

# **Basic Energy Sciences Facilities Prioritization**

**Co-Chaired by:**

**John C. Hemminger, BESAC Chair  
University of California, Irvine**

**and**

**William Barletta  
Massachusetts Institute of Technology**

**February 26-27, 2013**

Bethesda North Marriott Hotel and Conference Center  
5701 Marinelli Road  
North Bethesda, MD 20852



JOHN C. HEMMINGER  
VICE CHANCELLOR FOR RESEARCH  
OFFICE OF RESEARCH  
160 ALDRICH HALL

IRVINE, CALIFORNIA 92697  
Phone 949-824-5796 Fax 949-824-2095  
[JCHEMMIN@UCI.EDU](mailto:JCHEMMIN@UCI.EDU)  
[HTTP://SURFSCLPS.UCI.EDU](http://SURFSCLPS.UCI.EDU)

March 21, 2013

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

Dear Dr. Brinkman,

On behalf of the Basic Energy Sciences Advisory Committee I am forwarding to you the report that you had requested in your December 20, 2012 charge letter. This report, Basic Energy Sciences Facilities Prioritization, is the result of a meeting of a BESAC Subcommittee in February 2013 to address your charge. The Sub-committee heard presentations by each of laboratories that house the facilities.

Dr. William Barletta and I co-chaired this Subcommittee. The assessments of the Subcommittee and the contents of this report were discussed in detail, finalized, and unanimously accepted by the subcommittee and the members of the full BESAC on March 1, 2013 during our public BESAC 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 world-leading new science and discoveries that these facilities will enable.

Sincerely,

John C. Hemminger  
Chair, BESAC  
Vice Chancellor for Research  
Professor of Chemistry

C: Patricia Dehmer  
Harriet Kung  
BESAC Membership

## **Subcommittee on BES Facilities Prioritization**

John C. Hemminger* (co-chair)	University of California-Irvine
William Barletta* (co-chair)	Massachusetts Institute of Technology
Simon Bare*	UOP LLC, a Honeywell Company
Gordon Brown*	Stanford University
Robert Dimeo	NIST
Ernest Hall*	GE Global Research
William McCurdy*	LBNL/University of California-Davis
Robert McQueeney	Ames Laboratory
Keith Moffat	University of Chicago
Monica Olvera de la Cruz*	Northwestern University
Anthony Rollett*	Carnegie Mellon University
Gary Rubloff*	University of Maryland
Sunil Sinha	University of California, San Diego
John Spence*	Arizona State University
Douglas Tobias*	University of California-Irvine
John Tranquada*	Brookhaven National Laboratory

**\*BESAC members**

**Basic Energy Sciences Advisory Committee  
Subcommittee on BES Facilities Prioritization**

**Agenda  
Wednesday, February 27, 2013**

Bethesda North Marriott Hotel and Conference Center  
5701 Marinelli Road  
North Bethesda, MD 20852

**Linden Oak Room**

Wednesday, February 27, 2013		
7:30am - 8:00am	Continental Breakfast	
8:00am - 8:45am	Advanced Photon Source and Advanced Photon Source-Upgrade	Eric Isaacs Argonne National Laboratory
8:45am - 9:30am	National Synchrotron Light Source and National Synchrotron Light Source-II	Steve Dierker Brookhaven National Laboratory
9:30am - 9:50am	Break	
9:50am - 10:50am	Stanford Synchrotron Radiation Lightsource, Linac Coherent Light Source, and Linac Coherent Light Source-II	Chi-Chang Kao SLAC National Accelerator Laboratory
10:50am - 11:35am	Advanced Light Source and Next Generation Light Source	Paul Alivisatos Lawrence Berkeley National Laboratory
11:35am - 1:00pm	Lunch – Oakley Room (Subcommittee ONLY)	BESAC Subcommittee
1:00pm - 2:00pm	High Flux Isotope Reactor, Spallation Neutron Source and the Second Target Station	Thom Mason Oak Ridge National Laboratory
2:00pm - 2:20pm	Lujan Neutron Scattering Center	Mark Bourke Los Alamos National Laboratory
2:20pm - 3:00pm	Break	
3:00pm - 4:40 pm	Center for Functional Nanomaterials Center for Integrated Nanotechnologies Center for Nanophase Materials Sciences Center for Nanoscale Materials Molecular Foundry	Emilio Mendez (BNL) David Morris (LANL) Sean Smith (ORNL) Amanda Petford-Long (ANL) Omar Yaghi (LBNL)
<b>Subcommittee Only</b>		
4:40pm - 6:00pm	Discussion – Oakley Room	BESAC Subcommittee
6:00pm - 7:00pm	Dinner	
7:00pm - 9:00pm	Discussion and Report Writing	BESAC Subcommittee
9:00pm	Adjourn	

# **Subcommittee on BES Facilities Prioritization Report**

## *Executive Summary*

The Department of Energy's Office of Science plays an essential role in creating and supporting user facilities that attract users from across the U.S. and around the world. These facilities are indispensable as they allow users to produce world-leading science. Basic Energy Sciences (BES) has been a central player in this effort, particularly in envisioning, designing and advancing facilities that are critical to U.S. competitiveness in broad areas of science such as biology, chemistry, physics, materials science, optics and catalysis. Stewardship of the suite of scientific user facilities requires continuous evaluation of the existing facilities as well as foresight into what new facilities will be required to enable the discoveries of the future. The past highly effective management and foresight of the leadership of the Office of Science and the Office of Basic Energy Sciences is in no small part due to the close and highly professional relationship between the office leaders and the community of scientists that make up the BES science community. The present Subcommittee of the Basic Energy Sciences Advisory Committee (BESAC) has completed its prioritization study as a mechanism for assisting in the planning process for the Office of Basic Energy Sciences and the Office of Science.

