laboratories, offices and user support space, a high brightness cold source and guide system and five cold neutron beam lines with neutron science instruments. The proposed new guides would take advantage of the large diameter and high brightness of the HB-2 beam port at the HFIR to develop the world's most intense cold neutron facility offering approximately three times the neutron brightness of currently available sources including the cold neutron guide currently under development at the HB-4 beam port at the HFIR. The initial suite of instruments would include a polarized Laue diffractometer, grazing incidence reflectometer, a triple-axis spectrometer, a small-angle neutron scattering spectrometer and one guide devoted to neutron physics with future plans to add five additional instruments.

A strong case can be made for additional capabilities to support neutron scattering within the United States, and the critical need for new neutron scattering infrastructure is well documented in numerous DOE studies and reports and has been a concern of BESAC for many years. In response to this need, the DOE has made a significant commitment by funding a new spallation source, the SNS, and by making a considerable investment in the upgrade of existing neutron scattering facilities including the HFIR. DOE provided funding at HFIR for a new cold guide hall, which is currently under construction, and support for new instruments and other enhancements in the HFIR infrastructure. The BESAC Subcommittee considers this proposal for a second cold guide hall at HFIR as worthy of further consideration, but it did not have sufficient documentation on the mission need or how this request would fit into the broader activities currently supported or proposed within DOE. Even with the recognized need for enhancements to neutron scattering facilities beyond those currently being pursued, it is imperative that additional consideration be given to this request as it relates to other projects. For example, Oak Ridge National Laboratory has also proposed as part of this 20-Year BES Facilities Roadmap a power upgrade for the SNS taking it from its current plans to operate at 1.4 MW to 3.0 MW and eventually to 5.0 MW along with the addition

of a long wavelength target station at the SNS. How this project and the requested instrumentation complements current and proposed opportunities at SNS is not clear

The BESAC Subcommittee considers this project to be important but calls on the Oak Ridge National Laboratory and the neutron scattering community to carefully review this proposal in the context of the proposals for increased power at the SNS and for the long wavelength target station. Care should be given to documenting the various scenarios with regard to optimization of instrumentation leading to a prioritized list of instrumentation opportunities and challenges associated with the enhanced power for SNS, the addition of a long wavelength target station at SNS and a second guide hall at the HFIR. Input from the neutron user community on these priorities is essential as DOE further pursues opportunities to rebuild the United States neutron science infrastructure.

4. Other Facilities

Transmission Electron Aberration-corrected Microscope (TEAM): A Distributed Facility

The Lawrence Berkeley National Laboratory, National Center for Electron Microscopy (NCEM) has joined with the Argonne National Laboratory, Electron Microscopy Center (EMC), Brookhaven National Laboratory, the Frederick Seitz Materials Research Laboratory, Center for Microanalysis of Materials (CMM), and the Oak Ridge National Laboratory, Shared Equipment Research Program (SHARE) in a proposal for a national project to develop the next generation transmission electron microscope.

The goal of this project is to construct and operate several new aberration-corrected electron microscopes, and to make this capability widely available to the materials and nanoscience communities. The projected improvement in spatial resolution, contrast, sensitivity, and the flexibility of design of electron optical instruments will provide unprecedented opportunities to observe directly the atomic-scale order, electronic structure, and dynamics of individual nanoscale structures. The BESAC Subcommittee feels this project has central importance, and strongly recommends it go forward.

The TEAM instrument will serve as a platform for multiple aberration-corrected instruments optimized for different purposes such as wide-gap in-situ experimentation, ultimate spectroscopy, ultrafast high resolution imaging, synthesis, field-free high resolution magnetic imaging, diffraction and spectroscopy, and other extremes of temporal, spectral, spatial or environmental conditions. The TEAM proposal calls for the instruments to be remotely accessible as a distributed facility, which should serve to optimize both the accessibility and utilization of the instruments. A key aspect will be to make it the microscopes compatible with a variety of sample environments.

The BESAC Subcommittee has the following technical comments on the proposal:

1. This proposal for the construction and utilization of a new aberration-corrected microscope has a high probability of success. The technology is already proven. The methodology is established to go below one angstrom resolution. The existing facilities in Europe have been found to work well.
2. The theory for aberration correction is well advanced.
3. The people who are working on the optics for the microscope are the best in the field.
4. The proposed environmental cell in the third stage of the project will be the greatest challenge.
5. The TEAM project members are urged to work with the supplier/instrument community for the development and construction of the instruments.
6. The BESAC Subcommittee considers the proposed microscopes to be central to the DOE's mission. The reviews supporting the Mission Need have been completed. The TEAM project members should go forward to prepare a Conceptual Design Report and other prerequisites for CD-1.

