CD-0, Approve Mission Need for the Linac Coherent Light Source (LCLS)

Office of Basic Energy Sciences Office of Science

A. Justification of Mission Need

1. Office of Basic Energy Sciences Program Mission

The mission of the Office of Science is "To advance basic research and the instruments of science that are the foundations for DOE's applied missions, a base for U.S. technology innovation, and a source of remarkable insights into our physical and biological world and the nature of matter and energy." The Linac Coherent Light Source (LCLS) project is a unique opportunity for a major advance in carrying out that mission.

The Office of Basic Energy Sciences (BES) within the DOE Office of Science currently operates four major synchrotron facilities: the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory, the Stanford Synchrotron Radiation Laboratory (SSRL) at the Stanford Linear Accelerator Center (SLAC), the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory and the Advanced Photon Source (APS) at Argonne National Laboratory. These four facilities provide world-class X-ray probes of matter to an enormous user community that spans a broad range of the physical and biological sciences. BES is dedicated to the stewardship of the current light sources, as evidenced by the ongoing upgrades to SSRL, and to advancing the state-of-the art in X-ray probes of matter through the development of next-generation sources and instruments.

In the early 1990s, it became clear that the next-generation X-ray light source would be based on a linac-driven, x-ray free electron laser (XFEL). As early as 1992, workshops began to better define the properties of such an XFEL and the science that would be enabled. In 1994, the National Research Council published a study, *Free Electron Lasers and Other Advanced Sources of Light, Scientific Research Opportunities*, that reached the conclusion that FELs were not competitive with conventional lasers for scientific applications *except* in the X-ray region.

By 1997, SLAC had developed a concept for the Linac Coherent Light Source (LCLS), an XFEL based on the last third of the existing 50 GeV SLAC Linac. The proposed LCLS is truly a next-generation light source with properties vastly exceeding those of current synchrotron sources in three key areas: peak brightness, full spatial coherence, and ultrashort pulses. The peak brightness of the LCLS is some 10 orders of magnitude greater than current synchrotrons, providing 10^{12}-10^{13} X-ray photons at energies from 0.8 to 8 keV in a pulse with duration of 230 femtoseconds.

The Basic Energy Sciences Advisory Committee (BESAC) has been actively involved with the development of the next-generation light source and keenly interested in new realms of science to be explored with such an XFEL. In 1997, the BESAC report *DOE Synchrotron Radiation*

Sources and Science (known as the Birgenau-Shen Report) recommended funding an R&D program in next-generation light sources and that another BESAC panel be convened to focus on this topic. The result was the 1999 BESAC report *Novel, Coherent Light Sources* (known as the Leone Report). That report concluded:

> "Given currently available knowledge and limited funding resources, the hard X-ray region (8-20 keV or higher) is identified as the most exciting potential area for innovative science. DOE should pursue the development of coherent light source technology in the hard X-ray region as a priority. This technology will most likely take the form of a linac-based free electron laser using self-amplified stimulated emission or some form of seeded stimulated emission…"

In addition, the report observed for the first time that:

> "The is a symbiotic relationship between future accelerator-based sources and high-powered ultrafast lasers. Future light sources will involve a complete marriage of accelerator and laser principles…"

The latter observation had a profound impact on the nature of the development of scientific applications for the LCLS, setting in motion the merging of the community of scientists experienced in x-ray applications at synchrotrons with the community of scientists who use ultrafast lasers in the visible and ultraviolet spectral regions. The former is largely unfamiliar with the use of ultrashort pulses to probe dynamics and with the interaction of intense radiation with matter, while the latter is largely unfamiliar with the use of x-rays to probe matter. An extensive series of workshops has brought these two communities together to develop the scientific applications of the LCLS and to form the nucleus of a user community.

The Leone Report also recommended the start of an R&D program to explore key issues with regard to the LCLS. Following this recommendation, BES began funding a 4-year LCLS R&D program for the period FY1999–FY2002. SLAC and SSRL, in partnership with the APS, BNL, LANL, LLNL, and UCLA, formalized a broad program of R&D to address the technical issues. A Technical Advisory Committee (TAC) and a Scientific Advisory Committee (SAC) were formed by SLAC to review the progress of the R&D program, and each has met regularly.

2. Project Purpose and Justification

The LCLS will serve as a research and development center for XFEL physics in the hard x-ray regime and as a facility for the application of XFEL radiation to experimental science.

