

MISSION NEED STATEMENT

NATIONAL SYNCHROTRON LIGHT SOURCE-II (NSLS-II)

SYSTEM POTENTIAL: Major System

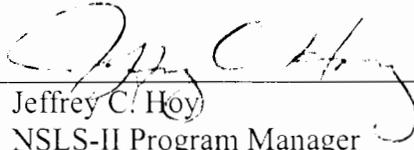
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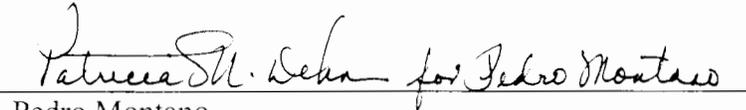
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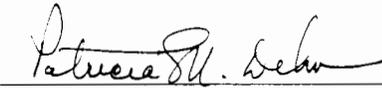
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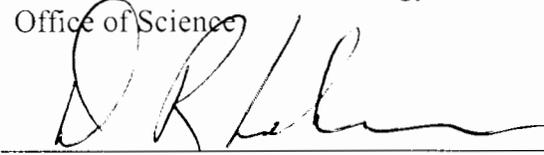
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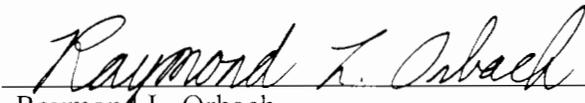
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MISSION NEED STATEMENT

for the

National Synchrotron Light Source-II (NSLS-II)

Office of Basic Energy Sciences

Office of Science

SYSTEM POTENTIAL: Major System

A. Statement of Mission Need

The mission of the Department's Basic Energy Sciences (BES) program – a multipurpose, scientific research effort – is to foster and support fundamental research to expand the scientific foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use. The portfolio supports work in the natural sciences: emphasizing fundamental research in materials sciences, chemistry, geosciences, and aspects of biosciences. As part of its strategic mission, the BES program plans, constructs, and operates major scientific user facilities to serve researchers at universities, national laboratories, and industrial laboratories, as set forth in Public Law 102-486 (Title 42, U.S. Code, Chapter 134—Energy Policy, Section 13503) and which is briefly summarized below.

Mission

The Department shall continue to support a vigorous program of basic energy sciences to provide basic research support for the development of energy technologies. Such program shall focus on the efficient production and use of energy and the expansion of our knowledge of materials, chemistry, geology, and other related areas of advancing technology development.

User Facilities

As part of the program referred to above, DOE shall carry out planning, construction, and operation of user facilities to provide special scientific and research capabilities, including technical expertise and support as appropriate, to serve the research needs of our Nation's universities, industry, private laboratories, Federal laboratories, and others.

In addition, the current DOE Strategic Plan (2003) contains a Science Strategic Goal that calls for providing a world-class scientific research capability and advancing scientific knowledge in order to protect our national and economic security. Within the framework of the Strategic Plan, this Strategic Goal translates to General Goal # 5, "Provide world-class scientific research capacity needed to: ensure the success of Department missions in national and energy security; advance the frontiers of knowledge in physical sciences and areas of biological, medical, environmental, and computational sciences; or *provide world-class research facilities for the Nation's science enterprise.*"

Major advances in energy technologies – such as the use of hydrogen as an energy carrier; the widespread, economical use of solar energy; or the development of the next generation of nuclear power systems – will require scientific breakthroughs in developing new materials with advanced properties. Examples include catalysts that can split water with sunlight for hydrogen production, materials that can reversibly store large quantities of hydrogen, materials for efficient power transmission lines, materials for solid state lighting with 50 percent of present power consumption, and materials for reactor containment vessels that can withstand fast-neutron damage and high temperatures. A broader discussion is given in several recent reports, including the Basic Energy Sciences Advisory Committee Reports *Opportunities for Catalysis in the 21st Century* and *Basic Research Needs to Assure a Secure Energy Future*, the BES report *Basic Research Needs for the Hydrogen Economy*, the Report of the Nanoscale Science, Engineering, and Technology Subcommittee of the National Science and Technology Committee *Nanoscience Research for Energy Needs*, and the Nuclear Energy Research Advisory Committee Report *A Technology Roadmap for Generation IV Nuclear Energy Systems*.

Collectively, these reports underscore the need to develop new tools that will allow the characterization of the atomic and electronic structure, the chemical composition, and the magnetic properties of materials with nanoscale resolution. Needed are non-destructive tools to image and characterize buried structures and interfaces, and these tools must operate in a wide range of temperature and harsh environments. The absence of any tool possessing these combined capabilities was identified as a key barrier to progress in the 1999 BES Report *Nanoscale Science, Engineering and Technology Research Directions*.

