Report from BESAC to the Office of Science on New and Upgraded National User Facilities

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BESAC Facilities Subcommittee

Charge to BESAC

On December 1, 2023, Dr Asmeret Berhe, Director of the DOE Office of Science (SC1), charged the Basic Energy Sciences Advisory Committee (BESAC) with considering new and upgraded facilities proposed or planned by DOE's Basic Energy Sciences Directorate that will be crucial for making forefront scientific discoveries. The primary elements of the evaluation are:

1. *Potential to contribute to world-leading science* in the next decade, categorizing each facility as: (a) absolutely central; (b) important; (c) lower priority; or, (d) don't know enough yet.
2. *Readiness for construction*, classifying as (a) ready to initiate; (b) significant scientific/engineering challenges to resolve before initiating; or (c) mission and technical requirements not yet fully defined.

BESAC was asked to further consider opportunities for cross-directorate partnerships within the Office of Science that would advance science and user effectiveness. The demographics of future user communities were another consideration, spanning research topics, the number and geographic origin of users, and their level of technical expertise.

In response to the SC-1 charge, a BESAC Subcommittee on Facilities led by Dr. Eric Isaacs and Prof. Serena DeBeer (Appendix 1) was created, consisting of eleven members with expertise that span the science and capabilities of X-ray and neutron facilities. The subcommittee was asked to assess eight facilities:

- Two Neutron Sources at Oak Ridge National Laboratory
    - High Flux Isotope Reactor Pressure Vessel Upgrade (HFIR PVR)
    - Spallation Neutron Source Second Target Station (SNS-STS)
- Upgraded synchrotron instruments at Brookhaven National Laboratory
    - National Synchrotron Light Source (NSLS)-II NEXT III instrument suite
    - NSLS II Upgrade
- X-ray Free Electron Lasers at SLAC National Accelerator Laboratory
    - Linac Coherent Light Source High Energy Upgrade (LCLS II HE)
    - Low Emittance Injector for LCLS II HE (LEI)
    - LCLS-X
- Future Light Source (FLS) – a 'green field' light source, location(s) TBD

Overview

Over the past four decades, the Department of Energy's (DoE) Office of Science Basic Energy Sciences light and neutron sources have had a profound impact on scientific discovery and technological innovation in the United States. Research at BES facilities has yielded more than 84,000 publications and nine Nobel Prizes, and served over 260,000 users (FY04-FY23).

The BES light and neutron sources, in conjunction with DOE's computing facilities, have been pivotal for significant breakthroughs in US research and development, in critical fields, such as, new materials for applications in quantum science, catalysis, semiconductor devices, and the energy transformation—all of which are critical for national security. These facilities also advance drug design, structural biology, and efficient manufacturing design, which impact human health and economic competitiveness.

While BES facilities are generally world-leading, global competition is fierce putting US leadership at risk. (See the BESAC International benchmarking report.) China and the EU are aggressively advancing next-generation XFELs, synchrotrons and neutron sources. The EU already has world leading reactor-based research facilities. Hence, there is great urgency for the US to advance the capability of these crucial facilities to ensure US leadership in discovery science and technological innovation.

The BESAC Subcommittee commends the forward-thinking leadership of ’BES aimed towards providing a portfolio of key, major user facilities that will drive discovery and innovation for US scientists and engineers for the future. Herein, the subcommittee provides insights into the status of emerging facilities that will enable future breakthroughs.

Summary of the BES Facilites Subcommittee assessments

The subcommittee concluded that all of the *X-ray and neutron facilities considered are absolutely central to the success of US science and technology*. A testament to the strength of BES planning, each new facility will provide capabilities that ensure the US continues to lead the world in discovery science and key technologies that address the DOE BES and the Nation’s top priorities. The basis for the evaluations is articulated below.

Neutron Facilities at Oak Ridge National Laboratories

Pressure Vessel Replacement for the High Flux Isotope Reactor (HFIR):

a) Is **absolutely central** to future world-leading science.
Rationale: The PVR is required for HIFR to produce isotopes critical for energy, medicine, and national security: materials irradiation for essential analytic tools including for reactor fuels and sensitive probes of magnetic and soft materials. *HIFR will be the only source of these isotopes in the western hemisphere.*

b) Has a **significant engineering challenge**—to secure regulatory approval before PVR achieves CD2/3. CD0 has been achieved and CD1 is approaching.

The **Second Target Station** at the Spallation Neutron Source:

a) Is **absolutely central** to future world-leading science.
Rationale: It will be the world’s brightest source of cold neutrons (up to 100x brighter than existing facilities), enabling discovery science and technologies, in the fields of quantum materials for computing and sensors, biological and soft materials for science, energy, national security and medicine.

b) STS will be **ready to proceed** to CD2 once the science case is refined and the instrument suite supports the science.

Synchrotron Sources of X-rays at Brookhaven National Laboratory

NSLS II NEXT III:

a) Is **absolutely central** to future world-leading science.
Rationale: Enables NSLS II to fulfil mission critical science in energy storage, catalysis science, and quantum materials science through an integrated multiscale, multimodal suite of beamlines.

b) The **technical requirements not yet fully defined**. The capabilities and capacity that the new beamlines will create for science should be clarified by CD1, scheduled for later in 2024.

NSLS II Upgrade

a) Is **absolutely central** to future world-leading science.
Rationale: The upgrade will provide the world’s brightest synchrotron source in the 1-10 keV range, by using a unique accelerator design. The upgrade will enable experiments to address key challenges in microelectronics, clean energy, bio-preparedness and quantum materials using a multiscale, multimodal approach for studies under operating conditions.

b) **Engineering challenges** remain for the unique Triple Complex Bend Achromat (TCBA) accelerator design that need to be addressed with additional research.