The LCLS will provide coherent radiation of unprecedented intensity and pulse duration in the wavelength range 1.5–15 Å. It is based on the SLAC linac, which can accelerate electrons or positrons to 50 GeV. The linac presently serves primarily as an injector of electrons and positrons for the PEP-II B Factory. The last one-third of the linac is available for the production of electron beams of up to 15 GeV, and with the endorsement of the SLAC faculty and the SLAC Science Policy Committee, a commitment has been made to provide a minimum of 70% of the operational time of the linac for LCLS.

For the LCLS, the linac will produce high-current, very low emittance 5–15 GeV electron bunches, nominally 230 fs in length, at a 120 Hz repetition rate. When traveling through the 120 meter long LCLS undulator, the electron bunches will lead to self-amplification of the emitted X-ray radiation constituting an X-ray free electron laser (XFEL). The LCLS makes use of technologies developed for the SLAC Linear Collider, progress in the production of intense electron beams with radio-frequency photocathode guns at SLAC and BNL, and the development of undulator technology at the APS. The LCLS will be the first XFEL in the world operating in the 1.5–15 Å wavelength range utilizing the first harmonic of the undulator (shorter wavelengths are possible using higher harmonics). The emitted coherent X-rays will have unprecedented brightness with 10^{12}–10^{13} photons/pulse in a 0.2–0.4% energy bandpass and an unprecedented time structure with a design pulse length of 230 fs.

The unique characteristics of the LCLS will open new realms of scientific applications in the chemical, materials, and biological sciences. Work on scientific applications of the LCLS began shortly after it was introduced conceptually in 1992. Most recently, at the request of BES, the LCLS SAC selected five experiments as those most likely to be initially mounted on the LCLS. These are summarized in the document, *LCLS: The First Experiments*, submitted to BES for review by BESAC and by a panel of independent experts in September 2000. In October 2000 BESAC expressed their support for the LCLS experimental plan and voted unanimously to recommend that DOE proceed with the Conceptual Design Report for the LCLS by approving CD-0, following receipt of the independent peer review comments. The independent reviews expressed clearly that the scientific case for the LCLS was strong, but suggested that some areas that could be strengthened further. In early May 2001, BES sponsored a workshop that significantly enhanced the case for the LCLS as a probe of ultrafast dynamics in condensed phases and more clearly defined the experimental science that can be accomplished with the initial operating parameters of the LCLS. Another significant result of the May workshop was the elucidation of schemes by which the longitudinal coherence of the LCLS could be improved and the pulse length reduced into the ten-femtosecond range.

These first five areas of experimentation currently envisaged for the LCLS are fundamental studies of the interaction of intense X-ray pulses with simple atomic systems, use of the LCLS as a pump source to create warm dense matter and plasmas, structural studies on single nanoscale particles and biomolecules, ultrafast dynamics in chemistry and solid-state physics, and studies of nanoscale structure and dynamics in condensed matter. The experiments fall into two classes. The first follows the traditional role of X-rays to probe matter without modifying it while the second utilizes the phenomenal intensity of the LCLS to excite matter in fundamentally new ways and to create new states in extreme conditions.

The fundamental studies of the interactions of intense X-rays with simple atomic systems are necessary to lay the groundwork for all interactions of the LCLS pulse with atoms embedded in molecules and condensed matter. They include investigations of multiple ionization and direct multiphoton excitation of core-level electrons. The penetrating power of hard X-rays, combined with the large number of photons in each pulse, make the LCLS an ideal pump source for the uniform excitation of nanoscale volumes of matter. This excitation can be mild or intense, ranging from the initiation of structural phase changes in condensed matter to the creation of new forms of matter, such as the mildly ionized plasma state known as warm dense matter that is found in both terrestrial and astrophysical environments. The LCLS initiated excitations can be probed by a time-delayed LCLS pulse or by the broadband wiggler radiation that accompanies the primary XFEL beam.

The structural studies of individual particles or molecules make use of recent advances in imaging techniques for reconstructing molecular structures from diffraction patterns of non-crystalline samples. The need for crystalline regularity in X-ray crystallography arises because of the need to amplify the diffraction process from a single particle through Bragg scattering. The enormous photon flux of the LCLS makes it feasible to determine the structure of a single biomolecule or small nanocrystal using only the diffraction pattern from a single moiety. This application has enormous potential in structural biology, particularly for important systems such as membrane proteins, which are virtually uncharacterized by X-ray crystallography because they are nearly impossible to crystallize. One of the most intriguing aspects of this research is that it utilizes the extremely short pulse duration of the LCLS to "beat" the problem of radiation damage. The biomolecule or nanoparticle exposed to such an intense LCLS pulse will explode as the result of the massive ionization of its constituent atoms. However, the LCLS pulse is so short that it appears to be feasible to capture a diffraction image before the molecule or nanoparticle flies apart.