In order to fill this capability gap and to further the accomplishment of its mission, the BES program will need a synchrotron light source that will enable the study of material properties and functions, particularly materials at the nanoscale, at a level of detail and precision never before possible. To achieve this, the light source will need to provide photon beams having ultra-high brightness and flux and exceptional stability. It will also need to provide advanced insertion devices, optics, detectors, robotics, and a suite of scientific instruments. No other synchrotron light source worldwide will have these beam characteristics and advanced instrumentation. For the purpose of this Mission Need Statement, the new synchrotron light source will be called the National Synchrotron Light Source II (NSLS II).

B. Analysis to Support Mission Need

The combination of brightness, flux, and stability will provide the world's finest capabilities for x-ray imaging. NSLS-II will enable the study of materials with ~ 1 nanometer (nm) spatial resolution and with ~ 0.1 millielectron volt (meV) energy resolution. It will be possible to focus both soft (several hundred eV) and hard (several thousand eV) x-rays to a spatial resolution of ~ 1 nm and to perform spectroscopy on a single atom. With the development of novel "lensless" imaging, it will be possible to capture x-ray images with a spatial resolution of ~ 1 nm. This resolution and sensitivity is unprecedented in x-ray imaging. If there is any doubt that this is needed for our future energy security, one only need remember that all the elementary steps of energy conversion (charge transfer, molecular

rearrangement, and chemical reactions), both for fossil fuels and for critical renewable energy sources, take place on the nanoscale, and many of these steps involve a combination of complex physical, chemical, and often biological, transformations.

The unique characteristics of NSLS-II will enable exploration of the scientific challenges faced in developing new materials with advanced properties, including: the correlation between nanoscale structure and function, including the profound effects of confinement, finite size, and proximity; the mechanisms of molecular self-assembly, which produces exquisite molecular structures in both the living and nonliving worlds; and the science of emergent behavior, one of the grand scientific challenges.

NSLS-II supports the BES *scientific mission* by providing the most advanced tools for discovery-class science in condensed matter and materials physics, chemistry, and biology – science that ultimately will enhance national and energy security and help drive abundant, safe, and clean energy technologies. Furthermore, NSLS-II supports the related BES *facilities operation mission* by creating the most advanced storage-ring-based light source to serve the Nation’s researchers. BES is the steward of user facilities for the Nation, a role formally recognized by Congress in the Energy Policy Act of 1992. Under BES leadership, these facilities have thrived and flourished. The synchrotron light sources have become one of the great success stories of the past 20 years. Once the province of a few hundred specialists, mostly physicists, the BES light sources are now used by more than eight thousand researchers annually from all disciplines and with support from DOE, the National Science Foundation (NSF), the National Institutes of Health, the Environmental Protection Agency, the U.S. Department of Agriculture, many other Federal agencies, and foreign countries.

NSLS-II supports elements of DOE’s Strategic Plan (2003) and the Office of Science’s (SC’s) Strategic Plan (2004). The DOE Strategic Plan includes among the eight strategies for enabling world-class scientific research capacity the following two: (1) advance nanoscale science leading to improved energy technologies and systems and (2) provide the Nation’s science community access to world-class research facilities, including light sources, which advance the physical sciences and enable the study of complex, interdisciplinary science questions. The SC Strategic Plan expands on the theme of world-class scientific research capacity discussed in the DOE Strategic Plan by specifically recognizing that we are now in the early stages of two remarkable explorations—observing and manipulating matter at the molecular scale (i.e., the nanoscale) and understanding the behavior of large assemblies of interacting components, a subject often referred to as the science of emergent behavior. Scientific discoveries in these two frontiers alone will accelerate our progress toward more efficient, affordable, and cleaner energy technologies.

NSLS-II also supports SC’s strategic plan for facilities that was developed in early 2003 and described in *Facilities for the Future of Science: A Twenty-Year Outlook* (2003). As input to that roadmap, the Basic Energy Sciences Advisory Committee considered 15 facility proposals. Of these, only three were given the top science rating. These were the NSLS-II, the Linac Coherent Light Source (LCLS), and the Transmission Electron Aberration-corrected Microscope; the latter two proposals already are funded and the projects are already underway.

The LCLS, a new x-ray light source facility being built at the Stanford Linear Accelerator Center (SLAC), is based on an x-ray free electron laser (XFEL). The LCLS will provide very high time average brightness, but it is optimized to deliver ultra-high peak brightness in very short pulses (230 fsec) at low duty cycles (120 Hz repetition rate). These extraordinary properties will make the LCLS an unrivaled source for studies of ultra-fast phenomena. However, LCLS will have a single beamline and will deliver photons over a limited energy range of 800 eV to 8 keV. The process of tuning the energy will be slower and more difficult than with a synchrotron, and the energy and intensity will be less stable than with a synchrotron. These capabilities are complementary to those of NSLS-II and both facilities are necessary to meet different mission needs.