The Sub-committee has categorized existing and proposed facilities at DOE National Laboratories based on its review of oral and written input from those facilities. The facilities fall into three categories: synchrotron light sources and free electron lasers, neutron sources, and nanoscience centers.

In its deliberations the subcommittee considered both the degree to which the facility will contribute to world-leading science in the period 2014 to 2024 as well as the readiness of the proposed facilities for construction. The relevant criteria are in the charge given to BESAC by Dr. William Brinkman, Director of the Office of Science. The charge letter is included as an appendix to this report.

In assessing the scientific impact of both existing and proposed facilities the Subcommittee considered (1) the degree to which a facility would answer the most important scientific questions, (2) the degree to which other facilities could answer these questions, (3) the breadth of the facility's contribution to many areas of research, (4) the degree to which the facility addresses needs of the broad community of users including those supported by other agencies, and finally (5) the level of user demand. We considered

existing facilities organized into the three broad categories mentioned above: (1) photon based facilities (light sources), (2) neutron based facilities, and (3) nanoscience centers. The BESAC subcommittee found exciting, world-leading science in all categories. BES has the dual responsibility of developing new, world-leading facilities to address future scientific needs and continuing to maintain and upgrade its currently operating world-class facilities to respond to the evolving, critical scientific needs of the nation and to take advantage of new technological developments that will allow significant enhancements of existing capabilities.

### **Existing facilities**

*Light Source Facilities* - The system of five operating DOE light sources is an absolutely central resource in America's scientific and technological enterprise. The light sources are heavily used by more than 11,000 scientists from across the country and around the world; each facility produces truly outstanding science. Within this system of photon sources, the committee did find a variation in the degree to which each of the facilities will contribute to world-leading science over the period from 2014 to 2024. That characterization is reflected in Table 1.

Much of that variation derives from the degree to which the capabilities of the facility will be matched or exceeded by other facilities over the assessment period (2014—2024). Nonetheless, all the facilities are highly over-subscribed by users producing outstanding scientific discoveries and are expected to remain so. The U.S. must maintain vital capacity in all of its light source facilities. One of these facilities, NSLS, will be closed in 2014 as its replacement, NSLS-II, begins operation. For that reason the nearly completed NSLS-II is included among the existing facilities. To continue to produce world-leading science in the face of fierce competition from new light source facilities overseas, continual modernization of these facilities is needed. Three proposed major upgrades or new facilities have received DOE Critical Decision-0 (approval of mission need) CD-0 and will be characterized separately.

*Neutron sources* - Leadership in the science of materials is needed to ensure economic competitiveness and enable innovation. For the U.S. to lead in materials research, it must have world-leading neutron science capabilities. Neutrons are a key scientific tool and a complement to photons, especially for studying disordered and aperiodic structures as well as inelastic processes and dynamics. Moreover, neutrons do not suffer from strong z-dependent scattering cross sections enabling studies of, for example, hydrogenous materials that are key to many energy technologies. To that end, BES developed, and runs the world's highest power neutron spallation source, the Spallation Neutron Source

(SNS), and operates two other neutron science facilities that produce outstanding science. All facilities are highly oversubscribed. It is important to note that in terms of total capacity of its neutron instruments the U.S. lags far behind Western Europe. The characterization of the BES neutron sources is summarized in Table 1.

*Nanoscale Science Research Centers (NSRCs)* – These five facilities facilitate world-leading science through their twin missions of pursuing top-quality science and enabling the same for external users through access to NSRC facilities and/or collaboration with NSRC researchers. The Subcommittee identified particular value in synergies between science programs of NSRC researchers, the unique facilities the NSRCs develop, and the benefits available to users. The overall characterization of the NSRCs is given in the third section of Table 1.

Table 1 – The ability of existing facilities to contribute to world leading science in the next decade

Facility name / institution	Ability to contribute to world-leading science in the next decade
<b>LIGHT SOURCES</b>	
Advanced Light Source (LBNL)	Important
Advanced photon Source (ANL)	Absolutely central
NSLS (BNL)	Lower priority
NSLS-II (BNL)	Absolutely central
SSRL (SLAC)	Important
LCLS (SLAC)	Absolutely central
<b>NEUTRON SOURCES</b>	
High Flux Isotope Reactor (ORNL)	Important
Spallation Neutron Source (ORNL)	Absolutely central
Lujan Neutron Scattering (LANL)	Lower priority
<b>NANOSCIENCE CENTERS</b>	
Center for Functional Nanomaterials (BNL)	Important
Center for Integrated Nanotechnologies (LANL)	Absolutely central
Center for Nanoscale Materials (ANL)	Absolutely central
Center for Nanophase Materials Sciences (ORNL)	Important
The Molecular Foundry (LBNL)	Absolutely central

## Proposed projects

*Light sources* - The BESAC and the BESAC Subcommittee strongly urge timely investment in the following major projects: the Advanced Photon Source Upgrade, and the Linear Coherent Light Source-II. To continue to produce cutting-edge science, upgrades at these facilities are needed **now** so that they will remain at the forefront in light source activities. The APS Upgrade and the LCLS-II have received CD-1 (approval of alternative selection and cost range) and are close to receiving CD-2 (approval of performance baseline). The Subcommittee considers both projects *absolutely central to US world leading science*. Both the APS Upgrade and LCLS-II *are ready for construction*.

