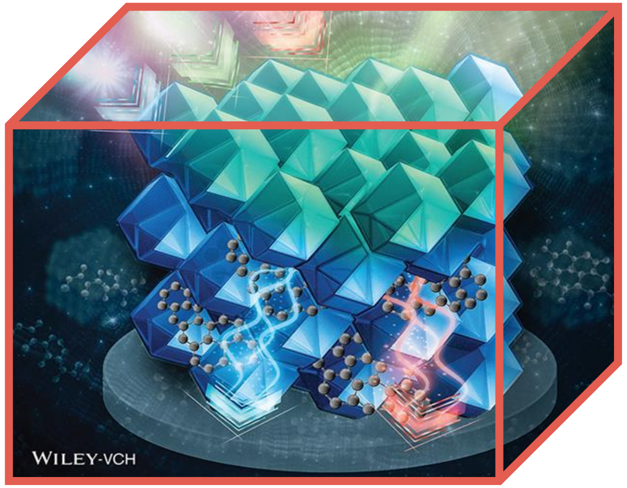
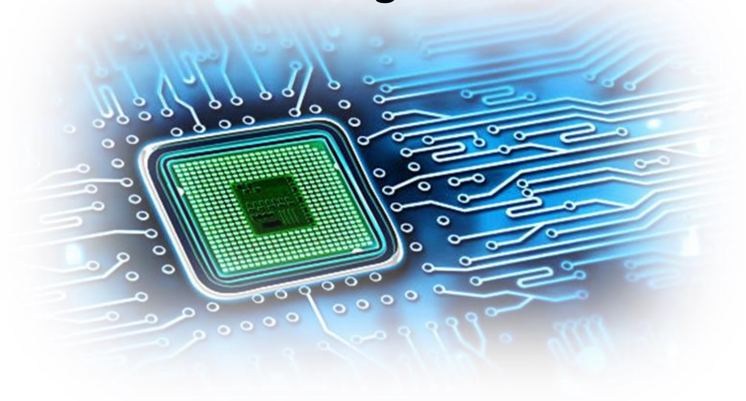
BESAC Subcommittee on BES Future Facilities

Eric Isaacs (chair), Serena DeBeer (vice-chair)



Transformational science and future technologies



Future science communities and new user modalities

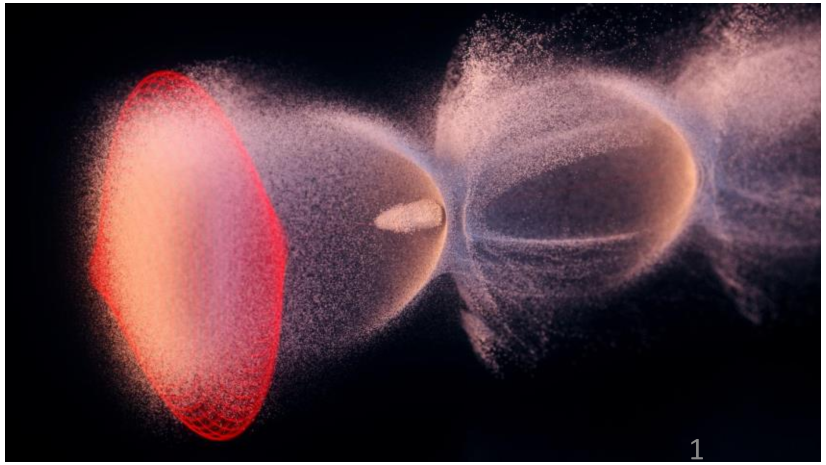
- New areas of research
- Multi-modal, multi-technique
- Non-expert users
- Digital controls/workflows
- Onsite + remote

Full digital integration of accelerators & sources, instrumentation and data analytics

AI/ML/SimMod/Data

Robotics & sample environments

New neutron and x-ray facility concepts



SC1 Charge to BESAC on Future Scientific Facilities on December 1, 2023

Consider new or upgraded facilities (>$100M) that will provide the capability to deliver world-leading, transformative science

a) absolutely central; b) important; c) lower priority; d) don't know enough yet

Readiness for construction of new or upgraded facility

a) ready to start construction; b) significant scientific/engineering challenges;
c) mission and technical requirements not yet fully defined

Also consider

- Cross-directorate partnerships within the office of science (ASCR, BER, FES, …)
- Future science communities – fields/topics, quantity, geography, user support

New Facilities and Upgrades Considered

Neutron sources (Oak Ridge National Laboratory)

- High Flux Isotope Reactor - Pressure Vessel Replacement
- Spallation Neutron Source - Second Target Station

Synchrotron sources (Brookhaven National Laboratory)

- NSLS-II Experimental Tools - NEXT-III
- NSLS – II Upgrade

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

- LCLS II High Energy Upgrade
- Low Emittance Injector
- LCLS-X next generation FEL

Future Light Source(s) (TBD)

- Green-field ideas

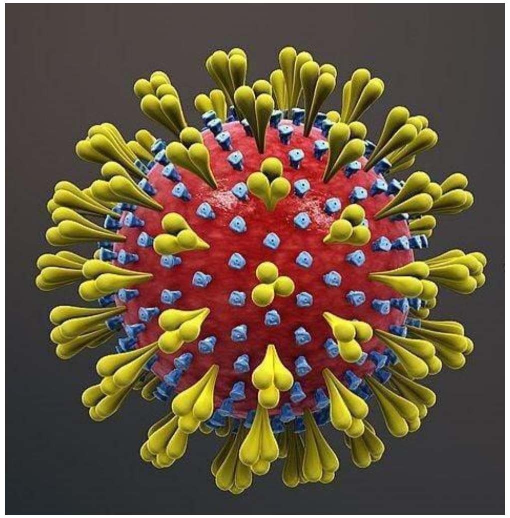
BES Neutron and X-ray Facilities Historic Impact: By-the-Numbers