Finally, NSLS-II supports the National Nanotechnology Initiative, which was launched in FY 2001 to accelerate the pace of revolutionary discoveries in nanoscale science, engineering, and technology and facilitate their incorporation into beneficial technologies. In support of this initiative, BES has established five Nanoscale Science Research Centers, each associated with a major synchrotron light source or neutron scattering center.

The analysis to support mission need includes three elements: (1) a summary of the scientific challenges for the mission described in Section A and the impact of NSLS-II in meeting those challenges; (2) a summary of the technical capabilities of NSLS-II that will enable this science; and (3) a summary of the range of alternatives that have been considered to meet the need, including the ability of other synchrotron radiation facilities worldwide, both operating and under construction, to provide the required technical capabilities.

1. Scientific Challenges and Impact of NSLS-II

NSLS-II will be the best synchrotron in the world, but, more importantly, NSLS-II will be transformational in that it will open new regimes of scientific discovery and investigation. The ability to probe materials with 1 nm or better spatial resolution and to analyze their dynamics with 0.1 meV energy resolution will be truly revolutionary. For example, it will be possible to investigate the atomic and electronic structure and chemical composition of nanometer-scale objects such as single-walled carbon nanotubes incorporated as the active element in a Field Effect Transistor (FET) under realistic in-situ device operating conditions. And it will be possible to investigate processes that change the energy or spin state of electrons, such as their interaction with the atomic lattice or other electrons or spins. These processes, occurring on the scale of ~ 1 meV, form the foundation of many diverse phenomena, such as photosynthesis and spin-based quantum computing, and the ability to study them with high spatial resolution will be unprecedented.

The importance of the scientific challenges described above and the impact of NSLS-II on meeting these challenges are summarized briefly below.

- *Nanoscale structure and function.* The nanoscale – the length scale from about 1 to 100 nanometers – is the scale at which fundamental properties of materials and systems are established. For example, melting temperature, magnetic properties, charge capacity, and even color are dictated by the arrangement of nanoscale structures. However, the

properties of matter at the nanoscale cannot necessarily be predicted from those observed at larger or smaller scales. Instead, they exhibit important differences that cannot be explained by traditional models and theories. Some of these differences result from continuous modification of characteristics with changing size. Others represent totally new phenomena, such as quantum size confinement, wave-like transport, and the predominance of interfacial phenomena. The major challenge for progress in this qualitatively new scientific frontier is developing the ability to directly observe fundamental material properties with nanoscale resolution and atomic sensitivity rather than being limited to globally-averaged information or secondary characteristics.

Because of its unprecedented spatial resolution and high sensitivity, NSLS-II will provide a powerful nanoscale laboratory, using the full range of synchrotron tools for *in-situ* characterization and three-dimensional visualization of *local* nanoscale structures, properties, and functions. Furthermore, this will be possible deep below surfaces, as well as at them, an absolutely critical and unique feature among material probes. Detailed understanding of growth and function will become possible with the ability to determine the real-time response to a wide range of external variables, such as temperature, stress, gaseous and liquid environments, chemical activity, and applied fields. Such studies may eventually lead to new electronic materials that scale beyond the limits of silicon technology or to designer catalysts that operate as selectively as enzymes but with greater robustness in real-world applications, with enormous implications for the nation's energy and economic security.

- *Self-assembly.* Self-assembly is the creation of structural organization from preexisting parts or disordered components without guidance or management from an outside source. Nature uses molecular self-assembly to integrate molecules into functioning three dimensional macrostructures. It is the basis for polymer formation, protein folding, the formation of cell components, and much more. Challenges to controlling molecular self-assembly include understanding how to incorporate multiple nanoscale components with one another and integrating them with larger-scale components to tailor properties, tuning dimensions from nanometers to microns, overcoming thermodynamic immiscibility, and manipulating kinetic pathways to produce both equilibrium and metastable structures.
- The high spatial resolution and rapid measurement times (resulting from the high brightness and flux) of NSLS-II will enable studies of molecular interactions in nano-confined environments, interactions between nanoscale building blocks, materials with hierarchical structures on length scales ranging from nanometers to microns, studies of the kinetics of assembly on faster time scales typical of nanoscale assembly, and determining the mechanisms whereby external applied fields influence self-assembled structures. Scientific advances in this area will lead to revolutionary changes in our ability to design new functional materials incorporating nanometer sized organic and inorganic molecules self-assembled into exotic hierarchical structures. This will result in significantly improved solar energy conversion, more energy efficient lighting, novel photonic bandgap materials for guiding and switching optical signals, stronger

and lighter materials, meso-porous hosts to trap and catalytically break down toxic substances for environmental remediation, greatly improved chemical and biological sensing, information storage, membranes, drug delivery, and more.