***In addition to the APS Upgrade and LCLS-II, the BESAC Subcommittee urges DOE to aggressively pursue a new future light source with unprecedented beam characteristics and thus unprecedented opportunities for world-leading science.*** The Director of the Office of Science has Charged BESAC to provide advice on the future of photon sources and science by July, 2013. The Next Generation Light Source (NGLS), which has CD-0 (approval of mission need), could dramatically change the landscape of photon science with soft X-rays; hence it *could be absolutely central to US world leading science*. The NGLS does have “*scientific/engineering challenges to resolve before initiating construction.*”

*Neutron sources* - The BESAC Subcommittee also urges the strong support of a major upgrade to DOE’s premier neutron facility, SNS. The SNS Second Target Station, STS, and the associated power upgrade of the SNS are both crucial to increase significantly facility capability and capacity. The STS *will be absolutely central to US world leading science*. However, this project, which has received CD-0, does have “*scientific/engineering challenges to resolve before initiating construction.*”

We summarize our rating of these proposed projects in Table 2.

Table 2. Characterization of BES facility projects

Facility name	Ability to contribute to world-leading science in the next decade	Construction readiness
<b>LIGHT SOURCES</b>		
Next Generation Light Source*	Could be absolutely central*	Scientific/engineering challenges to resolve before initiating construction*
Advanced Photon Source - Upgrade	Absolutely central	Ready for construction
Linac Coherent Light Source II	Absolutely central	Ready for construction
<b>NEUTRON SOURCES</b>		
SNS Second Target Station	Absolutely central	Scientific/engineering challenges to resolve before initiating construction.

\*The Director of the Office of Science has Charged BESAC to conduct a study and provide a report with advice on the future of photon sources and science by August, 2013.

## *Assessment of major existing and proposed facilities*

The charge from the Director of the Office of Science to the BES Facilities Prioritization Subcommittee was to evaluate the scientific merit of existing and proposed facilities and the technical readiness of proposed future facilities and upgrades. Only facilities and proposed facilities with a value in excess of \$100M were reviewed. Our Subcommittee was instructed not to rank-order the facilities and not to consider their overall budgetary impact. BES provided the BESAC subcommittee with a list of facilities and proposed projects that the Subcommittee was to consider. Consistent with the charge the Subcommittee was free to comment on other large projects beyond the list provided. The results of the Subcommittee's work were presented at a public meeting of BESAC on the two days immediately following the meeting of the Subcommittee.

### **Light sources**

The combined capabilities of the five DOE light sources are *absolutely central* to the advancement of *America's world-leading scientific research and technology*. Each light source offers unique beam characteristics and user support facilities. Each has been highly successful in its level of performance and service to the scientific user community. Together they produce world-leading research and serve more than 11,000 scientists from across the nation and abroad. However, each faces fierce international competition from a new generation of ultra-bright synchrotrons and free electron lasers (FELs) coming online in Europe, Asia, and South America. It is crucial that the DOE respond aggressively to the international challenge by providing adequate funds for facility upgrades in a timely manner. The Sub-committee strongly recommends that DOE continue its practice of continually upgrading its light sources, and building new sources such as FELs and diffraction-limited storage ring sources that can offer unprecedented beam characteristics to open new scientific frontiers.

### **Advanced Light Source**

The Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory, began operations in 1993 as one of the world's brightest sources of high-quality, reliable vacuum-ultraviolet (VUV) light and long-wavelength (soft) X-rays for probing the electronic and magnetic structure of atoms, molecules, and solids, such as those for high-temperature superconductors. The high brightness and coherence of the ALS light are

particularly well-suited for soft x-ray imaging of biological structures, environmental samples, polymers, magnetic nanostructures, and other inhomogeneous materials. The ARPES programs at the ALS have resulted in important world-class results on the electronic structure of new materials of interest to scientific communities, such as systems with highly correlated electrons, graphene, etc. Consequently the ALS has a worldwide reputation for excellence in the use of soft x-ray synchrotron radiation science. The ALS staff has a laudable record of invention and experimental innovation. They have continuously developed new instruments for x-ray science and have extended the capabilities of the ALS towards shorter wavelength (harder) X-rays that are in high demand by structural biologists. User demand for beam time is strong resulting in high scientific productivity with strong impact. During the next decade the ALS will face stiff international competition as new light sources come online with much brighter soft x-ray beams. An ALS upgrade program is planned to add (1) new instrumentation for improved photon-beam stability and control, (2) a lattice upgrade for higher horizontal brightness; and (3) a novel storage ring operational mode to serve multi- and single-bunch users simultaneously. In light of the very high level of international competition, the Subcommittee has characterized the ALS as *important to U.S. world leading science*. The three upgrades just mentioned would make the ALS a unique facility and would keep the U.S. at the forefront of soft x-ray science world wide.

### **Advanced Photon Source**

The Advanced Photon Source at Argonne National Laboratory is one of only three third-generation, hard x-ray synchrotron radiation light sources in the world. The 1,104-meter circumference facility began operations in 1996 and includes 34 bending magnets and 34 insertion devices, which generate a capacity of 68 beam lines for experimental research. Instruments on these beam lines attract researchers to study the structure and properties of materials in a variety of disciplines, including condensed matter physics, materials sciences, chemistry, geosciences, structural biology, medical imaging, and environmental sciences. The high-quality, reliable x-ray beams at the APS have brought about new discoveries in a wide range of fields from physics, chemistry, and materials science to structural biology. The Subcommittee finds that the APS is *absolutely central to U.S. world leading science*.