X-ray Free Electron Lasers (XFELs) at SLAC National Accelerator Laboratory

There are three projects inter-related projects for the XFEL at SLAC with major potential for transformational energy science; however, their impact will be strongly dependent on the timing of the start of operations due to strong global competition for development of XFELs. The EU XFEL is planning similar projects for later this decade.

The **Linac Coherent Light Source II High Energy (LCLS II HE)**:

a) Is **absolutely central** to future world-leading science.
Rationale: LCLS II HE will provide the world's brightest source of atomic-resolution X-rays with ultrafast pulse structure, increasing the average X-ray brightness in the hard X-ray range up to 13 keV by 3,000-fold.

b) The project **will be ready to initiate** since 90% of the facility design is already complete. CD-2/3 is planned for May 2024, major construction will begin in summer 2025, and an early finish date of readiness for CD-4 is anticipated by FY2027 end.

The Low Emittance Injector (LEI) for LCLS II HE:

a) Is **absolutely central** to future world leading science.
Rationale: The LEI will yield the world's brightest X-ray laser for model-free structural dynamics and insights into complex energy systems and quantum materials. It will provide a superconducting electron source that will: (i) improve the X-ray beam brightness to extend XFEL operation from 13 keV to 20 keV, enabling sub-angstrom atomic resolution. Furthermore, the LEI will be central to the future development of LCLS-X.

b) Is close to **readiness-to-construct** with essential R&D and modeling underway showing that the required emittance can be reached.

LCLS-X:

a) Is **absolutely central** to future world-leading science.
Rationale: LCLS-X will be the first 3rd-generation X-ray free electron laser in the world. Its advanced capability will enable understanding and control of structural dynamics that underpin 21st century science in technology and energy. With the proposed ten specialized XFELs and dozens of intruments, multiple parallel experiments will be possible, reducing the cost per experiment and scientific throughput dramatically.

b) Has **significant scientific/engineering challenges** to resolve before Critical Decision process after LCLS-II-HE is complete to determine if LCLS-II-HE accelerator will be sufficiently powerful to feed 10 undulators.

The Future Light Source:

a) Is **absolutely central** to future world-leading science.
Rationale: Planning for future accelerator projects beyond those currently imagined is essential for the science of the future. Because of the long lead time for imagining and designing new large-scale facilities, it critical to plan now for the future. Otherwise, the US will certainly lag in global competitiveness in science and technology.

b) The **mission and technical requirements not yet fully defined** for the FLS. Future-looking planning and design are necessary.

Detailed Assessment:

Neutron Facilities

Neutron sources provide essential and powerful tools that enable production of critical isotopes for medicine, national security, forensics and for basic research and development. (See BESAC 2020 report on US Domestic High-Performance Reactor-Based Research Facility). Neutrons have several unique characteristics as probes, including penetration through most materials; light element sensitivity (e.g. hydrogen, deuterium, and lithium); sensitivity to magnetism; and very high energy resolution (down to about 10 µV) and polarization, which together offer high-precision characterization of atomic and spin structure and dynamics. Oak Ridge National Laboratory (ORNL) has proposed an upgrade for the High Flux Isotope Reactor (HFIR) with a Pressure Vessel replacement and the Second Target Station, a second source at the Spallation Neutron Source. ORN'Ls *proposed upgrades, as part of a two-facility, three-source strategy, will offer the opportunity for the US to remain world leaders in both reactor-based and accelerator-based neutron science.*

The Second Target Station (STS) project at SNS is absolutely central for the US to maintain a world-leading position in neutron scattering science for the foreseeable future. STS will be the next-generation, short-pulse, cold neutron source that provides up to a factor of 100 increase in experimental performance in peak brightness at 5 angtroms and provides capabilities not currently available anywhere in the world. If construction begins promptly these capabilities could be available in the second half of the next decade.

That being said, it is imperative that the types of unique, transformational science that will be achievable with the STS, not possible today with any other source, be articulated. In other words, plans for the inaugural experiments using the first suite of instruments, be clearly stated to highlight the power of the STS.

SNS aims to construct a low-repetition-rate (15 Hz) facility at the existing ORNL Spallation Neutron Source (SNS) to augment and complement the capabilities of the First Target Station (FTS). STS will provide an initial suite of 8 novel neutron scattering instruments and capacity for 20 instruments. The project will leverage the ongoing Proton Power Upgrade (PPU) that doubles the available power from the SNS accelerator from 1.4 MW to 2.8 MW and provides the capability to seamlessly connect to the STS beam transport system. The closest competitor facility is the J-PARC MLF in Japan. Other sources with substantially lower peak and average brightness include ISIS-TS1/2 in the United Kingdom and the CSNS in China. The European Spallation Source (ESS) long-pulse facility is under construction in Sweden and will provide neutrons by 2027 with a ramp-up to a proton beam power of 2 MW serving 15 instruments at 14 Hz by ~2028. The facility is planning to upgrade to 5 MW and 22 instruments in the early 2030s but will not achieve the proposed STS peak brightness.

STS and its instruments will generate cold neutrons with unparalleled flux to address the scientific grand challenges identified by the Office of Science in the quantum universe, sustainable manufacturing methods and climate science among others. It is expected to be an integral and unique characterization enabler for the future technological era. The construction of this facility will also allow the United States to maintain and bolster its world leadership in producing high impact science and engineering research as stated in the BESAC International benchmarking report published in 2021.

The unique technical capabilities of STS will supply a range of transformational capabilities which are not accessible at any neutron facility worldwide: time-resolved measurements of kinetic processes in materials during synthesis and formation; exploration of the physics of out-of-equilibrium systems, as well as materials during phase transitions; experiments leveraging the unique interactions of neutrons with matter, to simultaneously measure hierarchical structures across a broad range of length and time scales in functional materials; and parametric studies on very small sample volumes of novel systems to accelerate materials discovery.