- *Emergent behavior.* Emergent behaviors arise from the collective, cooperative behavior of individual components of a system; in general, even exquisite knowledge of the components may not allow the prediction of the emergent behavior. For example, complete knowledge of a bird will not enable the prediction of its flocking patterns. The challenge of understanding how emergent behavior results from the complexity of competing interactions is among the most compelling of our time, spanning phenomena as diverse as phase transitions, high temperature superconductivity, colossal magnetoresistance, random field magnets, and spin liquids and glasses. Progress requires understanding the nature and origin of highly correlated states in strongly interacting systems that have spin, charge, lattice, and orbital degrees of freedom and that are often intrinsically inhomogeneous on nanometer length scales.

With the unparalleled energy resolution and coherence of NSLS-II, it will be possible to study many of these atomic- and molecular-scale phenomena. For example, it will be possible to study charge dynamics of stripe order and the dynamics of vortex liquids in high temperature superconductors; to probe orbital excitations (“orbitons”) in manganites; to visualize the magnetization of random field magnets and spin glasses with nm resolution and to follow their short length scale, slow dynamics; and to examine the response of these phenomena to external control parameters such as field, temperature, or pressure. Unlocking the mysteries of these systems will lay the scientific foundation for designing and engineering new multifunctional materials, devices and sensors with exquisitely sensitive properties.

2. Technical Capabilities of NSLS-II

Achieving the scientific discoveries outlined above requires the following technical capabilities provided by NSLS-II:

- *Spatial resolution of ~ 1 nm* to enable the study of the multitude of real-world nanostructures and of the changes in the physical, electronic, chemical, and magnetic properties of man-made nanostructures brought about by deliberate “tuning” of composition and structure of these nanostructures;
- *Electronic energy resolution of ~ 0.1 meV* to enable the study of electronic excitations on the energy scales relevant to materials of scientific and technical importance, such as high-temperature superconductors and giant magnetoresistive materials;
- *Sensitivity to atomic structure, electronic structure, chemical composition, and magnetic properties* to enable in-situ chemical imaging, with a sensitivity of a single atom, of scientifically and technologically important materials such as electrocatalysts; studies of the electronic and magnetic properties of novel multifunctional devices that result from the merging of electronics, photonics, and spintronics, such as spin Light Emitting Diodes;
- *Sensitivity to surface features* to enable studies of the fundamentals of surface growth and surface-mediated reactions such as heterogeneous catalysis at gas-solid interfaces;

- *Sensitivity to sub-surface features* to enable studies of buried interfaces and nanostructures, to perform truly three-dimensional microscopy, and to determine the hierarchical structure of biomaterials, multi-component polymers, and nanocomposites;
- *Ability to operate in extremes of temperature, pressure, and applied magnetic fields* to enable studies of materials growth, catalytic reactions, and materials under extreme conditions, such as superconductors, magnets, and other complex systems;
- *Ability to handle high sample throughput* to enable combinatorial approaches to materials synthesis in the search for new materials with advanced properties

Among the available materials probes – i.e., x-ray scattering, neutron scattering, and electron beam microscopy – only x-ray scattering offers the potential to meet all of these technical requirements; however, even beams of x-rays presently do not have the required spatial resolution and energy resolution to meet the high demands. Achieving these requires the combination of high brightness, flux, and beam stability that NSLS-II will provide.

Achieving high spatial resolution. The spatial resolution of x-ray measurements is limited primarily by focusing optics and by source brightness. NSLS-II addresses both of these and, in addition, forges new ground in developing diffractive (i.e., “lensless”) imaging. The spatial resolution of NSLS-II x-ray microscopes will be unmatched, and NSLS-II will provide the world’s finest capabilities for x-ray imaging.

- *Focusing optics.* The NSLS-II project will fabricate advanced optics sufficient to reach spot sizes of ~ 1 nm for both hard and soft x-rays. Samples will be scanned under these nanometer-sized x-ray probes using high precision robotic manipulators, including adaptive optics with feedback, and the full gamut of x-ray techniques applied with nm spatial resolution. With these intense beams, spectroscopy on a single atom will be possible. For comparison, the smallest spot sizes that are expected to be achieved with current synchrotron light sources in the next several years are 30 nm in the crucial hard x-ray region and 15 nm in the soft x-ray region. Spectroscopy measurement with other sources will require thousands of atoms instead of just one.
- *Diffractive imaging.* A newly developing alternative to using the conventional optics described above is an x-ray imaging technique based on coherent diffraction. In principle, the ultimate resolution of this “lensless” technique is limited only by the x-ray wavelength, suggesting that resolutions in the 1 nm range, or possibly even better, could be achieved. However, in practice, the resolution is limited by the x-ray brightness. The ultra-high brightness of NSLS-II will provide the greatly increased coherent flux required to enable imaging the three-dimensional physical, chemical, and magnetic structures of materials with a spatial resolution of 1 nm. Since this technique does not require scanning a small probe beam across a sample, it also offers the opportunity to follow dynamic processes in time-resolved imaging experiments. This technique will be unique in its ability to provide full three dimensional images of individual nanoparticles or nanometer-sized grains in complex nanomaterials, both at the surface and deep below it, with sensitivity to their density, composition, oxidation and spin states, strain, texture, magnetization, atomic and electronic structure, and dynamics. For comparison, the best resolution achieved to date with this technique at

today's high-brightness 3rd generation light sources such as SPring8 or the Advanced Photon Source (APS) is 50 nm.