## **Advanced Photon Source Upgrade**

As the APS looks to the future, renewal planning has focused on approaches that will revolutionize APS experimental capabilities. In the short term, the APS is looking toward enhanced x-ray optics and detectors to achieve at least an order of magnitude improvement. For the long term, the APS Upgrade (APS-U) project will optimize the opportunities for the facility users to observe, understand, and ultimately control material functions on both the nanoscale and mesoscale through two themes that reflect the scientific power of high-energy X-rays: mastering hierarchical structures through imaging and understanding real materials under real conditions in real time. The project will involve upgrades to the APS accelerator, new insertion devices located in the straight sections of the accelerator, the creation of new beam lines, upgrades to existing beam lines, and the creation and installation of new enabling technologies. The APS-U will provide high-energy, high-average-brilliance, short-pulse, penetrating hard X-rays in the energy range above 25 keV; nanoscale focal spots approaching 10 nm above 25 keV; time resolution approaching several picoseconds; new or improved x-ray beam lines; and the technical capabilities required to fully exploit these upgraded technical components. The upgraded capability will, in particular, position the APS well to support many aspects of the mesoscale science that was recently identified as a key priority by BESAC. The combination of these upgrades will provide a more intense beam at all beamline locations and provide capabilities unique among all facilities in the world. Especially in light of vigorous international effort in upgrading the competing hard x-ray light sources, the APS-U is *absolutely central to U.S. world leading science*. The APS Upgrade is *ready for construction* pending a successful review of the technology for producing X-ray pulses of  $\sim 2$  ps.

## **National Synchrotron Light Source**

The National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL), commissioned in 1982, consists of two distinct electron storage rings. The X-ray storage ring is 170 meters in circumference and can accommodate 60 beamlines or experimental stations, and the vacuum-ultraviolet (VUV) storage ring can provide 25 additional beamlines around its circumference of 51 meters. Synchrotron light from the x-ray ring is used to determine the atomic structure of materials using diffraction, absorption, and imaging techniques. Experiments at the VUV ring help understand the electronic structure as well as the magnetic properties of a wide array of materials. The NSLS has regularly updated its technology and expanded its scientific capabilities to

provide internationally competitive, scientific tools to about 2,200 users/year from more than 400 institutions, including universities, national laboratories, and industry.

As the boundaries of scientific discovery have been expanded, however, many researchers are looking for additional capabilities well beyond those that can be provided by the NSLS. The Subcommittee finds that the NSLS is *of lower priority to U.S. world leading science*. The facility will cease operations in 2014 as a new facility (NSLS-II) at BNL comes online.

### **National Synchrotron Light Source-II**

To respond to user needs for a broad spectrum of ultra-bright beams, BNL is building NSLS-II, a replacement for its present synchrotron facility. NSLS-II will be a new synchrotron light source, highly optimized to deliver ultra-high brightness and flux and exceptional beam stability, which will enable the study of material properties and functions with a spatial resolution of 1 nanometer, an energy resolution of 0.1 milli-electron volt, and the ultra-high sensitivity required to probe atomic-scale features. Its unprecedented capabilities will be *absolutely central to world-leading U.S. science*, enabling scientists to explore the challenges they face in developing new materials with advanced properties. The NSLS-II *construction is on schedule and on budget* to begin operations in 2014.

### **Stanford Synchrotron Radiation Light Source**

The Stanford Synchrotron Radiation Light Source (SSRL) at the SLAC National Accelerator Laboratory was built in 1974 to use the intense x-ray beams from the Stanford Positron Electron Asymmetric Ring (SPEAR) that was built for particle physics. The SPEAR 3 upgrade, completed in 2008, provided major improvements that increase the brightness of the ring for all experimental stations. The research program conducted at SSRL has emphasized both the x-ray and ultraviolet regions of the spectrum. A broad group of scientists and engineers from many disciplines and their students are users of SSRL since its original commissioning.

It will become increasingly important in the future to create micro- or nano-sized x-ray beams with high intensity, and well defined polarization and time structure. Such studies promise unique insight into, for example: (1) materials under extreme conditions (e.g., high pressure or high magnetic fields); (2) materials that exhibit nanoscale dynamics (i.e.,

respond to excitations on the second to picosecond time scale); (3) artificial nanostructures or those intrinsically inhomogeneous on the micro- and nanoscale; and (4) biological crystals that only exist on the microscale. SSRL is known for outstanding user support and important contributions to science and instrumentation. The Subcommittee considers it well poised to make *important contributions to world-leading science*, in ways that also train the future scientific and technical workforce.

### **Linac Coherent Light Source**

The Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory (SLAC) is the world's first hard x-ray free electron laser facility. The first operation of LCLS in 2010 has advanced the state-of-the-art of x-ray user facilities from storage-ring-based, third-generation synchrotron light sources to a fourth generation. The LCLS provides radiation in the x-ray region of the spectrum that is 10 billion times greater in peak power and peak brightness than any existing coherent x-ray light source. The SLAC linac drives the LCLS with high current, low-emittance, 5–15 GeV electron bunches at a 120 Hz repetition rate. The LCLS is used for ultra-fast imaging at times scales as short as several femtoseconds, illuminating the fundamental processes of physics, chemistry, and biology. This FEL has the potential for even shorter duration x-ray pulses. In every respect the LCLS has already exceeded all of its performance expectations. The Subcommittee finds that LCLS is *absolutely central to U.S. world-leading science*.