- **9 Nobel Prizes** (7 in biology, 2 in physical sciences)

- **Publications**: total ~84,000 from CY04 to CY23
  - Grew from 2850 (CY04) to 6041 in (CY23)
  - While BES facilities grew from 7 in CY04 to 12 in CY23

- **Users**: total from FY04 to FY23: 263,138
  - Unique users: 14,730
  - 8,545 users in FY04 to 13,789 users in FY23
  - Oversubscription rates: 3 for neutrons; 5 for LCLS; 2 for x-rays

- BES facilities rapid response to SARS CoV-2 was critical for developing COVID vaccines and therapies
  - 55 BES beamlines generated ~500 structures
  - 750 unique users (including most of major Pharma)



Key considerations

- Enables transformational science and new technologies
  - Powerful, crisp and distinctive science case
- Provides new capabilities that will answer important questions that cannot be addressed today
- Includes full [digital] integration of accelerator, source, sample environment, detectors and data analysis from facility inception (‘source to sample’)
- Enhances, or grows a new, skilled, robust, and geographically diverse national user community
  - Develops mechanisms to train new generations of users and access for non-experts
- Recruits and trains highly qualified facility staff to ensure the most productive user experience; also, accelerator scientists, data scientists, …
- Identifies cross-cutting capabilities for science and technology, computing and data, from other Office of Science directorates, e.g., ASCR, BER, HEP, NP and FES, as well as other cognizant agencies such as NSF, NIH, DOD, EPA, …

Subcommittee Members

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	FLS*/Free Electron Lasers
Thomas Epps	University of Delaware	Neutron Sources/Synchrotrons
Yan Gao	GE (retired)	Synchrotrons
Jamie Garcia	IBM	Free Electron Lasers/FLS
Ashfia Huq	Sandia National Lab (CA)	Neutron Sources
Eric Isaacs (Chair)	Carnegie Institute of Science	Free Electron Lasers/FLS
Kevin Jones*	European Spallation Source	Neutron Sources
Sakura Pascarelli*	EU XFEL	Free Electron Lasers*/FLS

*Subgroup Lead

FLS = Future Light Sources

Subcommittee Approach

- White papers and presentations prepared by each facility for subcommittee consideration
  - Future Light Source science and concepts were presented by an expert panel
- Assessments and writing by four expert subgroups in neutron, synchrotron, XFEL, and future light sources, respectively
- Subgroups met as needed
- Subcommittee met monthly; chair and vice-chair met with BESAC chair and BES leadership as needed

Four subgroups for eight projects

Subgroup I Neutron Sources (HFIR and SNS Second Target Station @ ORNL)
Kevin Jones (Lead), Ken Anderson, Thomas Epps, Ashfia Huq

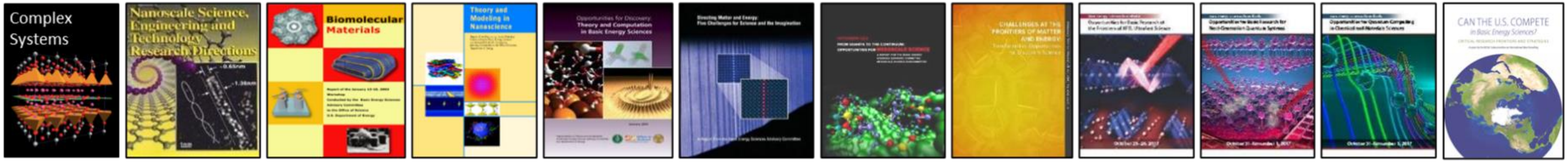
Subgroup 2 Synchrotron Sources (NSLSL II NEXT III and Upgrade @ BNL)
Tabbetha Dobbins (Lead), Serena DeBeer, Thomas Epps, Yan Gao,

Subgroup 3 X-ray Free Electron Lasers (LCLS II HE, LEI & LCLS X @ SNAL)
Sakura Pascarelli (Lead), Serena DeBeer, Jamie Garcia, Eric Isaacs

Subgroup 4 Future Light Sources
Helmut Dosch (Lead), Jamie Garcia, Eric Isaacs, Sakura Pascarelli

Science Goals: 20+ Years of Community-driven Input

Science for Discovery



Science for National Needs

National Scientific User Facilities, the 21st century tools of science

Summary Statement

- The subcommittee concluded that scientific mission for all of the *X-ray and neutron facilities considered are* ***absolutely central*** *to the future 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 for decades to come
- Each facility is in a different state of technological readiness
- Global competition is very strong. Urgency is encouraged