The next generation of quantum computers will require a complete understanding of qubit physics and of individual qubit interactions with the materials and defects in its vicinity, in order to be sufficiently scalable and fault tolerant. This understanding requires major advances in the microscopic examination of the materials that will form the basis of any future devices, as well as a robust materials discovery pipeline. Cold neutrons are a powerful probe for characterizing quantum materials due to their unparalleled sensitivity to unpaired electron spins and their low-energies that are perfectly matched to magnetic excitation energies of these systems. This precision will allow the quantitative comparison with theory and models that will be so essential for developing new quantum materials and shaping them into functional qubits for the next generation of quantum computers.

The spatial and temporal resolution needed for operando studies of industrially relevant environments will be crucial to improve our manufacturing methods to produce environment-friendly, sustainable products. The high penetration depth of neutrons ensures that these studies can be performed *operando* (*e.g.,* in materials growth chambers of the type that may be used in industrial process). Robust polymers that can be rapidly manufactured rely on developments made possible using neutron scattering techniques that exploit neutron sensitivity to light elements not easily accessible to x-rays (e.g., H, O, C), deep penetration, and sensitivity to a broad range of length scales, along with the ability to use Hydrogen and Deuterium contrast matching. The development of new polymers with the required characteristics also requires *in situ* and *operando* investigations of out-of-equilibrium structure and dynamics that are uniquely enabled by the high brightness of cold neutrons at STS.

The instruments at STS will provide capabilities that far exceed those of existing instruments, responding to needs of the current user community, and anticipating those in the future. Instruments at SNS today are oversubscribed by a factor of 3 over capacity on average. The instrument types that stand to gain the most from STS are generally more oversubscribed than the average. This level of demand indicates that a strong user base already exists to take advantage of the new capabilities and increased throughput that STS will provide. This being said, it is incumbent upon the SNS to actively engage with potential new research communities to ensure the highest impact in science across the US.

The HFIR Pressure Vessel Replacement (PVR) project aims to replace the HFIR Pressure Vessel to extend the life of the reactor and increase operating power to 100 MW thus enabling continued availability of neutron scattering and irradiation capabilities at the facility. When combined with small vessel changes for beam tube HB-2, the facility used for assembly during the PVR will be re-purposed to a new guide hall to increase thermal neutron scattering capabilities. A small change to beam tube HB-4 would improve beam quality and flux by factors of 4-9. Changes to the vessel head will enable increased in-cycle access to irradiation positions for isotope production and materials irradiation, including neutron activation analysis. The pressure vessel replacement was a central priority of the BESAC report on Neutron Facilities issued in 2020.

The Institut Laue-Langevin (ILL) in France is the acknowledged world leader in reactor-based neutron scattering capabilities for science currently. The NIST Center for Neutron Research (NCNR) in the US is a lower power reactor-based neutron scattering source. The Belgian Reactor 2 (BR2) operates up to 100 MW for the purposes of materials irradiation and isotope production. The Jules Horowitz Research Reactor (JHR) is a mixed-field materials test reactor (100 MW) under construction in France and estimated to become operational in 2032-2034.

The HFIR core design that provides the highest thermal neutron flux density of any reactor operating in the western world allows for unique capabilities in isotope production, materials irradiation, and neutron activation analysis. It is the sole source of critical isotopes of importance to industry and is *the sole non-Russian producer of* ^{252}Cf. Medical applications continue to grow, for example for targeted a-radiotherapy (TAT), for which HFIR is the sole source of the important parent radioisotope ^{227}Ac. HFIR also plays a key role in the production of heavy nuclei for fundamental research. The HFIR irradiation facilities offer unique mixed-field capabilities that enable both fast and thermal flux irradiation positions, which are used to study advanced fuels, helium generation in reactor materials, and fusion materials irradiation capabilities. Neutron activation analysis, important to non-proliferation activities, is also a critical element of the HFIR's capabilities that take advantage pneumatic systems to allow flexible irradiation times shorter than the normal duration of the reactor fuel operating cycle.

While the scope of the PVR project does not include new neutron scattering capabilities, it opens up future possibilities for significant enhancement by accommodating a new design for an additional cold source that can substantially increase both capacity and capability for the future. A newly constructed beam tube could deliver neutron beams to up to 10 new instruments and significantly improve signal-to-noise ratios for experiments that require the intense monochromatic brightness of the upgraded reactor.

This project, which would likely occur in the late 2030s/early 2040s, is essential to ensure a continuing national/international resource for isotope production, materials irradiation, neutron scattering, and neutron activation analysis beyond the 2030s. The project is ready to proceed with engineering design necessary to obtain regulatory approval before commencing construction.

The premier reactor and accelerator-based neutron sources in the U.S. are currently located at ORNL, and both are over-subscribed with sound user bases. The co-location of these two facilities means that significant effort must be expended by ORNL to maintain and expand the user base throughout the U.S. scientific community. Although the U.S. has NCNR, also on the east coast, it does not benefit from the distributed user communities that exist and have existed in Europe around smaller research reactor facilities.

Synchrotron Sources of X-rays at Brookhaven National Laboratory

NSLS-II NEXT III Project

The NSLS-II NEXT III Project is an initiative aiming to address the complex, multi-scale challenges of contemporary science. Today's scientific inquiries demand multiscale and multimodal solutions, necessitating various measurements to examine a single problem from multiple perspectives, including different length and time scales. A critical component of the project involves identifying gaps in NSLS II's current capabilities, together with the user community. Among the missing key capabilities are gaps in high throughput scattering, spectroscopy and imaging. The NEXT-III initiative aims to bridge these gaps through the development of 8-12 proposed beamlines, the first four of which have already been identified through joint efforts with the user community.