### **Linac Coherent Light Source-II**

The LCLS-II project, which is near to receiving CD-2, will expand the capabilities and capacity of the LCLS. It enhances scientific opportunities by installing additional beam paths allowing harder X-rays (>10 keV) for the 3D imaging of materials, an extended soft x-ray spectral range below the carbon absorption edge at 280eV, and generation of ultrashort x-ray pulses (< 1 femtosecond) to explore the attosecond temporal region for molecular dynamics. None of these capabilities exist with LCLS. LCLS-II will allow for understanding (1) disordered systems such as liquids, glasses, amorphous systems and mesoporous assemblies and their dynamics; (2) photosynthetic water splitting; (3) materials in extreme states; (4) real-time observation of surface reactions in catalysis; and (5) highly correlated materials. The Subcommittee finds that LCLS-II is *absolutely central to U.S. world-leading science*. LCLS-II is *ready for construction*.

## **Next Generation Light Source**

The Office of Science has granted CD-0 to a Next Generation Light Source (NGLS). The scientific case for the NGLS spans many important areas of science, including photosynthesis, fundamental energy and charge dynamics, advanced combustion science, catalysis, nanoscale materials synthesis, quantum materials, spin and magnetization, and imaging dynamics and function in materials, chemical and biological systems. The NGLS is envisioned as transforming the field of attosecond science, impacting the material, chemical, and biological sciences that underpin DOE missions in energy, environment, and national security. The present design concept for the NGLS is an array of fully coherent x-ray free electron lasers (FELs) powered by a superconducting accelerator capable of delivering electron bunches to a suite of independently configured FEL beamlines. As presently envisioned, the NGLS will be optimized for specific applications requiring high repetition rates, time resolution to the attosecond regime, high spectral resolution, tunability, and polarization control. High repetition rates are essential for capturing rare or low-scattering-rate events, to probing the structure of heterogeneous ensembles in situ, and for maintaining the requisite average brightness for experiments in which the peak brightness is necessarily restricted to avoid significant perturbation of the sample.

The NGLS is still in the conceptualization phase and requires National Environmental Policy Act evaluation of environmental impact prior to establishing the preferred alternative for the project. The Subcommittee concludes that the NGLS has the *potential to be absolutely central to U.S. world-leading science*. However, *significant R&D is required to resolve scientific/engineering challenges before initiation of construction*.

## **Neutron sources**

There is a strong global argument that U.S. leadership in materials is needed to ensure economic competitiveness and enable innovation. For the U.S. to lead in materials, it must have world leading neutron science capabilities in addition to world leading photon science capabilities. The recent BESAC report, “From Quanta to the Continuum: Opportunities for Mesoscale Science,” argues strongly for neutron science as a key scientific tool and a complement to photons, especially for studying so-called “soft matter” and complex fluids, magnetic materials and disordered and aperiodic structures (for which coherent x-ray imaging is just emerging) as well as for studying inelastic process and dynamics.

## **Spallation Neutron Source**

The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, which began operation in 2006, is presently the most powerful accelerator-driven neutron source in the world, operating at a power of 1 MW. Sub-microsecond proton pulses from the accelerator complex hit the liquid-mercury target at 60 Hz, generating pulses of neutrons that feed 13 operating instruments, with 6 more instruments in commissioning or under construction and space for a maximum of 5 more. The funding for two instruments was provided by Germany and Canada, while a third instrument was funded by the Office of Nuclear Physics in DOE's Office of Science. The number of unique users served has grown rapidly, reaching 799 in 2012. Beam time is oversubscribed by factors of 3 to 4, reflecting both the demand for this facility and the overall lack of capacity in terms of neutron instruments in the U.S., an area in which the U.S. lags far behind Europe.

Beams of neutrons are particularly well suited for measuring the positions as well as the fluctuations in the positions of atoms, the structure of atomic magnetic moments in solids, and the excitations in their magnetic structure. Such studies lead to understanding of phenomena such as melting, magnetic order, and superconductivity in a variety of materials. The importance of high proton beam power—and consequently high neutron flux—to technological innovation means that the SNS will be the nation's premiere neutron facility for many decades to come.

Research at SNS over the next decade will focus on studies of small samples, complex molecules and structures, time-dependent phenomena, and very weak interactions. The high flux at the SNS will enable studies of complex materials in real time and relevant to all disciplines—physics, chemistry, materials science, geosciences, and biological and medical sciences. Over the coming decade, the SNS is *absolutely central to world leading science* in the U.S.

## **Spallation Neutron Source Second Target Station**

It is essential that the SNS realize its full potential, as it represents the best opportunity for expanding the capability and capacity of advanced neutron instrumentation in the U.S. The SNS second target station (STS) project will design, build, install, test and commission a second target station at SNS. Key components include a new spallation target and supporting systems, an enhancement and extension of the SNS accelerator systems, conventional support buildings, and initial neutron beam instruments.

Presently SNS has the capacity to provide high intensity bursts of neutrons to approximately twenty instruments. The potential to gain an order of magnitude in performance for experiments that require long-wavelength neutrons would be realized with the construction of a second target station, an option that was anticipated in the layout of the original SNS project. The plan for STS leverages the investment in the SNS proton accelerator, including an upgrade of the linac for operation at higher power, which also benefits the first target station.

Many important scientific problems require characterization of structures with a long length scale (compared to atomic spacing) or very slow dynamics (motion of large objects). Examples include large molecular structures such as polymers, biological membranes, and magnetic heterostructures. Such measurements require the use of long-wavelength neutrons. The efficient detection of such neutrons requires a longer time between neutron bursts than that provided by the 60-Hz pulse rate on the first target station of SNS. The second target station will be designed to operate at 10 or 20 Hz, using one out of six or one out of three of the proton pulses that presently go to the first target station. A further option is to use longer pulses directly from the linear accelerator, creating a long-pulse source, as is planned for the European Spallation Source under development in Sweden. An essential component of the STS project would be a power upgrade to the accelerator system, increasing the capacity of the linac to 3 MW, thus more than compensating the first target station for the protons directed to the STS.