Achieving high energy resolution. The energy resolution of x-ray measurements is limited by x-ray monochromators and by x-ray source brightness and flux. NSLS-II addresses each of these and will bring about a new era in high resolution inelastic x-ray scattering.

- *Monochromators.* The charge and spin excitations governing emergent behavior described in Section B-1 have energies of order 1-100 meV and are difficult to study because x-ray scattering is a weak process. The situation is made even more difficult, because the energy resolution of state-of-the-art monochromators is inadequate (~120 meV for x-ray energies of 5-10 keV and ~ 1 meV for energies of 20-30 keV), and new monochromator designs are required. The NSLS-II project will provide the required resolution of ~ 0.1 meV over a broad energy range by developing a new monochromator and analyzer based on a novel design. The design achieves higher energy resolution than existing ones by utilizing the high angular dispersion of x-rays in highly asymmetric reflections from the monochromator crystals, rather than relying on the intrinsic spectral properties of Bragg reflections. Its performance will be further improved by utilizing sapphire crystals rather than the traditional silicon crystals used in current designs. The high brightness of the NSLS-II will permit the use of these new monochromators and analyzers for the study of the weak scattering processes.

The importance of source brightness and flux. Optics capable of nanometer focusing will have reduced acceptance aperture and efficiency, placing greater demands on the brightness of the source. NSLS-II will provide the ultra-high brightness necessary to enable x-ray nanoprobe measurements with enhanced sensitivity and high throughput. Achieving nanometer resolution with diffractive imaging requires sensitivity to weak scattering at high momentum transfers. The high brightness of NSLS-II will provide the high coherent flux required to reach nanometer, or even better, spatial resolution. The monochromators described above provide very high energy resolution at the cost of reduced x-ray throughput. In order to use these devices for weak inelastic scattering measurements, a source with greater brightness and flux than presently exists is necessary. NSLS-II will provide this ultra-high brightness and flux. The high brightness of NSLS-II will also extend the reach of the coherence-based technique of x-ray photon correlation spectroscopy to sub-nanosecond timescales, which is more than a factor of 10,000 times faster than routinely possible today. This will allow this form of time-domain spectroscopy to explore the short length scale fluctuations of a host of materials and phenomena, such as spin glasses, random field magnets, orbital order, and others.

The importance of beam stability. NSLS-II will have exceptional beam stability to enable the ultra-small beams to be focused without undesirable blurring due to beam motion; repeated measurements over long time scales with nanometer precision and reproducibility; and sensitive coherent imaging techniques to achieve the highest spatial resolution and coherent dynamics measurements.

The initial suite of instruments at NSLS-II will include five undulator beamlines. Their precise capabilities will be specified via continued consultation with the scientific community. However, in order to meet the mission need identified here, it is anticipated that they will be optimized for nanoscale imaging, diffractive imaging, inelastic scattering, small angle scattering, and magnetic scattering measurements. The NSLS-II project will also advance the state-of-the-art in experimental instrumentation, including advanced large array detectors with high efficiency and high readout speed.

3. Summary of Alternatives

The alternatives identified for consideration at Critical Decision 1 (Approve Alternative Selection and Baseline Range) are: (1) use other light sources worldwide, (2) upgrade one of the existing U.S. synchrotron radiation light sources, or (3) construct a new light source with the capabilities of NSLS II. Comparisons of the important technical parameters of NSLS-II with leading U.S. and foreign synchrotron radiation light sources – both operating and under construction – are given in Table 1.

Use foreign light sources. Analysis will focus on the impact to U.S. scientists on relying on foreign light sources in terms of gaining adequate access to those facilities. In addition, there are no foreign facilities in the near-term that will be able to provide capabilities comparable to those of NSLS II.

Upgrade an existing U.S. synchrotron light source. The analysis will focus on the four major synchrotron facilities operated by BES: the National Synchrotron Light Source (NSLS-I) at Brookhaven National Laboratory, the Stanford Synchrotron Radiation Laboratory (SSRL) at SLAC, the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory, and the APS at Argonne National Laboratory. The analysis may also consider upgrades to the smaller light sources operated by NSF.