Science Case. The case for NSLS-II NEXT III is strongly supported by the power of multimodal approaches to tackle pressing scientific questions, such as those related to microelectronics, aqueous batteries and grid storage. A notable report by Kankanallu et al. in Energy & Environmental Science (2023) highlights the project's potential. This study, conducted at a Department of Energy EFRC, utilized five beamlines for scattering, imaging, and spectroscopy in situ during the charge and discharge processes of batteries, demonstrating how multimodal measurements were pivotal in verifying cathode dissolution and reformation.

Future advancements facilitated by NEXT-III, include improvements in temporal resolution (from minutes to less than 0.1 seconds), length scales (from 1µm to 100nm), and field of view (from 40µm to 1mm). The project also aims to broaden the energy range from 6-18 keV to 1-25 keV, significantly enhancing the facility's capabilities for applications in microelectronics, Quantum Information Science (QIS), and beyond, with a promise of improving resolution and acquisition times from 10nm in 10 hours to 10nm in just 1 hour.

NSLS-II NEXT III Initial Observations. The evaluation team felt that the NSLS-II NEXT III project has great potential. However, in order to give a fully informed opinion, an expert evaluation of each of the proposed beamlines is needed within the context of other similar beamlines in the US (and internationally). In particular, there is a need to clearly establish the needs of the broader DOE user community, to quantitatively assess the demands for enhanced data collections speeds for specific experiments, and also to evaluate potential requirements for new optic designs on the proposed beamlines. Aspects such as high-resolution and high-throughput Powder Diffraction (PWD), and the capacity for full-field nanoprobe analysis, are highlighted as unique, especially for fields working with biological materials. The importance of co-location and a unified beam time proposal system is viewed very positively, as is the need for high-speed, high-resolution capabilities enabled by the proposed wiggler beamline and its use of multiple crystal analyzers.

NSLS-II NEXT III Readiness. The NSLS-II NEXT III was deemed as “ready to initiate construction”. Of the 8-12 beamlines planned as part of the NEXT III project, 4 have already been identified - two scanning probes, one full field imaging and one scattering (ANI, TXN, HRD, QCT). The selection and design process for these new beamlines has actively involved the user community through workshops and detailed proposal evaluations, ensuring that the new facilities will address the most pressing and unique scientific challenges. The continued engagement of a broad user community through the next two subproject phases is strongly encouraged.

Summary. The NSLS-II NEXT III Project is central to addressing the evolving needs of the scientific research community and presents a unique approach to solving complex problems through advanced, multiscale and multimodal scientific instruments and methodologies. The approach provides the opportunity to develop standardized sample environments and fiducials needed for performing multiple measurements on the same sample with different methods. In addition, the development of associated data analysis and visualization tools for disparate data sets will be beneficial to the broader community. There is also an opportunity for NSLS II to utilize NEXT III for developing the data infrastructure and metadata structure that will be needed for NSLS II U, and for other modern facilities. The evaluation team acknowledges the significance of the multiscale and multimodal challenges presented by the planned NSLS-II NEXT III project. While the scientific cases are compelling and hold promise for groundbreaking contributions to global research, an ongoing assessment of the planned beamlines with other facilities worldwide needs to be conducted, particularly as the remaining 4-8 beamline specifications are defined. NEXT III is clearly prepared for advancement, and we eagerly anticipate its eventual realization to introduce innovative approaches for tackling complex issues.

NSLS-II U (Upgrade) Project

The NSLS-IIU Project aims to fill a critical niche in the United States' scientific infrastructure by developing a multimodal ring capable of operating at high flux within the 1-10 keV energy range, a capability that outperforms other facilities in the U.S. and internationally over this energy range. The project addresses the tender X-ray gap, introduces new accelerator design concepts developed at Brookhaven National Laboratory (BNL), and will enable multilength and multi-time scale questions to be addressed in a wide range of scientific disciplines.

NSLS-II U Science Case. The science case for NSLS-II-U spans a broad array of applications, allowing for peak intensities in the 5-13 keV X-ray regime and beyond, and spanning timescales from microseconds to weeks. The project is poised to impact multiple research areas by offering unparalleled brightness and advanced multimodal techniques necessary for exploring phenomena on multi-length and multi-time scales. Key areas of focus include overcoming Moore’s law limitations for nodes below 1nm through enhanced photon concentration, advancing energy-efficient computing technologies such as neuromorphic computing and AI by addressing stochastic switching challenges, and improving clean energy battery materials through innovative use of tender X-rays for in-situ/operando full cell imaging. Additionally, NSLS-II-U introduces the novel concept of "ghost X-ray imaging" and explores quantum correlations for spectroscopy, promising significant advances in the study of X-ray sensitive samples.

NSLS-II U Initial Observations. The evaluation team deems this project as **absolutely central** in its potential to contribute to world-leading science in the next decade. If the overall improvement across the energy spectrum could be realized, then this is truly essential for NSLS-II. The improvements in the tender range will make this a world-leading facility for capabilities in that 1-10keV range. The lab should go further in defining the critical experiments in this tender range.

Initial observations underscore the project's compelling potential, highlighting an expected 10-20 times brightness increase over current state-of-the-art sources within the U.S., thereby asserting leadership internationally in this domain. This technology opens numerous opportunities, including the application of AI/ML for data processing, the necessity for detector development capable of on-pixel processing and fast frame rates, and the exploration of superconducting undulators for adaptive gap adjustments. The evaluation team felt that despite the white paper's focus on the 1-10 keV range, it is crucial to clarify that the significant benefits that were highlighted in the science case extend to ranges beyond 10 keV.