The higher intensities for both target stations translate into the ability to study much smaller samples, more weakly scattering processes and/or higher-rate kinetic behaviors. This increase in performance brought by the second target station will lead to qualitatively new scientific capabilities complementary to those at the first SNS target station, while roughly doubling the user capacity.

The Subcommittee recognizes that the STS is *absolutely central to U.S. world-leading science*; however, there are *significant scientific/technical issues that must be resolved before construction can be initiated*. The choice of a long-versus a short- pulse source is intimately tied to the choice and optimization of the instrument suite. This evaluation requires further detailed study.

### **High Flux Isotope Reactor**

The High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory provides the highest time-averaged neutron flux of any facility in the western hemisphere. Operating

at 85 MW of thermal power, it supports 11 instruments, with one more in commissioning. Five of these instruments benefit from the cold neutron source, commissioned in 2007, that has world-leading brightness. Altogether, there were 442 unique users in FY 2012.

The reactor requires periodic replacement of its beryllium reflector; the next such replacement will be in a decade. During the last replacement in 2000, larger beam tubes were installed for two beam ports, along with instrumentation improvements that enabled the use of greater neutron flux. The neutron-scattering experiments at HFIR reveal the structure and dynamics of a very wide range of materials. The high time-averaged flux is extremely valuable for detailed studies of a system as a function of a variable such as temperature, pressure, or magnetic field. The state-of-the-art neutron scattering instruments on one of the world's brightest beams of steady-state, long-wavelength neutrons are used in fundamental studies of materials of interest to solid-state physicists, chemists, biologists, polymer scientists, metallurgists, and colloid scientists.

While BES stewards HFIR for the neutron scattering capabilities, the facility is essential in other ways. In particular, it is a unique producer of a number of special isotopes, which are distributed through the isotope program of the Office of Nuclear Physics. For example, californium-252 is used by oil companies to monitor the progress of well drilling; several other isotopes are produced for medical therapies. A significant program of irradiations performs high-dose neutron irradiations of materials for Fusion Energy Sciences as well as for the commercial nuclear power industry and gamma-ray irradiations of samples for NASA. Finally, the Neutron Activation Analysis program provides ultra-sensitive measurements of certain elements in a material, with regular customers such as the International Atomic Energy Agency. An unresolved, future issue for HFIR is the potential fuel conversion of the reactor core from highly enriched to low-enriched uranium.

The Sub-committee finds HFIR to be *important to US world leading science* in the BES research portfolio, and also notes the importance and uniqueness of the facility for a number of other programs crucial to U.S. science and security.

### **Lujan Neutron Scattering Center**

The Lujan Neutron Scattering Center (Lujan Center) at Los Alamos National Laboratory supports 16 flight paths, which receive intense pulsed neutron beams at LANSCE. The LANSCE proton accelerator operates at a power of 100 kW, providing pulses at a frequency of 20 Hz. At present, the Office of Science supports 8 instruments, 7 through

BES, plus 1 through BER: these have served an average of 310 unique users per year (2005 through 2011). Three other existing instruments could be added to the BES user program if funding were available.

The Lujan Center features instruments dedicated for measurement of atomic, magnetic, and local structure, especially at high-pressure and high-temperature, as well as for measurement of residual strain, liquid surfaces, magnetic thin films, and texture. The facility has a long history and extensive experience in handling actinide samples. A 30 Tesla magnet is also available for use with neutron scattering to study samples in high magnetic fields.

The Los Alamos Neutron Science Center (LANSCE) consists of a high-power 800-MeV proton linear accelerator, a proton storage ring, production targets at the Lujan Center and the Weapons Neutron Research facility, and a variety of associated experiment areas and spectrometers for national security research and civilian research operated by the National Nuclear Security Administration (NNSA). The Lujan Center's reliability is dependent on NNSA's stewardship of LANSCE and its 30+ year-old accelerator. NNSA has recently begun to fund the LANSCE Risk Mitigation Project (to be completed in 2018), an effort that is essential for reliable operations in the future.

The Subcommittee considers the Lujan Center to be of *lower priority for U.S. world leading science* with respect to the other neutron facilities in the BES portfolio. Nevertheless, the Sub-committee notes that the Lujan Center enables excellent scientific research in a very cost-effective fashion, and that the work performed there cannot easily be transferred to other U.S. facilities because of the lack of capacity at the other facilities, and the specialized sample environments that exist at the Lujan Center.

## **Nanoscale Science Research Centers**

The five Nanoscale Science Research Centers (NSRCs) add a large contribution to U.S. world-leading science through their twin missions of pursuing top-quality science and enabling the same for external users through access to NSRC facilities and/or collaboration with NSRC researchers. The Subcommittee commends the quality of their research, strong connections to relevant research centers, and their achievements in enabling successes of external users. The Subcommittee identified particular value in synergies between science programs of NSRC researchers, the special facilities the NSRCs develop for their own staff and external users, and the consequent benefits available to users.