Facility	Capability for science/DOE BES mission relevance	Readiness for construction
HFIR	Absolutely central – brightest continuous US source, and only source in the Western Hemisphere for many critical isotopes	Ready for CD1, engineering challenge - regulatory approval prior to CD2/3
SNS - STS	Absolutely central – world's brightest source of cold neutrons; science case and instruments need refining	Ready to proceed to CD2 once science case is refined and instrument suite defined
NSLS II NEXT III	Both important and central depending on beamline - capability vs capacity	Tech requirements need to be fully defined by CD1
NSLS II U	Absolutely central; worlds brightest synchrotron for 1-10keV	Engineering challenges for Triple Complex Bend Achromat; additional research needed
LCLS-II HE	Absolutely central; world's brightest (x3000 LCLS), ultrafast XFEL to 13 keV	Ready to initiate; design 90% complete; CD2/3 in May 2024
LCLS - LEI	Absolutely central; brightest XFEL, extends LCLS II HE to 20keV	Getting close to ready with essential R&D underway for emittance target
LCLS - X	Absolutely central; first 3rd generation XFEL; 10 specialized XFELs, integrated ops	Significant engineering challenges before CD process
FLS	Absolutely central to plan facility for future US leadership; science mission/case TBD	Readiness requires technical layout, following science case

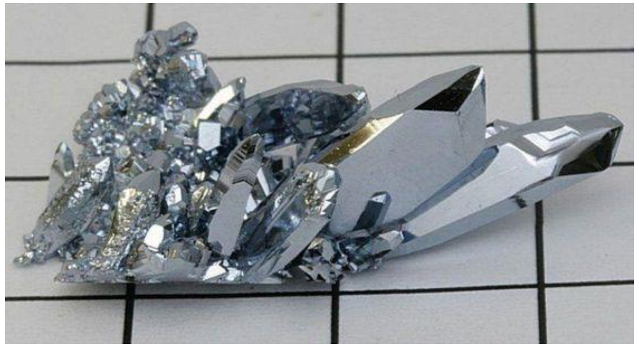
Facility	Partnerships with other SC programs, EERE and others agencies
HFIR	Advanced Scientific Computing Research (ASCR), Biological and Environmental Research (BER), Nuclear Physics (NP), Fusion Energy Sciences (FES), Nuclear Energy (NE) ; NIH, NSF, DOD
SNS - STS	ASCR, BER, Energy Efficiency and Renewable Energy (EERE), Nuclear Physics (NP)/High Energy Physics (HEP), NSF, NIH
NSLS II NEXT III	ASCR, BER, NP/HEP
NSLS II U	ASCR, BER, NP/HEP, EERE
LCLS-II HE	ASCR, BER, HEP NIH, NSF, DOD
LCLS - LEI	ASCR, BER, HEP NIH, NSF, DOD
LCLS - X	ASCR, BER, NP, HEP, EERE, ; NSF, NIH
FLS	ASCR, BER,HEP, EERE, NP, NIH, NSF, DOD….

Neutron sources are essential for U.S. competitiveness

The SNS and HFIR at ORNL are core elements of the BES facility portfolio and are well positioned for a world-leading role

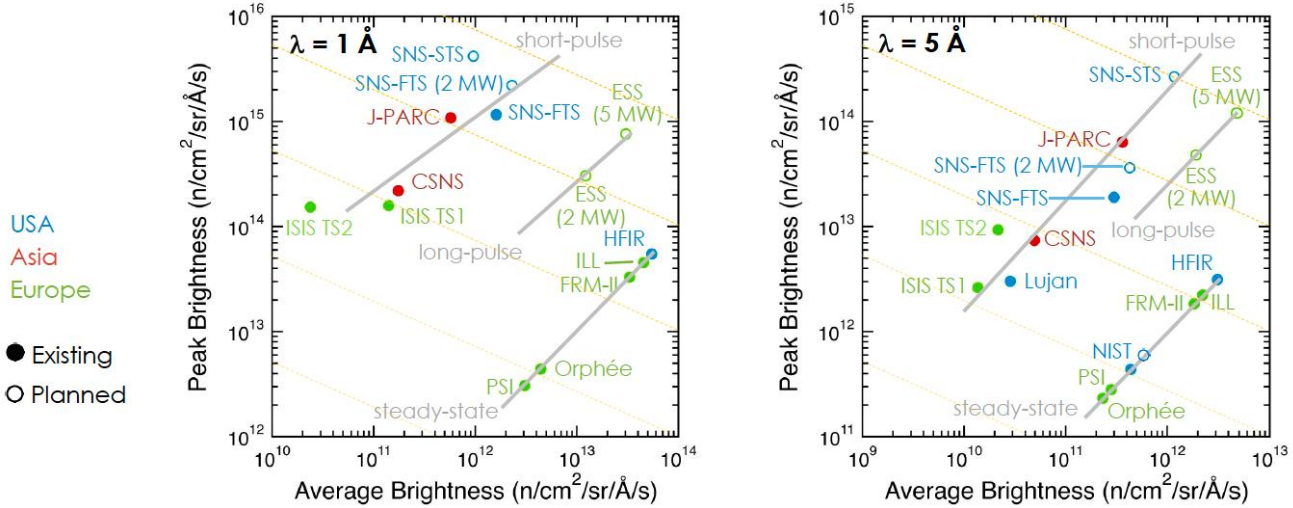
Neutrons offer a combination of capabilities that are unique probes of matter, and isotope production and materials irradiation

- High penetrating power
- Light element sensitivity, particularly to H and D
- Exquisite sensitivity to atomic and magnetic structures and dynamics with very high energy resolution (>10μV)



Isotopes: Cf-252 (~$27M/gm)

Quantum materials



ORNL proposes a two-facility, three source strategy to enable US leadership in neutron science

A complete and comprehensive neutron portfolio is necessary to address the most pressing material challenges

Two neutron user facilities
Three advanced sources

Every source serving an optimized portfolio

HFIR:
- Highest steady-state brightness of thermal and cold neutrons
- Parametric studies
- Kinetics