Plant Metabolomics – Iowa State University

This is a proposed national facility for Plant Metabolomics, to be established on the campus of Iowa State University and to be equipped with sophisticated analytical equipment for high throughput plant cell analysis, using techniques such as capillary electrophoresis, MRI, NMR, AFM, optical imaging, etc. The BESAC Subcommittee feels that this research is important and endorses the move towards closer collaborative research linking Ames Laboratory with Iowa State University, recognizing that the scientists involved are among the leaders in this field. The BESAC Subcommittee feels that this research trust by this group of scientists is important but believes that any decision on a facility such as this would need to be reviewed in the context of competing proposals from other institutions and laboratories.

Proposal for a Complex Interfacial Catalysis Facility

Pacific Northwest National Laboratory (PNNL) has proposed a user facility for catalysis research. The purpose of the Complex Interfacial Catalysis Facility is to provide the tools needed to advance catalysis science by enabling the development of the fundamental principles underlying catalytic phenomena.

The Subcommittee found this report to be interesting. Catalysis is an important part of the BES portfolio and PNNL has many good scientists in this area. However, the Subcommittee believes that any decision on a facility such as this would need to be reviewed in the context of competing proposals from other institutions and laboratories.

5. Cross Cutting Issues

Detectors and other Instrumentation

Scientists across the nation using US facilities are experiencing an urgent need for optimized new instrumentation to successfully tackle scientific measurements in condensed matter, nanotechnology, catalysis, biotechnology, and complex materials. As we enhance the source brightness at our facilities, we must ensure that we can continue to take full advantage of our investment with parallel advances in scientific instrumentation, especially in end stations, detector technologies, automation, robotics, and sample environments.

The 1996 Facility Instrumentation Initiative enabled many advances in science. Now it is time for another facilities instrumentation initiative to enable advances in detector performance and in advanced instrumentation that will allow scientific breakthroughs. Addressing the need to upgrade instrumentation in an effective and timely manner enables advances in science and progress in a variety of research and technologically important areas.

Electron Gun Development

The evolution of light sources toward diffraction limited radiation at high energy, to sub-picosecond photon pulse lengths, and with FEL operation places increasingly stringent demands on the three dimensional phase space density of the electron beam. For linear accelerators, these performance requirements translate directly into the necessity of smaller emittance, higher charge bunches generated at the electron gun. In addition, increased repetition rates at the gun allow higher average flux, multiple undulator end stations, and ultimately the generation of storage-ring-class currents in energy recovery linacs. Also, with lowered emittance, the resulting higher gain will enable important cost savings. For example, undulator lengths and electron beam energy could be reduced.

The critical enabling technology to advance linac-based light sources is the electron gun. At low repetition rates, the present RF photocathode technology generates 1 mm-mrad normalized emittance bunches with a charge of a nanocoulomb at 100 Hz repetition rates. For projects such as an LCLS upgrade to higher energy photons or for

the “Greenfield” FELs, emittances at the 0.1 mm mrad level will be necessary to increase photon beam energies to 30 keV and above. Repetition rates to tens of kilohertz are envisioned for optimal facility performance. Performance enhancements in RF photocathode guns are crucial to advanced FELs and extended capability undulator sources such as LUX.

For energy recovery linear accelerators, improvements of injector performance to 100 mA average current at 1 mm mrad emittance will yield photon beam specifications possibly bettering that obtainable in the storage ring approach to 4th generation light sources. The shorter bunch lengths inherent in linac beams, into the femtosecond regime, offer another potential benefit. For an ERL, the current state of the art at 10 mm mrad at 100 pC bunch charge at 10 mA average current (100 MHz repetition rates) needs to be extended to 1 mm mrad at 100 mA (1 GHz repetition rates). The current technology of DC photocathode guns may yield these gains, but work on RF and superconducting RF guns should also be pursued.

These order of magnitude improvements in electron guns (DC, RF, and superconducting RF) will allow qualitative advances in light sources capabilities at reduced costs. They are the highest-leveraged technology for next generation light sources. The BESAC Subcommittee recommends that DOE BES strongly support and coordinate research and development in this unique and critical technology. The strengths and core competencies of Office of Science laboratories (and also across agency boundaries) should be integrated into a comprehensive high performance national electron gun R&D program.

Energy Recovery Linac (ERL) Development

The DOE BES should take a lead role in the development of the basis for energy recovery linear accelerators (ERL), which may outperform the conventional hard X-ray storage ring sources envisioned for a decade from now in both brightness and short bunches. Given that ERLs might be a competitive technology for 4th generation light sources, the BESAC Subcommittee recommends that DOE BES actively support ERL research and development.

An ERL R&D program would address the following key issues to demonstrate whether or not it is a viable technology for future light sources:

1. Electron gun development (the top priority), as discussed in the electron gun development section of the report.
2. Developing of superconducting RF cavities with sufficient damping for 100 mA beams, both from beam breakup and energy deposition points of view.
3. Energy recovery at high average current and high energy.

4. Energy recovery with the manipulations of phase space envisioned for light source optimization (e.g., bunch compression, transverse deflection, chirping), given the adiabatic antidamping (i.e., increase) of the beam geometric emittance and relative energy spread as the beam is decelerated for energy recovery.
5. Stability of ERL sources, with sufficient diagnostics of ERL performance through the generated photon beam.