## **Center for Functional Nanomaterials**

The Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory (BNL) focuses on three research thrusts (interface science and catalysis, electronic materials with emphasis on photovoltaic materials, and soft and bio-nanomaterials) with cross-cutting programs in electron microscopy and theory and computation. The three thrusts are well aligned with key Brookhaven research programs. Unique capabilities at CFN include wide-area assembly via block copolymer templating, aberration-corrected environmental TEM, scanning tunneling microscopes that operate under reactive conditions, and ambient-pressure x-ray photoelectron spectroscopy. This capability, currently operated at the NSLS, will be an integral part of the electron spectro-microscopy (ESM) beamline at NSLS-II.

CFN plans are now in place for strong coupling with NSLS-II. An aberration-corrected low energy electron microscopy (LEEM) system to be installed at NSLS-II will offer an unprecedented 10 nm resolution in photoelectron microscopy (PEEM), 3 to 5 times better than currently possible at NSLS. The Subcommittee judges that presently the Center for Functional Nanomaterials is *important to US world leading science*. The Subcommittee also recognizes that as the NSLS-II comes on line CFN with its strong coupling to this new light source will be critical to a broad user community.

## **Center for Integrated Nanotechnologies**

The Center for Integrated Nanotechnologies (CINT) is administered jointly by Los Alamos National Laboratory (LANL) and Sandia National Laboratories. CINT makes use of a wide range of specialized facilities including the nanofabrication facilities at Sandia and the neutron scattering and high magnetic field facilities at LANL. CINT focus areas are nanophotonics and nanoelectronics, complex functional nanomaterials, nanomechanics, and the interfaces at the nanoscale as well as at the bio/microscale. Research at CINT over the next decade will address four scientific thrusts: (1) *Nanophotonics and Optical Nanomaterials*—synthesis, excitation and energy transformations of optically active nanomaterials and collective or emergent electromagnetic phenomena; (2) *Nanoscale Electronics, Mechanics and Systems*—control of electronic transport and wave functions, and mechanical coupling and properties using nanomaterials and integrated nanosystems; (3) *Soft, Biological and Composite Nanomaterials*—solution-based materials synthesis and assembly of soft, composite and artificial bio-mimetic nanosystems; (4) *Theory and Simulation of*

*Nanoscale Phenomena*—assembly, interfacial interactions, and emergent properties of nanoscale systems.

With special recognition of CINT's creation of a growing number of new MEMS-based, discovery science platforms that are readily delivered to users or employed in collaborations with CINT scientists, the Subcommittee concludes that the Center for Integrated Nanotechnologies is *absolutely central to US world-leading science*.

### **Center for Nanophase Materials Sciences**

The Center for Nanophase Materials Sciences (CNMS) at Oak Ridge National Laboratory (ORNL) combines nanoscale science research with neutron science, synthesis science, and theory, modeling, and simulation. CNMS provides state-of-the-art clean rooms, wet and dry laboratories for sample preparation, fabrication and analysis. Equipment to synthesize, manipulate, and characterize nanoscale materials and structures is included. The facility is co-located with the Spallation Neutron Source complex. The CNMS's major scientific thrusts are in nano-dimensioned soft materials, complex nanophase materials systems, and the crosscutting areas of interfaces and reduced dimensionality that become scientifically critical on the nanoscale. The Subcommittee notes that these thrust areas are particularly important to users of the SNS, both present and future.

Research at CNMS over the next decade will focus on understanding, designing and controlling the dynamics, spatial chemistry, and energetics of the functionality and properties of nanoscale materials and architectures. Scientific themes will include: (1) origins of functionality at the nanoscale; (2) functional polymer architectures, and (3) emergent behavior in nanoscale systems. In view of its excellence in theory, coupling to a leadership scale computing platform (Titan) at ORNL, and scanning probe experimental capabilities, the Subcommittee considers the Center for Nanophase Materials Sciences to be *important to US world-leading science*.

### **Center for Nanoscale Materials**

The Center for Nanoscale Materials (CNM) at Argonne National Laboratory contains clean rooms and specialized equipment explicitly tailored to create and characterize new functional materials on the nanoscale, particularly research in advanced magnetic materials, complex oxides, nanophotonics, and bio-inorganic hybrids. The State of

Illinois provided funding for construction of the building, which is appended to the APS. CNM operates and exploits the hard x-ray nanoprobes at APS, a unique facility for a host of collaborations with key industrial laboratories as well as universities. The CNM also provides users excellent access to environmental nanoprobes.

Research at CNM over the next decade will address six scientific themes: (1) electronic and magnetic materials and devices, (2) nano-bio interfaces, (3) nanofabrication and devices, (4) nano-photonics, (5) theory and modeling, and (6) X-ray microscopy. The Subcommittee finds that the Center for Nanoscale Materials is *absolutely central to US world-leading science*.

### **The Molecular Foundry**

The Molecular Foundry at Lawrence Berkeley National Laboratory (LBNL) has a strong cross-disciplinary portfolio to support users in one six-story, laboratory building fully equipped with state-of-the-art, sometimes one-of-a-kind instruments. It includes modular clean room space consisting of labs for nanofabrication/lithography and clean measurement, and a low-vibration, low-electromagnetic-field laboratory housing state-of-the-art imaging and manipulation tools. The Foundry building has controlled environmental rooms, equipped with a wide range of state of the art imaging, and spectral characterization equipment in addition to equipment to support synthetic chemistry and chemical biology. These capabilities enable staff and users to take their projects all the way to screening and prototyping. Research at the Molecular Foundry over the next decade will integrate research within four major themes: (1) combinatorial synthesis of nanomaterials, (2) multimodal in situ imaging and spectroscopy, (3) interfaces in nanomaterials and (4) nanofabrication with sub-10 nm precision.