The last two sets of experiments make use of the extremely short pulse of the LCLS to follow dynamical processes in chemistry and condensed matter physics in real time. The coherence properties of the LCLS beam are utilized in experiments on condensed matter that employ X-ray Photon Correlation Spectroscopy (XPCS) or X-ray Transient Grating Spectroscopy. XPCS is currently being applied to the study of near-equilibrium dynamics at synchrotron sources, but is limited by coherent photon flux and the ability to time delay excitation pulses. The XTGS technique stems from the laser community, where it is commonly practiced in the optical spectrum. The use of ultrafast X-rays will open up whole new regimes of spatial and temporal resolution to both techniques.

The last set of experiments planned for the LCLS use X-ray diffraction as a probe of dynamics initiated by another ultrafast laser. At 230 femtoseconds, the LCLS pulse does not yet have sufficient temporal resolution to follow atomic motion in simple molecules, which occurs on the timescale needed to break or make individual chemical bonds in isolated molecules (~50 femtoseconds). However, it will be very useful for probing larger scale molecular dynamics, such as protein folding, molecular re-arrangement in photosynthetic centers following light excitation, or chemical reactions in solution where solvent effects are significant. As noted above, there are now proposals for R&D on the XFEL physics that will enable LCLS operation at pulse lengths as short as ten femtosceconds that would enable X-ray diffraction to be performed on the timescale of atomic motion.

3. Project Description

The project proposed is to build an X-Ray FEL Facility at SLAC. It requires <u>a new 150 MeV injector</u> to be built at Sector 20 of the 30-sector SLAC linac to create the high brightness electron beam required for the FEL. The last one third of the linac will be modified by adding <u>two</u>

magnetic bunch compressors. Most of the linac, and its infrastructure, will not be changed. The existing components in the Final Focus Test Beam tunnel will be removed and replaced by a new 120 meter undulator and associated equipment. Provision will be made for housing instrumentation and controls for the initial experiments.

B. Project Cost Range

The preliminary Total Estimated Cost (TEC) is in the range of $165M to $225M. The current estimate is $175M (design, project management, quality assurance, construction, and contingency at 25% of the TEC). The expected source of funding is the Basic Energy Sciences program. Project Engineering and Design funds will be provided in FY03 to begin Title I and II design.

Upon approval of CD-0, the project will initiate development of the Conceptual Design Report (CDR) and the National Environmental Policy Act (NEPA) documentation. The cost to prepare the final CDR, after CD-0 approval, is estimated at $225K. The cost for the NEPA documentation is estimated at $75K.

C. Project Schedule and Funding Profile

The preliminary schedule is as follows:

CD-0	Approve Mission Need	June 2001
CD-1	Approve Preliminary Baseline Range	January 2002
CD-2	Approve Performance Baseline Range	May 2002
CD-3	Approve Start of Construction	October 2003*
CD-4	Approve Start of Operations	October 2006

* The CD-3 approval may be phased with initial approval for key elements in October 2003 and approval for the remaining phased over FY 2005.

This preliminary schedule is based on receiving the following funding levels in thousands of dollars:

Fiscal Year	Total Estimated Cost		Other Project Costs		TPC
	Project Engineering & Design	Construction	Research and Development	Pre-operations	Total
Prior			4,425		4,425
2002			1,500		1,500
2003	6,000		3,000		9,000
2004	15,000	40,000	500		55,500
2005	10,000	55,000		2,000	67,000
2006	2,500	46,500		4,000	53,000
Total	33,500	141,500	9,425	6,000	190,425
	175,000*		15,425		190,425

* The TEC is a preliminary estimate and the projected TEC range is $165M to $225M.

D. Acquisition Strategy

The acquisition of the LCLS will be conducted through SLAC as an M&O contractor. The project makes extensive use of existing SLAC facilities including 1/3 of the linear accelerator. The installation must be carefully coordinated with other research activities at the laboratory. Therefore, it is infeasible to have a separate subcontract with another organization to manage this project. The project is similar in scope to the recently completed B-Factory at SLAC which was conducted successfully by SLAC management. SLAC has the resources to direct this project and the resources, with collaborators, to execute the project.