STS:
- Highest peak brightness of cold neutrons
- Broader perspective
- Materials in action

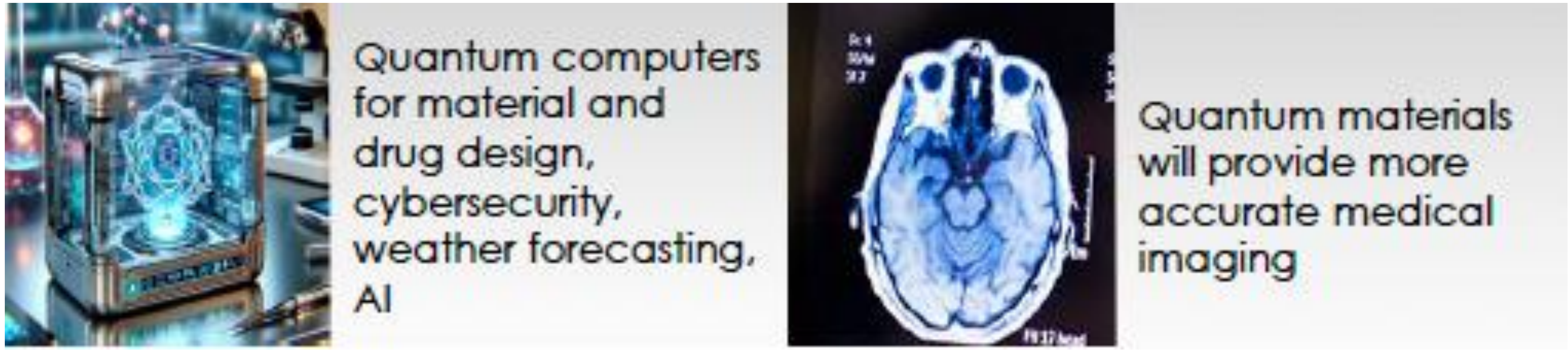
FTS:
- Highest peak brightness of thermal neutrons
- High-resolution crystallography
- Fast and high-energy dynamics

Second Target Station (SNS-STS)

Worlds brightest source of cold neutrons with up to 100x increase in performance for high impact science and engineering research
Jens Dilling, ORNL

Polarized, cold neutron scattering techniques determine low-lying excitations in quantum materials which allows quantitative comparisons with theory and models

Interrogate the development of hierarchical polymer structures for science and industry



Readiness of Second Target Station

- The project received CD-1: Total Project Cost optimization in progress to prepare for CD-2
- The machine concept is well-developed, beam transport technology is well established
- Civil construction designs for the facility are well along and are ready to proceed
- ***What compelling science will be done on the first instrument suite that highlights the full capabilities of STS?***
  - **The first instrument suite needs to be refined**
- ***How will the SNS develop and train new user communities by CD-4?***

HFIR Pressure Vessel Replacement (PVR)

Unique U.S. capabilities for isotope production, materials irradiation, and neutron activation analysis as well as thermal and cold neutron scattering capabilities - Robert Dimeo, ORNL

Isotope Production:

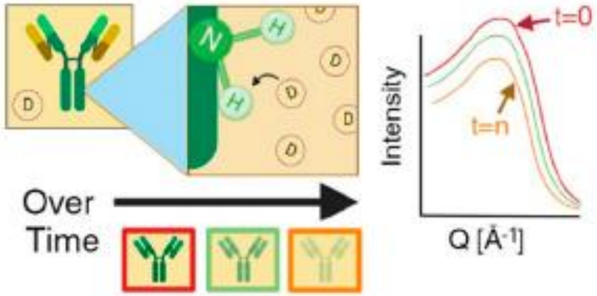
- Sole source in Western Hemisphere
- Cf-252 for military and industrial applications (oil) and radiography
- Ni-63 for explosives detection
- Pu-238 for thermonuclear power generation

Materials Irradiation and Activation Analysis:

- Reactor fuel and materials testing
- Activation analysis for nuclear and criminal forensics

Neutron Scattering:

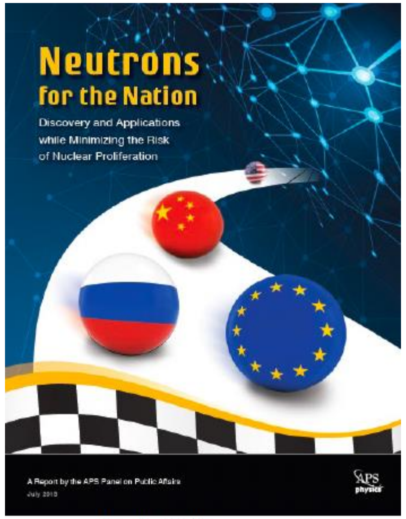
- Low-lying magnetic dynamics
- Structure and dynamics of soft matter/macromolecules



HDX-SANS informs conformational fluctuations and stability

HFIR PVR Readiness

- The project has received CD-0 and and with available funding could be ready for CD-1 in 2027
- Early progress is essential to satisfy regulatory requirements to achieve CD-2/3
- The PVR would likely take place in the late 2030s/early 2040s



Wells-Phillips report

The project is ready to proceed with engineering design necessary to obtain regulatory approval before commencing construction