Especially notable is a record of very strong rational chemical synthesis of nanoscale materials integrated with characterization/measurements. The research program is well coupled to the leadership scale computing platform at LBNL and to the ALS. The Subcommittee finds that the Molecular Foundry is *absolutely central to US world-leading science*.

## Appendix I

Charge letter from William Brinkman to Office of Science Advisory Committees



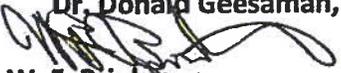
Department of Energy  
Office of Science  
Washington, DC 20585

Office of the Director

December 20, 2012

To: **Chairs of the Office of Science Federal Advisory Committees:**

**Professor Roscoe C. Giles, ASCAC**  
**Professor John C. Hemminger, BESAC**  
**Professor Gary Stacey, BERAC**  
**Professor Martin Greenwald, FESAC**  
**Professor Andrew J. Lankford, HEPAP**  
**Dr. Donald Geesaman, NSAC**

  
From: **W. F. Brinkman**  
**Director, Office of Science**

I am writing to present a new charge to each of the Office of Science Federal Advisory Committees. I would like each Advisory Committee to help us with an important task—the prioritization of proposed scientific user facilities for the Office of Science. To meet a very compressed timetable, we will need your final report by **March 22, 2013**.

This charge derives from Administration efforts to improve the efficiency, effectiveness, and accountability of government programs and requirements of the Government Performance and Results Modernization Act of 2010. In order to improve the agency's performance, and in compliance with this Act, DOE has established several Priority Goals, including the following goal for the Office of Science:

***Goal Statement: Prioritization of scientific facilities to ensure optimal benefit from Federal investments. By September 30, 2013, formulate a 10-year prioritization of scientific facilities across the Office of Science based on (1) the ability of the facility to contribute to world-leading science, (2) the readiness of the facility for construction, and (3) an estimated construction and operations cost of the facility.***

To accomplish this goal, DOE will undertake the following steps. We will need your help with step #2, as described below.

1. *The DOE/SC Associate Directors will create a list of proposed new scientific user facilities or major upgrades to existing scientific user facilities that could contribute to world leading science in their respective programs from 2014 to*



2024 (the timeframe covered by this goal).

This step is complete. The Associate Directors have developed material describing the nature of a number of proposed new or upgraded facilities, the scientific justification for the facility or upgrade, and the various inputs from the scientific community that provided motivation for the proposal. Additionally, the Associate Directors have provided assessments of their existing scientific user facilities to contribute to world-leading science through 2024. The Associate Directors will be in touch with their respective FACA chairs shortly to submit this material directly to you.

2. *The information developed by the DOE/SC Associate Directors will be used by the DOE/SC as the basis for engagement with the DOE/SC Federal Advisory Committees and others to seek advice and input on new or upgraded scientific user facilities necessary to position the DOE/SC at the forefront of scientific discovery. The Federal Advisory Committees will seek additional outside input as necessary. In particular, for programs that have a significant existing or potential user base outside of the DOE/SC, the Federal Advisory Committees will be encouraged to seek input from the broader scientific community and existing facility user committees.*

In order for your Advisory Committee to execute step #2, I suggest that you empanel a subcommittee to review the list of existing and proposed facilities provided to you by the program Associate Director, subtracting from or adding to the list as you feel appropriate. To address the concerns of the broad facilities user community, the subcommittees should include representatives of the broad, multi-disciplinary community that stands to benefit from these facilities, including representatives whose research is supported by other Federal agencies. In its deliberations, the subcommittees should reference relevant planning documents and decadal studies. If you wish to add facilities or upgrades, please consider only those that require a minimum investment of \$100 million. More detailed instructions for the report are given below.

3. *Finally, with input from the DOE/SC Federal Advisory Committees and other stakeholders, the DOE/SC Director will prioritize the proposed new scientific user facilities and major upgrades across scientific disciplines according to his/her assessment of the scientific promise, the readiness of the facility to proceed to construction, and the cost of construction and operation. In making this prioritization, the DOE/SC Director will consider the resource needs for research support and for robust operation of existing facilities and will engage leaders of other relevant agencies and the Administration to ensure priorities are coordinated with related investments by other agencies and reflect cross-agency needs where appropriate.*

Please provide me with a short letter report that assigns each of the facilities to a category and provides a short justification for that categorization in the following two areas, but do not rank order the facilities:

1. **The ability of the facility to contribute to world-leading science in the next decade (2014 – 2024).** Please include both existing and proposed facilities/upgrades and consider, for example, the extent to which the proposed or existing facility or upgrade 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 and especially whether the facility will address needs of the broad community of users including those supported by other Federal agencies; 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 (sometimes many) scientific communities that use the facility. **Please place each facility or upgrade in one of four categories: (a) absolutely central; (b) important; (c) lower priority; and (d) don't know enough yet.**
2. **The readiness of the facility for construction.** For proposed facilities and major upgrades, please consider, for example, whether the concept of the facility has been formally studied; 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. **Please place each facility in one of three categories: (a) ready to initiate construction; (b) significant scientific/engineering challenges to resolve before initiating construction; and (c) mission and technical requirements not yet fully defined.**

Each SC program Associate Director will contact the Chair of his or her Federal Advisory Committee to discuss and coordinate the logistics of executing this charge. We realize that the six SC programs will require somewhat different approaches, in part based on recent and future community planning activities. In addition, if you would like to discuss the charge further, please feel free to contact Pat Dehmer ([patricia.dehmer@science.doe.gov](mailto:patricia.dehmer@science.doe.gov)). Thank you for your help with this important task.