NSLS-IIU Readiness. NSLSII-U is currently in an advanced planning stage toward CD-0. It is estimated that 8 years after CD-0 first light can be delivered. The plan is to preserve the present source locations in order to utilize existing beamlines and those new beamlines that may be developed during NEXT-III. The project utilizes a novel accelerator concept - a Triple Complex Bend Achromat (TCBA) lattice, which is based on BNL LDRD efforts and for which prototype complex bends already exist and have been tested. The complex bends would replace long dipole electro-magnets with permanent magnets, thus greatly reducing energy consumption. However, there are some open questions about the **engineering challenges** regarding the durability of permanent magnets against radiation damage. The committee recommends further evaluation by accelerator experts prior to committing to the planned designed. The engagement of experts who participated in the recent APS-U, CHESS-U, ALS-U, and other upgrade projects around the world is strongly encouraged. A further issue that was raised was how the large volumes of data that will be generated can be handled. Here there is opportunity for machine learning and AI integration, perhaps building on initial efforts learned from the NEXT-III beamlines. Addressing these hurdles is critical for transitioning from prototype to full-scale operational readiness.

Summary. The Subcommittee recognizes the NSLS-II-U project as filling vital gaps within the US scientific infrastructure. It will be the worlds brightest synchrotron source in the energy range of 1-10 keV, making it **absolutely central** for US scientists in the next decade. The project's readiness evaluation is deferred to experts familiar with storage ring and new accelerator concept of the TCBA. Recommendations in our report suggest avenues for accessing such expertise, leaving it to the NSLS-II-U team and BES to determine the best approach for incorporating these experts' insights into the project's development.

X-ray Free Electron Laser Facilities at SLAC

LCLS-II-HE: An ultrafast ultrabright X-ray nanoscope for transformative insights into the atomic-scale function of materials and devices, dynamics of chemical transformations, and complex biological systems.

LCLS-II-HE at SLAC will be a transformational X-ray tool providing deep insights into the atomic structural dynamics that underpin the function of broad classes of complex matter, including: chemical and catalytic assemblies, quantum materials, structural materials, and biological systems in physiologically relevant environments. LCLS-II-HE will deliver a 3,000-fold performance increase in average X-ray brightness in the hard X-ray range up to 13 keV (~ 1 Å atomic resolution), and spanning the core levels of earth-abundant 3d transition metals that will play a central role in sustainability, clean energy transformation processes, and energy storage materials of the future. The unique and powerful capabilities of LCLS-II-HE will be indispensable for bridging crucial knowledge gaps, by providing the world's brightest source of atomic-resolution X-rays with ultrafast pulse structure to capture the coupled motions of atoms and electrons.

In the area of renewable energy and sustainable catalysis, LCLS-II-HE will measure entire time sequences of non-equilibrium chemical transformations as they happen. This insight will inform the directed design of a new generation of efficient catalytic assemblies, via multi-modal characterization of the coupled electronic and nuclear degrees of freedom that determine reaction pathways in complex chemical systems. In the area of pharmaceuticals and bio-inspired technologies, a much deeper understanding is needed that links the structural evolution of a biomolecular system to its function. This is crucial for human health and biosecurity, and to inform synthetic approaches for harnessing biochemical approaches for green industrial, agricultural and energy solutions. The unique capabilities of LCLS-II-HE will be able to map the full range of spontaneous motions and evolving conformations of bio-sample ensembles as they function – for the first time in solvated and room temperature environments. It will start an era of atomic-resolution structural dynamics measurements that will likely be as profound as the impact of X-ray static structures over the past decades.

The project has completed 90% of the facility design. The suite of high-performance cryomodules in an advanced state of delivery. CD-2/3 planned for May 2024. Major construction activities are planned to begin in summer 2025, with a projected early finish date of readiness for CD-4 by the end of FY2027.

LEI: The world's brightest X-ray laser for model-free structural dynamics and insights into complex energy systems and quantum materials. The Low Emittance Injector (LEI) for LCLS-II-HE provides a superconducting electron source that will: (1) improve the X-ray beam brightness to extend XFEL operation from 13 keV to 20 keV (sub-Å atomic resolution), with improvement across the full X-ray spectral range, (2) provide essential operational redundancy to maximize scientific delivery, and (3) support ongoing injector performance improvements to maintain US leadership in this rapidly evolving field. The extension of X-ray energy reach from 13 to 20 keV is motivated by the need to observe the evolving atomic structure and transport of ions, electrons, spins and phonons within the interior of complex matter, bulk materials, and devices under relevant operational conditions. The penetrating power of hard X-rays (20 keV penetrates ~1 mm of Si), combined with the ultrafast time structure from LEI will be indispensable for revealing the atomic-scale dynamics that determine material properties and functionality. The average coherent X-ray power of LEI in this crucial energy range will exceed that of any proposed diffraction-limited storage ring (DLSR) by nearly 1,000-fold – enabling powerful new approaches for coherent imaging of the structure and dynamics of real-world materials, and chemical and biological systems in the environments in which they naturally operate.

The higher photon energy enables revealing atomic pair distributions for direct (model-free) structure interpretation and the investigation of structural dynamics, disorder, and metastable phases at sub-Å resolution, in complex materials without long-range order. Applications include novel metastable phases created by coherent light-matter interactions and local atomic arrangements in energy materials (e.g. perovskite photovoltaics, phase-change memory materials, nanocatalysts, and batteries). Higher photon energy also enables access to bulk properties, *operando* or tailored sample environments (pressure, strain, magnetic field, etc.) and coupling with tailored transient stimuli (resonant THz, optical etc) – all necessary for a leap to be made in the understanding of the behavior of complex and quantum materials (phonons, electron/phonon coupling, magnons etc.)

LEI is in an advanced state of readiness-to-construct with essential R&D underway. The design of the injector is largely complete, with modeling showing the required emittance can be reached.