Recommendations: Neutron Sources at ORNL

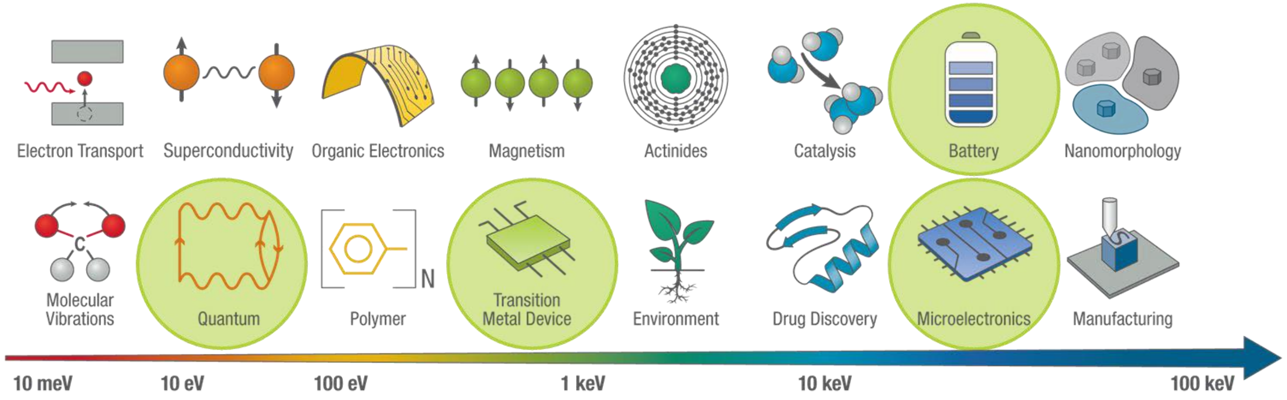
- The two facilities, three sources strategy in one location at ORNL is compelling
- The case for the **HFIR PVR** is **absolutely central** for the BES mission – the 100 MW reactor will be the brightest continuous neutron source for science in the US and the only source in the Western Hemisphere for many isotopes.
  - CD0 achieved and ready to start planning for CD1; **engineering challenge** to secure the regulatory approval before CD2/3
- The **SNS STS** will be the world's brightest source of cold neutrons (up to 100x) for structure and dynamics in quantum and biological/soft materials with very high energy resolution
  - Science is **absolutely central.** The science case needs refining: suggest a focus on a few grand challenges unaccessible today.
  - Readiness: CD1/0 achieved; **ready to proceed** to CD2 once science/user case is articulated and a realistic scope/cost/schedule can be established

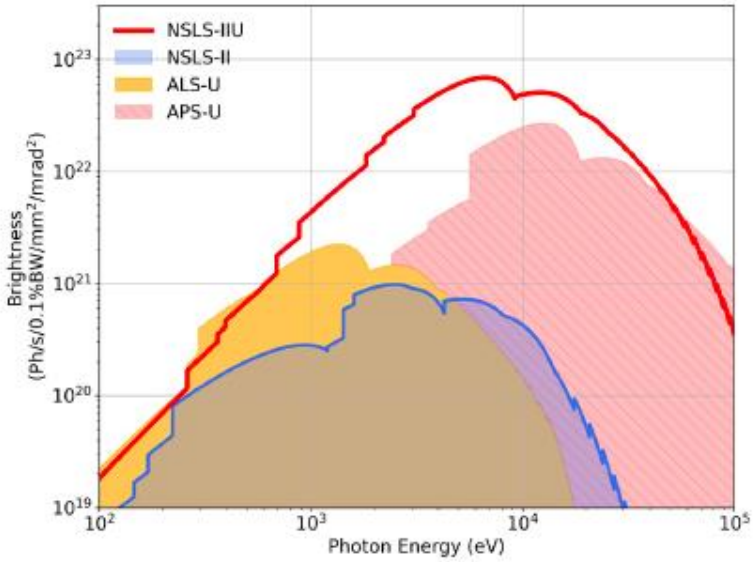
Two NSLS projects for US Leadership in Synchrotron Science

John Hill, BNL

- **NSLS II NEXT III:** provides 8 to12 additional beamlines to fill capability gaps, broaden the research community, and realize the full potential of NSLS II.

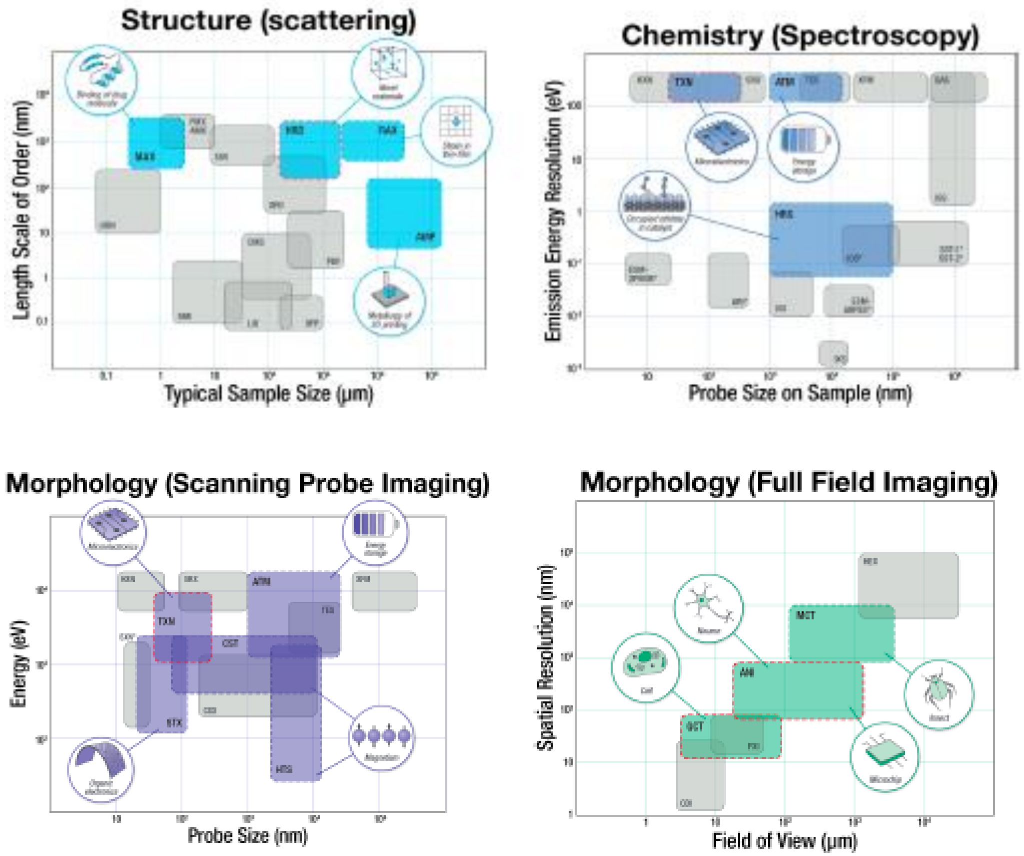
- **NSLS-II U:** the World's brightest (first?) multi-modal storage ring