In general, the strengths and core competencies of Office of Science laboratories (and across agency boundaries) should be integrated into a comprehensive ERL R&D program.

Superconducting Short Period Undulators

The next generation of X-ray sources either based on synchrotron radiation or free electron lasers presented to the committee require the development of a large number of undulators with high magnetic field quality. Undulators presently in use in light sources and FELs are made of permanent magnet material. Recent developments indicate that short period superconducting undulators should, in the near future, outperform permanent magnet based undulators by providing a higher magnetic field, a shorter period, a larger beam aperture and a higher resistance to radiation damage. These benefits have been recognized by the majority of the proposed upgrades or new facilities (NSLS, ALS, APS, LUX, “Greenfield” FEL) which are basing their future undulator sources on this yet immature but promising technology. Such undulators will reduce the requirement on electron energy for reaching a particular photon energy or alternatively extend the high brightness photon energy range in existing facilities.

The BESAC Subcommittee recommends that DOE support and coordinate the development of superconducting undulators to preserve the long-term competitiveness of its VUV and X-ray sources.

6. Workforce for Development and Use of these Facilities

Looking to the future of DOE facility implementation and operation, a highly educated technological workforce is critical. We recommend that every effort be made to retain our current workforce and to recruit and train the next generation of the best minds to design, build and exploit the capabilities of these world-class facilities. It is particularly critical to train and grow the next generation of accelerator designers.

The success of these facilities is only as good as the scientists that design, operate and use these facilities. It is imperative that DOE address workforce infrastructure issues on the same level of priority that they address construction and operation issues in order to realize the full range of outstanding opportunities that these future facilities offer.

7. Recommendation for Follow-up

A one time Roadmap such as this is extremely valuable, but it cannot possibly accommodate all future innovation and discovery. We urge that facilities road-mapping not be limited to one workshop, but become a regular part of the BES strategic planning process, with 20-year facilities roadmaps conducted every five years. Furthermore, we suggest additional periodic long-range evaluations of the science program needs of BES over 20 years, so that large facilities can be considered in the context of the overall BES science program and mission. This is the best way to ensure that the large facilities of the future will continue to effectively serve the BES program.



Department of Energy
Washington, DC 20585

December 18, 2002

Professor Geraldine Richmond
Professor of Chemistry
1253 University of Oregon
Eugene, Oregon 97403-1253

Dear Professor Richmond:

For more than a half-century the Department of Energy's Office of Science has envisioned, designed, constructed and operated many of the premiere scientific research facilities in the world. More than 17,000 researchers and their students from universities, other government agencies, private industry and from abroad use Office of Science facilities each year—and this number is growing. For example, the light sources built and operated by DOE now serve more than three times the total number of users, and twenty times as many users from the life sciences, as they did in 1990.

Creating these facilities for the benefit of science is at the core of our mission and is part of our unique contribution to our Nation's scientific strength. It is important that we continue to do what we do best: build facilities that create institutional capacity for strengthening multidisciplinary science, provide world class research tools that attract the best minds, create new capabilities for exploring the frontiers of the natural and physical sciences, and stimulate scientific discovery through computer simulation of complex systems.

To this end, I am asking all the Office of Science's advisory committees to join me in taking a new look at our scientific horizon, and to discuss with me what new or upgraded facilities will best serve our purposes over a timeframe of the next twenty years. More specifically, I charge the committees to establish a subcommittee to:

- A. Consider what new or upgraded facilities in your discipline will be necessary to position the Office of Basic Energy Sciences at the forefront of scientific discovery. Please start by reviewing the attached list of facilities, assembled by Dr. Patricia Dehmer and her team, subtracting or adding as you feel appropriate, with prudence as to cost and timeframe. For this exercise please consider only facilities/upgrades requiring a minimum investment of \$50 million.



B. Provide me with a report that discusses each of these facilities in terms of two criteria:

1. The *importance of the science* that the facility would support. Please consider, for example: 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 will create new synergies within a field or among fields of research; and what level of demand exists within the scientific community for the facility. In your report please categorize the facilities in three tiers, such as "absolutely central," "important," and "don't know enough yet," according to the potential importance of their contribution. Please do not rank order the facilities.
2. The *readiness* of the facility for construction. Please think about questions such as: 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. Group the facilities into three tiers according to their readiness, using categories such as "ready to initiate construction," "significant scientific/engineering challenges to resolve before initiating construction," and "mission and technical requirements not yet fully defined."

Many additional criteria, such as expected funding levels, are important when considering a possible portfolio of future facilities, however for the moment I ask that you focus your thoughts on the two criteria discussed above.

I look forward to hearing your findings and discussing these with you in the future. I would appreciate at least a preliminary report by March, 2003.

Sincerely,



Dr. Raymond L. Orbach
Director
Office of Science