Construct a new light source with NSLS II capabilities. As a comparison, in the hard x-ray region, a “new facility” NSLS-II would be 120 times brighter and have 12 times higher flux than the APS, and it would be 33 times brighter and have 4 times higher flux than SPring8. In the soft x-ray region, NSLS-II would be 380 times brighter and have 12 times higher flux than the ALS, and it would be 30 times brighter and have 5 times higher flux than Diamond. NSLS-II would also provide smaller beams than other facilities and superior beam stability, critical features for an x-ray nanoprobe.

Table 1. Comparison of Technical Parameters of NSLS-II with U.S. Synchrotron Facilities and Leading Foreign Facilities.¹

| Parameter | NSLS-II | ALS | APS | NSLS-I | SSRL | Diamond | SLS | ESRF | SPring8 |
|---|---------|-----------|-----------|----------|---------|-----------|----------|----------|---------|
| Energy [GeV] | 3.0 | 1.9 | 7.0 | 2.8 | 3.0 | 3.0 | 2.4 | 6.0 | 8.0 |
| Current [mA] | 500 | 400 | 100 | 280 | 500 | 300 | 400 | 200 | 100 |
| Top-off | Y | N | Y | N | Y | N | Y | N | N |
| Emittance [nm] | 0.5 | 6.8 | 3.5 | 63. | 18.0 | 2.7 | 5.0 | 3.8 | 3.0 |
| Insertion Device Beam Size (σ_x, σ_y) [μm] | 85, 4.3 | 309, 23.2 | 238, 10.8 | 369, 7.2 | 435, 30 | 179, 12.6 | 77, 11.4 | 404, 7.9 | 285, 10 |
| Insertion Device Straights | 22 | 9 | 35 | 8 | 14 | 22 | 9 | 28 | 38 |
| Soft X-ray Brightness ² | 4,193 | 11 | NA | 1 | 24 | 139 | 77 | NA | NA |
| Hard X-ray Brightness ² | 88,900 | NA | 733 | 1 | 29 | 311 | 93 | 1,667 | 2,667 |
| Soft X-ray Flux ³ | 25.2 | 2.1 | NA | 1 | 1.1 | 4.8 | 5.6 | NA | NA |
| Hard X-ray Flux ³ | 18.6 | NA | 1.5 | 1 | 1.9 | 0.5 | 0.7 | 3.1 | 5 |

¹ NSLS = National Synchrotron Light Source (Brookhaven National Laboratory, Upton, New York)
 ALS = Advanced Light Source (Lawrence Berkeley National Laboratory, Berkeley, California)
 APS = Advanced Photon Source (Argonne National Laboratory, Argonne, Illinois)
 SSRL = Stanford Synchrotron Radiation Laboratory (Stanford Linear Accelerator Center, Palo Alto, California)
 Diamond = Diamond Light Source (Rutherford Appleton Laboratory, United Kingdom)
 SLS = Swiss Light Source (Paul Scherrer Institut, Switzerland)
 ESRF = European Synchrotron Radiation Facility (Grenoble, France)
 SPring8 = Super Photon Ring – 8GeV (Hyogo, Japan)

² Brightness relative to that of NSLS-I, which is 3.1×10^{17} for soft x-rays (taken to be 800 eV) and 4.5×10^{16} for hard x-rays (taken to be 8 keV) (units are $\text{ph/s}/0.1\% \text{bw}/\text{mm}^2/\text{mrad}^2$).

³ Flux relative to that of NSLS-I, which is 2.7×10^{14} for soft x-rays (taken to be 800 eV) and 2.2×10^{14} for hard x-rays (taken to be 8 keV) (units are $\text{ph/s}/0.1\% \text{bw}$)

C. Importance of Mission Need and Impact if Not Approved

The economic and energy security of the United States requires that we develop alternative energy and pollution control technologies. Achieving this will require development of new materials with previously unimagined properties. The National Nanoscience Initiative is predicated on the promise of exploiting the remarkable changes in properties of materials when structured on the nanoscale to develop new nanodevices with enhanced properties.

To realize this promise, it is essential that we have the world's most advanced scientific tools. The Nanoscale Science Research Centers are dedicated to making new nanomaterials; the Transmission Electron Aberration-corrected Microscope will push electron microscopy to its ultimate limits; and the Spallation Neutron Source will push neutron scattering measurements to the best in the world. Although synchrotron radiation is unmatched in its ability to determine the physical, chemical, electronic, and magnetic properties of materials, it is currently impossible to do so with nm spatial resolution and 0.1 meV energy resolution. NSLS-II will deliver this capability.

Should NSLS-II not be approved, the needed ability to characterize materials with x-rays at nm spatial resolution and 0.1 meV energy resolution will not exist. Our ability to understand

materials and thus guide the research of the other facilities and research programs will be greatly diminished. Our efforts to develop zero-emission fossil fuel based power generation technology, hydrogen, and renewable energy may be less successful than required.