The Stanford Synchrotron Radiation Laboratory (a Division of SLAC), in close cooperation with the Technical Division, will be responsible for accomplishing the project under the terms of Stanford University's contract with the Department of Energy. SLAC will execute those parts of the project associated with the acceleration and control of the electrons as well as overall system integration and management. The Advanced Photon Source Division of Argonne National Laboratory will design and fabricate the undulator and associated systems. The Physics and Advanced Technologies Directorate at Lawrence Livermore National Laboratory will design, fabricate, qualify, and commission the front-end X-ray optics. Project management at SLAC using Memoranda of Understanding and project reporting tools will control this work at these laboratories.

The activities will be accomplished to the extent feasible by using fixed-priced subcontractors selected by SLAC on the basis of best value, price and other factors. A detailed acquisition plan will be developed as part of the conceptual design process.

E. Environmental Strategy

SLAC will comply with all requirements of the National Environmental Policy Act (NEPA) and its implementing regulations. A NEPA evaluation will be performed during the design phase of the project to ensure any possible adverse effects of the project are addressed. No negative impacts to the environment are anticipated as a result of this project.

F. Integration with Site Activities

The project will be integrated with site activities through the establishment of a project management team that will include members from operations, facilities management, project management and other organizations that could be affected by the project. The project requirements are within the capabilities of SLAC and the collaborating institutions.

G. Feasibility of Other Alternatives and Risk of Doing Nothing

Building the LCLS at other sites would incur a major increase in cost because of the availability of the 1 km linac between sectors 20 and 30 at SLAC. The cost of a new 16 GeV linac would be around $300 M. A superconducting undulator was considered but rejected on the basis of unwarranted increase in technical risk.

If this project does not go forward, a major opportunity will be lost. For a modest cost (modest because this project is able to use extensive infrastructure at SLAC including the linac) a tool can be built to access fundamental questions about molecular structure. The LCLS will produce an intense beam of coherent X-rays with a wavelength comparable to the interatomic spacing in molecules that, as well, has very short time structure that will enable dynamic studies. There are no tools available currently that come within orders of magnitude of this capability.

The science accessible with the LCLS is so compelling that if this machine is not built another machine will be built, most likely in Germany or Japan. This would be a loss to science in general since the capability would be available much later at more cost and would be a loss to the United States because of a lost opportunity to be a world leader in this field.

H. Risk Management

The three areas of technical risk are associated with the electron source and the undulator. Both of these are extrapolations of existing technology to more demanding specifications.

The first technical risk is achieving the required brightness in the electron beam. A research and development program on the electron source is underway at the Gun Test Facility (GTF) at SSRL. This R&D program is expected to demonstrate a source with the desired specifications before CD-2 thus eliminating this technical risk. In the meantime, the FEL physics group is investigating techniques for relaxing the tolerances.

The second technical risk is the demanding tolerances on the undulator. A full-scale prototype of one section of the undulator is being built as part of the undulator R&D program. This prototype will be carefully measured and then put in a beam line. This program will uncover any deficiencies in the design early enough to make corrections to the production undulator sections. This will significantly reduce the undulator technical risk.

The third technical risk is the extraordinary energy density of the LCLS X-ray beam at the X-ray optics. New techniques are being developed to handle this energy density. Prototype optical elements are being constructed at LLNL. These elements will be tested under simulated conditions using high power lasers that are available at LLNL.

The most significant cost risk is the civil construction. A proposed experimental hall involves a significant excavation. Such construction is subject to delays due to unexpected rock conditions, weather, etc. Test boring before going out for bid will mitigate this risk. Prospective bidders will be prequalified based on previous safety, quality, and schedule performance. The San Francisco bay area construction market has been very tight and could well continue so through this project. SLAC will be building similar buildings on site prior to the experimental halls so will have recent cost performance experience. Extra contingency may be required on the civil construction to keep this project under the baseline estimate.

Submitted by:

__________________________________ _________________

Iran L. Thomas Date
Director, Materials Sciences and Engineering Division
Office of Basic Energy Sciences
Office of Science

Reviewed by:

__________________________________ _________________

Daniel Lehman Date
Director, Construction Management Support Division
Office of Science

Recommendation

The undersigned Does Recommend (Yes) or Does Not Recommend (No) approval of CD-0 as noted below.

__________________________________ __________________ Yes ____ No ____

Patricia M. Dehmer Date
Associate Director, Office of Basic Energy Sciences
Office of Science

Approval

Critical Decision-0, Approve Mission Need, for the Linac Coherent Light Source (LCLS) is approved, and the Stanford Site Office (SSO) is authorized to proceed with development of the Conceptual Design for this project.

__________________________________ ____________________

James F. Decker Date
Acting Director of the Office of Science