LCLS-X: The world's first 3rd Generation X-ray Free Electron Laser, providing a suite of dedicated platforms for understanding and controlling the multi-scale structural dynamics that underpin 21st century technology and biologically-inspired solutions for energy sustainability and health**.** LCLS-X is a next-generation infrastructure with an array of X-ray lasers that are each optimized to address urgent science challenges requiring XFEL capabilities. Simultaneous operation of ten *specialized scientific* beamlines and dozens of instruments – analogous to modern synchrotron (SR) facilities – with the requisite stability, reliability, integrated data systems, and ease-of-use to maximize the impact across broad areas of science. LCLS-X will bring XFEL science into a SR-like era, with a large number of parallel experiments supporting a broad critical mass of the science community, and with an associated order-of-magnitude change in cost per experiment, scientific throughput and impact.
LCLS-X will usher in a new era of X-ray science to maintain long-term U.S. leadership across a wide range of fundamental and applied areas – from clean energy, to sustainability, to economic competitiveness and human health – where there is an essential need to understand and control the multi-scale structural dynamics that underpin the properties and function of complex matter. One overarching challenge for a sustainable economy is accelerating the discovery and design of new materials with exceptional properties. LCLS-X will characterize with high precision the fundamental processes at play in hierarchical structures fabricated by combinations of novel materials, rationally guiding the design of long-lasting, high efficiency and high-performance devices. LCLS-X will enable significant leaps in performance that are needed to respond to the scientific drivers from a disparate set of communities. For example:

1. Cavity-based XFEL sources will be fielded for the first time (providing 100-1000x increase in average spectral brightness compared to LCLS-II-HE). One of the many applications is in enabling *operando* studies of the fundamental processes controlling ion diffusion and bridging our present knowledge gap of the atomic-scale processes that mediate ionic diffusion in complex electrode and solid-electrolyte matter. Systematic campaigns will reveal how ion transport processes depend on electrode nanostructure, material crystal structure, diffusion direction, and ion concentration and make fundamental steps towards meet the demands for high-capacity efficient and reliable energy storage devices.
2. LCLS-X will build dedicated multimodal platforms to exploit unprecedented coherent X-ray capabilities for real-time non-destructive 3D imaging at the atomic scale – to see how materials form in manufacturing processes, and how devices function in real-world conditions. Multi-modal methods will be transformative for identifying and imaging heterogeneous nucleation processes and related microstructural black swan events that underpin both the formation of new material phases (e.g. under the nonequilibrium conditions of advanced processing) and represent initial steps in materials degradation and failure. The crucial transition in these processes is the emergence of the critical and stable nucleus from fluctuating clusters. Mastery of these processes comes from controlling the emergence of critical nuclei. It will be possible to monitor simultaneously the fluctuation in the "disorder" state prior to nucleation as well as the changes in the local chemical/bonding environment. The former provides revealing insights into the role of nucleation accelerators and inhibitors, while the latter provides a powerful first-order indicator that a critical nucleation (rare event) has emerged from the fluctuation.

LCLS-X is ready to construct after LCLS-II-HE; the existing LCLS-II-HE accelerator will be sufficiently powerful to feed 10 undulators. Delivery of end stations and instruments will be phased to allow staged growth, responsive to new discoveries and emerging national priorities.

Summary assessment: overall recommendations and/or action points for future planning. The potential of the three projects to significantly contribute to world-leading science and allow the US to maintain leadership in the fundamental science that underpins complex matter in the next decade is very high. Their performance leap, science scope and impact will extend significantly beyond current X-ray facilities.

For LCLS-II-HE and LEI, matching or exceeding capabilities may be available in China (SHINE, Shanghai) by the end of the 2020s, and at the European XFEL in the 2030s. Both LCLS-II-HE and LEI are therefore essential next steps for the U.S. to remain competitive. The two projects are absolutely critical, but their relevance and uniqueness for transformational science will be dependent on the timing of the start of operations.

For LCLS-X, there are as yet no known concrete proposals for similar facilities. But the US is lagging behind Europe and Asia in the number of optimized XFEL sources, beamlines and instruments.

XFEL science and technology have made huge advances in the past 15 years, mostly initiated and led by LCLS. However, the scientific output of these facilities is critically limited by efficiency and limited amount of endstations. This context hampers the production of a critical mass of publications in any specific science area, a necessary condition to have real impact. LCLS-X has here a world-wide unique opportunity to project the relevance and the impact of XFEL science to similar levels reached today by SR, and with it, an unchallenged potential to advance fundamental scientific discovery and translate to address pressing national challenges for renewable energy, environmental sustainability, economic competitiveness, human health, national security (and many other areas). This is achieved by supporting deep and sustained research programs led by broad mainstream science communities, with ready access to a suite of XFEL sources, beamlines, and instruments optimized for critical science areas.

A more detailed assessment of readiness of LEI will be enabled after RF gun prototype tests, planned for 2025. Revolutionary advances in data science and the development of a new generation of detectors are needed to fulfill the scientific potential of LCLS-II-HE and LEI. The multiplication of end-stations and increased multi-modal operation at LCLS-X will exacerbate this need. Programs have been launched and progressing well, but regular progress assessments to be performed.

A Future Light Source

Accelerator-based light sources will remain a key component of the United States' energy and technology strategies, making proactive research into their future design crucial. As such, the BESAC Subcommittee commends the forward-thinking approach of the Department of Energy's Office of Basic Energy Sciences (BES) to seek ideas for how a future, 'green-field' light source could transform our understanding of nature and technology. Anticipating the research environment over the next 15 years involves uncertainties, yet we offer preliminary insights into the science and emerging technologies that will shape FLSs, alongside recommendations beyond 2035.