NSLS II NEXT III

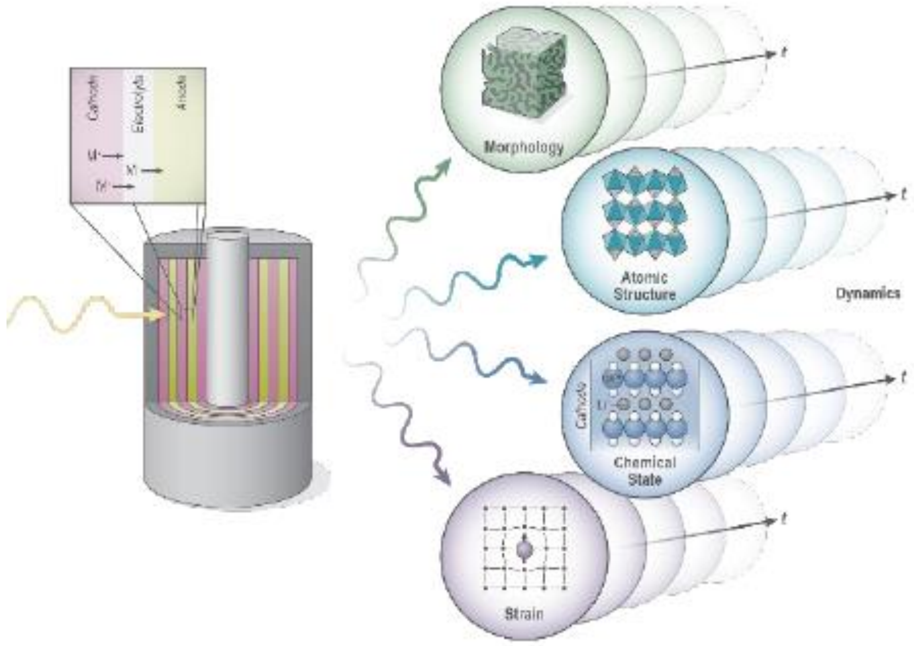
- **NSLS-II - world's largest medium-energy storage ring with 29 BLs delivering high-brightness photons from the far infra-red to the hard x-ray regime**
- **NEXT III – addresses critical gaps in current BL portfolio in scattering, spectroscopy and imaging**
- **8-12 are beamlines to be constructed in consultation with the broader user community**
- **Driven by multimodal and multiscale needs of modern science**

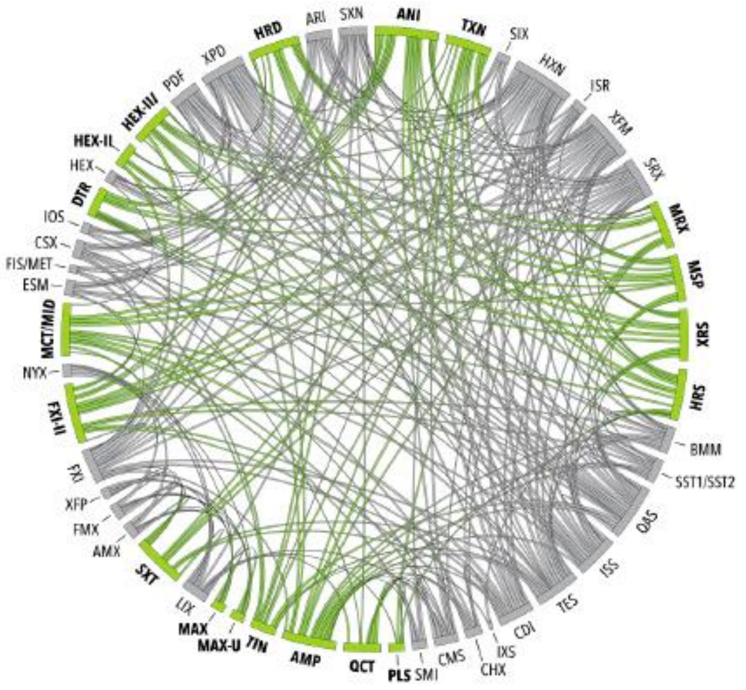


- **Planning based on strong community engagement, first four beamlines have been identified: Quantitative Cellular Tomography (QCT), High Resolution Diffraction (HRD) Advanced Nanoscale Imaging (ANI) and Tender X-ray Nanoprobe (TXN)**