There are thirteen 3rd generation synchrotron light sources operating in the world today, including three in the U.S. (ALS, APS, and SSRL). By 2009, there will be thirty 3rd generation synchrotron light sources worldwide. Of these thirty, fully 13 will be equal to or significantly more powerful than the two strongest U.S. sources, ALS and APS. Some of the scientific goals of the community could be pursued on a limited basis at foreign facilities. However, experiments at these facilities will not achieve the spatial or energy resolution required by the BES program mission. In addition, U.S. researchers would be competing for scarce beam time, and they would be unlikely to have the opportunity to maintain a strong leadership position in these areas of science and technology. The priorities for beamline development and access would not be based on U.S. policy needs.

D. Constraints and Assumptions

1. Operational Limitations

There are no foreseen operational limitations in regards to effectiveness, capacity, technology, or organization. The criteria for the reliable operation of synchrotron accelerators are well established from years of experience in operating facilities such as the APS, ALS, SSRL, and NSLS-I. Radiation damage to accelerator components can be mitigated by careful design and is not an issue.

2. Geographic, Organizational, and Environmental Limitations

There are no unusual geographic or environmental limitations to siting NSLS II. The site would need to have adequate electrical power and an existing cadre of scientists, engineers, and technicians with experience in designing, building, and operating a major synchrotron light source facility. Radiation hazards for synchrotron x-ray sources are well understood and robust controls are available in order to protect personnel and the environment.

3. Standardization and Standards Requirements

The NSLS-II facility will conform to the applicable design, construction, and operational standards of a facility of this type.

4. Environment, Safety and Health Requirements

NSLS-II will fully comply with DOE Accelerator Order 420.2B, "Safety of Accelerator Facilities." The DOE will comply with the requirements of the National Environmental Policy Act (NEPA) and its implementing regulations (10 CFR 1021 and 40 CFR 1500-1508) prior to taking any action on the proposed project that could have adverse environmental effects. A NEPA evaluation will be prepared to evaluate the potential environmental consequences of constructing and operating NSLS-II.

5. Safeguards and Security Considerations

None of the work at NSLS-II will be classified and no safeguard or security issues are foreseen during the design, construction, or operation phases. Access to the accelerator site will be controlled primarily to ensure worker and public safety and for property protection. Appropriate safeguard and security requirements will be implemented.

6. Interfaces with Existing and Planned Acquisitions

The BES Nanoscience Research Centers (NSRCs) will provide scientific expertise and advanced instrumentation, including specialized e-beam lithography equipment, high resolution electron microscopes, and scanning probes, that will be essential in carrying out R&D on, and fabrication of, the advanced optics required to achieve ~ 1 nm spatial resolution. Once operational, the scientific programs of the NSRCs will create nanostructured materials using their advanced nanofabrication equipment. NSLS-II will provide unique and indispensable capabilities for characterizing these materials with nm spatial resolution and 0.1 meV energy resolution. These studies will, in turn, guide the design and creation of new nanomaterials that have optimized properties and enhanced functionality.

7. Affordability Limits on Investments

At this preliminary stage, the NSLS II Total Project Cost (TPC) is estimated at \$600 to \$800 million (as spent). All funding would be provided by the BES Program. This project will require funding above the current Office of Science out-year funding target.

One possible constraint associated with success of the NSLS-II project is achieving the funds to construct and operate this facility. As with all large capital projects, NSLS-II will be vulnerable to budget and funding variations from the planned profile. Such multi-year construction projects need to have the planned funding appropriated each year of the construction project in order to ensure that the project can be completed on time and within the agreed upon baseline budget.

8. Goals for Limitations on Recurring or Operating Costs

Appropriation of an adequate operational funding level is of great important to ensure full utilization of this state-of-the-art facility. Based on experience with operating and maintaining DOE's existing synchrotron light sources, the annual operational cost for NSLS II is estimated to be approximately \$90 million (in 2005 dollars) and this would be funded entirely by the BES Program.

9. Legal and Regulatory Constraints or Requirements

The NSLS-II project will be in full compliance with all applicable Federal, state and local requirements. The legal and regulatory requirements to construct this facility will include typical construction permits. No significant hurdles are anticipated. Accelerator Readiness Reviews will ensure compliance with the accelerator order prior to commissioning activities.

10. Stakeholder Considerations

No significant stakeholder issues are anticipated. The synchrotron radiation scientific user community of the U.S., presently consists of ~ 8,000 scientists and, if current growth trends

continue, the user community may increase by 50 percent by the time NSLS-II becomes operational. The user community has been extensively involved in the planning of this project, and it is expected that NSLS-II will attract university, national laboratory, industry, and international users. Congressional support for the synchrotron light sources operated by BES has been strong.