Sections 1 and 2 explore scientific drivers and enabling technologies, as well as anticipated user needs that are vital for FLS design. These elements not only address urgent scientific challenges, but enhance the global leadership of the US in science and technology by making the FLS accessible to a wide range of users, including non-experts. The Subcommittee emphasizes the urgency of developing these aspects to justify the swift establishment of an FLS. The global race to develop such transformative facilities is intense and accelerating. Section 3 shortly comments on possible outlines the FLS layout. Section 4 suggests actions in the next 5 - 10 years to solidify the FLS concept.

Science Drivers. In our analysis of future science drivers, we examined three areas: the design of new materials, the field of soft and bio-matter and medical applications, and the domain of atomic, molecular and optical physics (AMO).

The design of new materials. Non-destructive, atomic scale data generation and investigating material metastability are two key scientific areas that can be addressed with the FLS.

Non-destructive, atomic-scale precision data generation is essential for:

- Advancing key [nano]electronics (such as described in the "Chips Act") by characterizing single defects with dramatically enhanced sensitivity and understanding of how to control their properties, safeguarding US leadership in semiconductors.
- Enhancing quantum technology development (e.g. computing, cybersecurity) by exploring individual pairs of entangled electrons (*terra incognita*), quantum energy landscapes, and decoherence mechanisms (lifetimes), vital for US technology competitiveness.
- Understanding and controlling material behavior under extreme conditions (high pressure, temperature, radiation) for material design, national security, planetary and Earth science, and space exploration.

Investigation of material metastability focusing on:

- Transients in chemical reactions (e.g., catalysis), non-equilibrium material states (*terra incognita*), and designing ultrafast functions for potential femtotechnology applications.
- The increasing complexity of material structures with embedded multifunctionality necessitates advanced understanding of local structures akin to crystallography for complex materials.

Soft/Bio Matter and Medical Research. Public health and the fight against disease will remain a primary focus of our society. Future X-ray sources like the FLS must make important contributions to this effort. A key topic will be how to achieve X-ray imaging techniques with the highest spatial resolution while minimizing radiation dose. New concepts on the horizon include novel X-ray imaging techniques that utilize, among others, entangled X-ray quanta ("ghost imaging") or other X-ray channels.

Some FLS applications in soft- and biomatter include: (1) high-throughput screening of cells, tissues, and organs for the broad bio-medical user community; (2) nanotoxicology, which involves understanding how the size, shape, surface structure, and chemistry of nanoparticles relate to their toxicity; (3) rapid electronic processes in biomaterials, such as radiation damage to DNA or the bio-catalytic processes of plant photosynthesis (femto- to attosecond timescale); and (4) the broad area of biological structures and processes in aqueous environments, which requires coherent X-ray light with corresponding temporal resolution for study.

Atomic, Molecular and Optical (AMO) Physics. In the field of AMO, we generally view the attosecond sector as a central science driver. If this area can be made accessible via X-ray technology, it opens many highly interesting and fundamental questions, the solutions to which can lead to the highest scientific honors. Images and movies of individual molecules or atoms and their dynamics are believed to be an achievable 'Holy Grail' of X-ray physics. Being able to film the formation and breaking of bonds delves deeply into the workings of quantum mechanics from the molecular dynamics in water to quantum computing. This is particularly significant in electronic transients in chemical reactions, representing a crucial milestone towards the quantum control of matter and energy.

Enabling technologies and advanced user operation modes. The operation of a future light will be revolutionized by data-driven methodologies, leveraging Artificial Intelligence and Machine Learning (AI/ML) to create materials with specific functionalities and properties more efficiently. High-resolution X-ray techniques will be crucial for innovators and Future Light Source (FLS) users, enabling standardized, extremely precise analytics for science and technology.

Importantly, the FLS will be greatly influenced by new digital concepts. This concerns the operation of the entire facility, from the accelerator to the detector, the sample environment, the collection and analysis of data, and real-time simulations, up to new modalities in remote operation. AI/ML is certain to play a dominant role in all these fields.

The options that digital transformation provides for the FLS include, among others:

- Digital twinning of critical components of the facility, to enable developers, operators, and users to run complex simulations of all aspects of the facility. This will greatly improve outcomes and efficient use of the facility.
- A fully automated AI/ML-supported operation of the accelerator complex, from “source to sample,” allowing for rapid startup of the accelerator and user-driven real-time switching between operating modes. This can also be crucial in difficult times with travel restrictions, as we have experienced during the pandemic.
- Experimental stations equipped with state-of-the-art robotics in sample handling and automated with AI/ML support, with user interventions à la carte. This will lead to an acceleration of the analytical processes by several orders of magnitude.
- Real-time data analyses for direct feedback to users for improved control of the experiments (e.g. anomaly detection, intelligent process automation, etc.).

Full-fledged data analyses for users without expertise in X-ray methods will lead to a broader use of an FLS and significantly increase its impact (from "data factories" to "solution factories"). In the area of remote or hybrid access, a wide range of modalities for FLS users can be offered, also highly interesting for industrial users and in the educational field at schools and universities ("training beamlines").

Access to the experiment must be adapted to the new needs of a broad user base, who typically have projects with which they are in fierce international competition. At the moment, pilots at synchrotron radiation sources are testing what is called a rolling access procedure. Here, a user can apply for beam time at any time, which, similar to publications, is quickly reviewed. In individual cases, the time between application and execution of the experiment can be reduced to just a few weeks.

The digital transformation needed is dependent on significant advances and exploitation of cross-cutting computing infrastructure and associated expert staff.