NSLS II NEXT III: Science Drivers

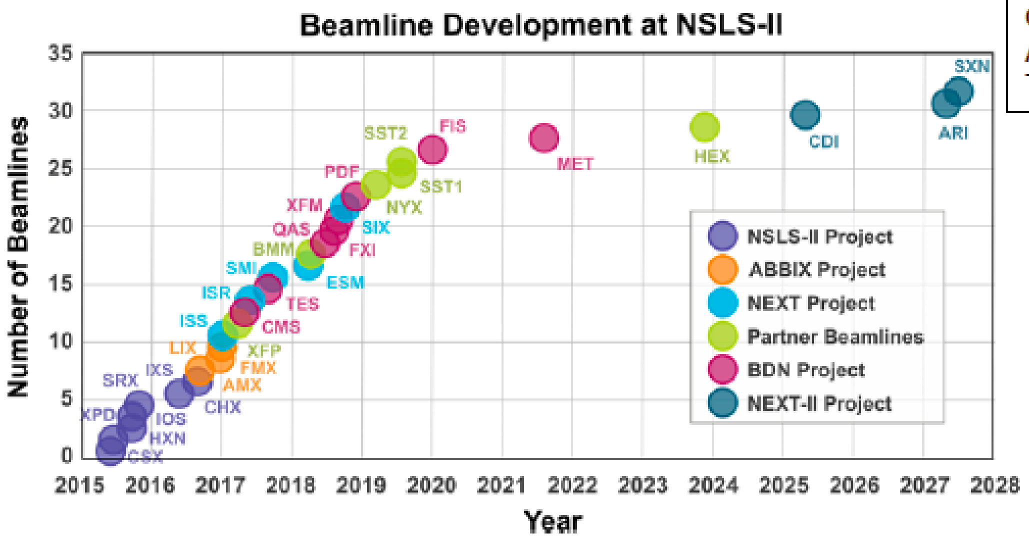
Addresses key missing capabilities needed for future science and engineering challenges in a multimodal, multiscale approach





NSLS II NEXT III Readiness

- A clear plan is in place to select and deliver beamlines based on the needs of the broader user community
- First four subproject beamlines have been identified
- **Ready to proceed to CD-1** (August 2024)
- NSLS II has a strong record of delivering new beamlines to the user community

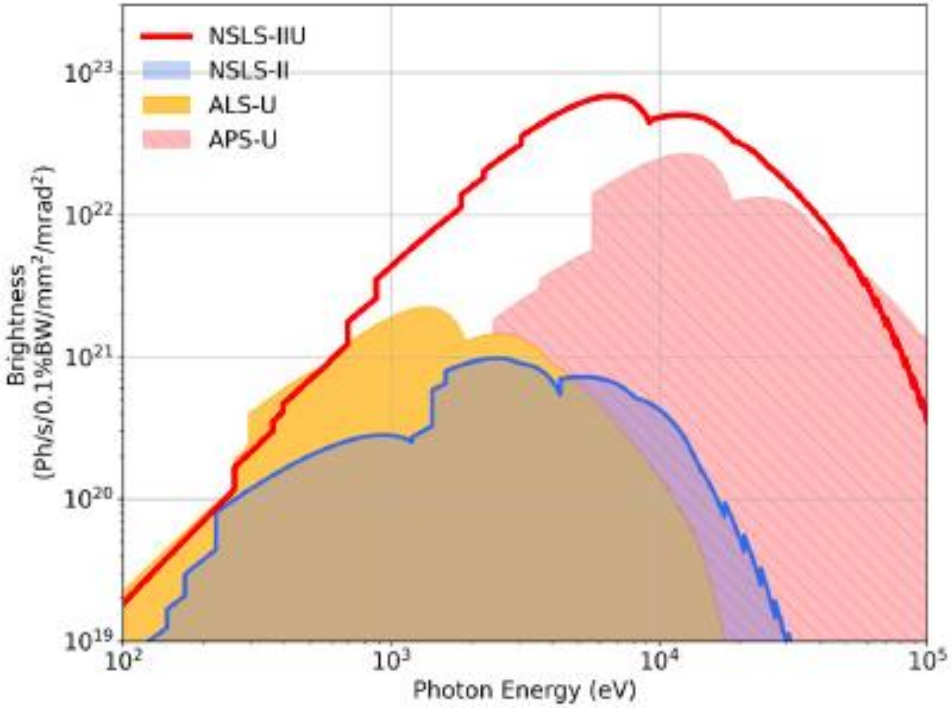


HRD
QCT
ANI
TXN

- The multimodal and multi-scale approach to developing the NEXT III suite of beamlines would be very **important** for the broad scientific community
- The continued engagement of the US (and global) user community is needed to quantitatively define required capabilities and their potential for unique impact.