11. Limitations Associated with Program Structure, Competition and Contracting, Streamlining, and Use of Development Prototypes or Demonstrations

There are no technical limitations to the construction of NSLS-II since it can be built based on extrapolation of existing technologies. Some research and development must be completed as part of this project, including development of superconducting undulators, advanced optics, advanced detectors, and robotic sample manipulators.

E. Applicable Conditions and Interfaces

Operation of the present NSLS-I facility will be discontinued at the time that the NSLS-II facility goes into operation.

F. Resource Requirements and Schedule

The NSLS II TPC is estimated to be in the range of \$600M to \$800 million (as spent). This would include design, R&D, civil construction, equipment procurement and installation, project management, quality assurance, pre-operations, and contingency. There is reasonable confidence in this estimate because it is based on a substantial pre-conceptual design effort, comparison with other recent synchrotron construction projects, and experience with building and operating NSLS-I.

The rationale for initiating CD-0 at this time is driven by SC's evaluation of the strong demand by scientific users for NSLS-II's unique capabilities as well as by the need for the U.S. to remain competitive in this economically important field of scientific research. A conceptual design report and NEPA review could be completed by calendar year 2006. A preliminary milestone schedule to construct NSLS-II is shown in Table 2.

Table 2. Preliminary Milestone Schedule

| Major Milestone Events | Preliminary Schedule |
|---|---------------------------|
| CD-0 (Approve Mission Need) | 2 nd Qtr, 2005 |
| CD-1 (Approve Alternative Selection and Cost Range) | 2 nd Qtr, 2006 |
| CD-2a (Approved Long-lead Procurement Budget) | 3 rd Qtr, 2006 |
| CD-2b (Approve Performance Baseline) | 3 rd Qtr, 2007 |
| CD-3a (Approve Start of Long-lead Procurement) | 3 rd Qtr, 2007 |
| CD-3b (Approve Start of Construction) | 3 rd Qtr, 2008 |
| CD-4 (Approve Start of Operations) | 2013 |

A hypothetical funding profile for the top of the TPC range, shown in Table 3, illustrates the time phasing of project funding. The funds for long-lead procurement (LLP) would be for

items that require little or no design effort. Other Project Costs (OPC) would include funds for conceptual design, R&D, NEPA, and pre-operation activities. The timing of CD-3a and CD-3b is in anticipation of the availability of LLP funds at the beginning of FY 2008, and construction funds at the beginning of FY 2009.

Table 3. Preliminary Annual Funding Profile (in millions of \$)

| | All Prior Years | FY 2007 | FY 2008 | FY 2009 | FY 2010 | FY 2011 | FY 2012 | FY 2013 | Totals |
|--------------|-----------------|---------|---------|---------|---------|---------|---------|---------|--------|
| OPC | 1.0 | 11.0 | 12.0 | 5.0 | 5.0 | 10.0 | 20.0 | 50.0 | 114.0 |
| PED | | 34.0 | 35.0 | | | | | | 69.0 |
| LLP | | | 30.0 | | | | | | 30.0 |
| Construction | | | | 140.0 | 150.0 | 150.0 | 100.0 | 47.0 | 587.0 |
| Totals | 1.0 | 45.0 | 77.0 | 145.0 | 155.0 | 160.0 | 120.0 | 97.0 | 800.0 |

The key measure of the success of the NSLS-II project will be to design, build, and install the relevant accelerator hardware, experimental apparatus, civil construction, and central facilities within the Performance Baseline cost and schedule constraints, while meeting the technical performance parameters specified in its Project Execution Plan.

G. Development Plan

While NSLS-II will deliver unprecedented levels of brightness, flux, and stability, the technology for it is based on extrapolation of existing designs and hardware to more demanding specifications. The major procurements require no R&D and present low technical risk. There are no known technical “show stoppers” in constructing NSLS-II, but pre-construction R&D on four key elements will be conducted to explore cost reductions and enhanced performance. These technical risks include: demonstrating the ability to fabricate undulators using superconducting magnets with the required high field precision and uniformity for generating high brightness x-rays; demonstrating the ability to fabricate optics that are capable of focusing hard x-rays to 1 nm; demonstrating monochromators and analyzers that are capable of achieving 0.1 meV energy resolution, and demonstrating x-ray array detectors that have large area and high efficiency. R&D is underway at BNL in all four areas and prototypes will be developed and tested to demonstrate the required performance prior to CD-3b, thus eliminating these technical risks. Furthermore, these elements represent relatively small fractions of the overall effort so the cost risk for the project as a whole is low. Technical scope, cost, and schedule risks are minimal, and so the overall technical risks are judged to be low. There are no known operational constraints or ES&H issues that would entail significant difficulties.