Facilities Layouts. As the technical layout for a FLS depends on the Scientific Cases, the desired user modalities, and future instrument technologies, it will take careful consideration to weigh and identify the synergies and tradeoffs required to optimize for these aspects. Currently, there are some established layouts, at synchrotron radiation sources, the Hybrid Multi-Bend Achromat concept, and at Free Electron Lasers, the superconducting technology and the seeding concept. Furthermore, plasma acceleration is emerging as a completely new technology, which can be 1000 times more efficient than current linear accelerators (LINACs). The development in this field is rapid (including in China) and thus, in 10-15 years, the technology may be mature enough for an FLS. Finally, among other pioneering technologies that have been tested are the FEL oscillator (XFELO), which can significantly increase the longitudinal coherence of the radiation, and the Energy Recovery Linacs (ERL), which link the SR- and FEL-worlds.

Future Light Source Recommendations. The subcommittee sees a clear need for the development of a national Future Light Source for the US to remain a leader in science and technology development. The process should be initiated with urgency to develop strong Science Cases and an approach for a concrete layout. The global community, from the EU to China, will also be pressing ahead with their own ideas for a FLS.

This includes various actions that we recommend starting to address now:

(1) Consultation of national and international experts and organization of dedicated workshops to sharpen the focus on Science Drivers and to anticipate which user needs could be prevalent in 10 to 15 years with a view towards to democratizing access to areas not yet incorporated advanced X-ray sources into their research agenda or in their value chain. In addition to BES, involve representatives from other DOE Divisions, including ASCR (AI/ML), BER (science), FES (extreme materials), and HEP and NP (accelerator concepts) and EERE (energy, nuclear) as needed.

(2) Initiate pilots at the current light sources at an early stage to test feasibility in specific cases. This particularly applies to all new technologies (autonomous operating modes, ghost imaging, etc.) and user modalities (remote operating modes, robotics beamlines) that rely on AI/ML concepts.

(3) Consider how to balance "enterprise beamlines" with "pioneer beamlines."

(4) Given the diverse X-ray requirements of upcoming scientific drivers, a single FLS facility might not suffice. In turn, a distributed FLS system, with satellites tailored to specific scientific needs, technologies, and access models, should be taken into consideration. Additionally, a hybrid approach, combining a centrally located, state-of-the-art facility operated by a specialized team with strategically placed, institutionally distributed data analysis centers, could be viable.

(5) An FLS project with entirely novel enabling technologies and user modalities will require new skills. BES, with Office of Science (SC) divisions and National Laboratories, are encouraged to develop a strategy for building relevant capacity.

Overall BESAC Facilities Subcommittee Recommendations

- Global competition for state-of-the art X-ray and neutron facilities is energized, creative, and acquiring funding. This includes spallation neutron sources, X-ray free electron lasers, and synchrotrons. **Urgency** is critical if the US is to retain its leadership.
- While it is natural that there will be scientific overlap among the facilities. the subcommittee recommends that all of the facilities further refine their early targets for grand challenge science that will utilize the first instrument suites. Each of the facilities science targets should be clearly distinct from the other facilities**.**
- BES should consider a coordinated effort by all of the aforementioned facilities to ensure that the science cases and instrument portfolio are synergistic and optimized to serve the US science communities and overall US leadership in science and technology. This would help DOE with funding, help build new user communities, and inform facility/instrument design.
- Each of the eight projects should consider how to deliver an integrated, multimodal facility: from accelerator, X-ray and neutron sources and beam optics to experimental stations, sample environments, detectors and data analysis.
- BES leadership could work with each of the facilities to engage with the other relevant SC divisions that support their science – ASCR, BER, NP/HEP, FES; include EERE and NNSA; explore involvement with other agencies - NSF, NIH, EPA, NOAA and NASA.
- The facilities all should have active program informing and collaborating with existing users and developing new user communities. As a start, they could articulate potential future research topics and capabilities. This way users can be prepared to be productive soon after CD4. Provide clear approaches for building and accommodating current users and training new user communities and what new modalities will be most effective for them.

Appendices

Appendix 1: BESAC Subcommittee membership

Name	Institution	Subgroup(s) Assigned
Ken Andersen	Institut Laue-Langevin (ILL)	Neutron Sources
Serena DeBeer (Vice-Chair)	Max Planck Institute	Free Electron Lasers/Synchrotrons
Tabbetha Dobbins*	Rowan University	Synchrotrons
Helmut Dosch*	DESY	Future Light Source*/Free Electron Lasers
Thomas Epps	University of Delaware	Neutron Sources/Synchrotrons
Yan Gao	GE (retired)	Synchrotrons
Jamie Garcia	IBM	Free Electron Lasers/Future Light Source
Ashfia Huq	Sandia National Lab (CA)	Neutron Sources
Eric Isaacs (Chair)	Carnegie Institute of Science	Free Electron Lasers/Future Light Source
Kevin Jones*	European Spallation Source	Neutron Sources
Sakura Pascarelli*	EU XFEL	Free Electron Lasers*/Future Light Source

- Subgroup Lead
- FLS = Future Light source

Appendix II: ***Key subcommittee considerations***

Throughout our deliberations, the BESAC subcommittee considered the following key elements:

1. Enables transformational science and technology
2. Provides new capabilities and capacity that will answer important research questions that cannot be addressed by the facilities that are available today.
3. Include integration of accelerator, source, sample environment, detectors, and data analysis from facility inception (source to sample)
4. Enhances or grows a new, skilled, robust and geographically diverse national user community. Develops mechanisms to train the next-generation of users
5. Recruits and trains highly qualified facility staff
6. Identifies cross-cutting opportunities for science, computing and data, and from other Office of Science directorates (BER, ASCR, HEP, NP and FES)

Appendix III: Subcommittee Approach

1. White papers and presentations prepared by each facility
2. Four subcommittee subgroups for neutrons, synchrotron, XFELs, and a future light source
3. Subgroups met as needed, conducted analyses and benchmarked, and prepared summary recommendations and slides to address the SC1 charge.
4. Subcommittee met monthly, chair and vice chair met with BESAC chair and BES leadership as needed