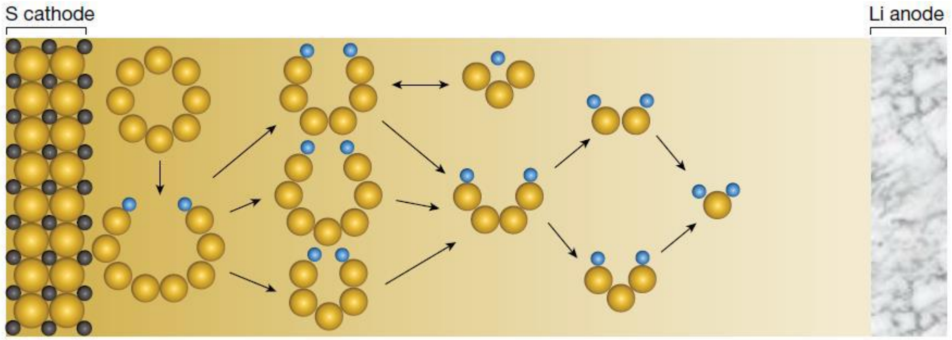
NSLS-II U

- The World's brightest multimodal storage ring
- World-leading brightness between 1 and 10 keV (10 x brighter than APS-U or ALS-U)
- Addresses challenges in microelectronics, clean energy, quantum materials, bio-preparedness, and beyond
- All need a multimodal facility to study operando phenomena from Angstrom to cm and microseconds to weeks.

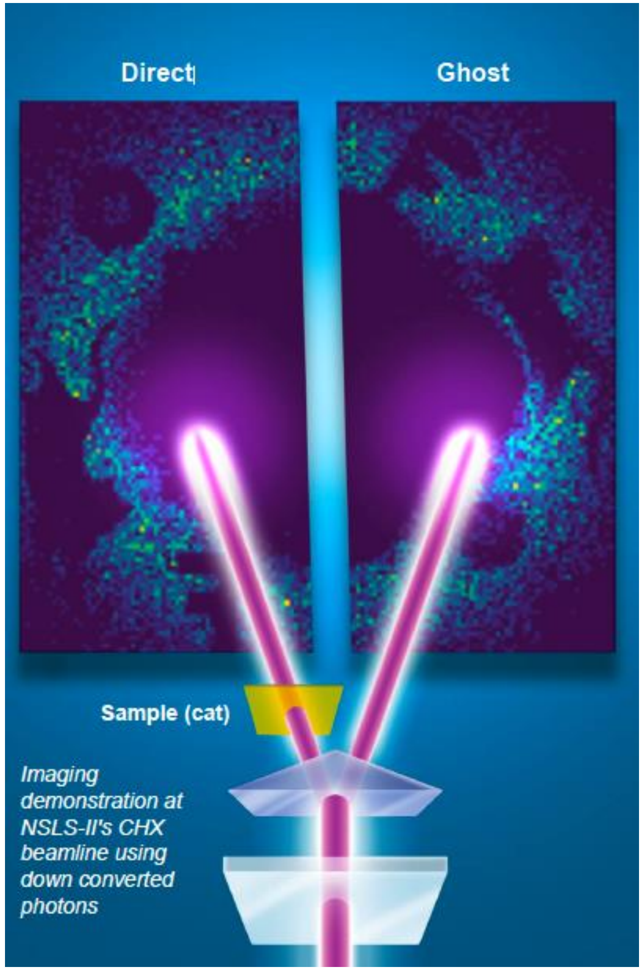


- NSLS-II U is for addressing future science challenges and maintaining US global competitiveness in synchrotron science.

NSLS II U: Science Drivers



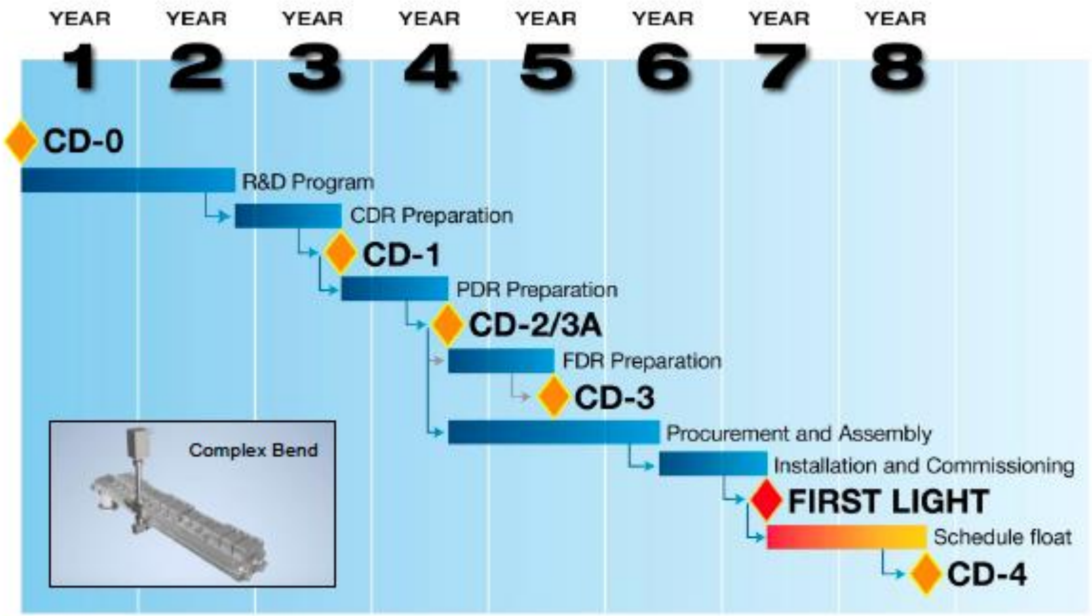
- Enable microelectronics beyond Moore's Law
- Develop high energy-density batteries with earth-abundant materials
- Facilitate catalysis for a cleaner environment
- Understand the processes of life in action
- Drive the quantum revolution
- Enable ghost x-ray imaging



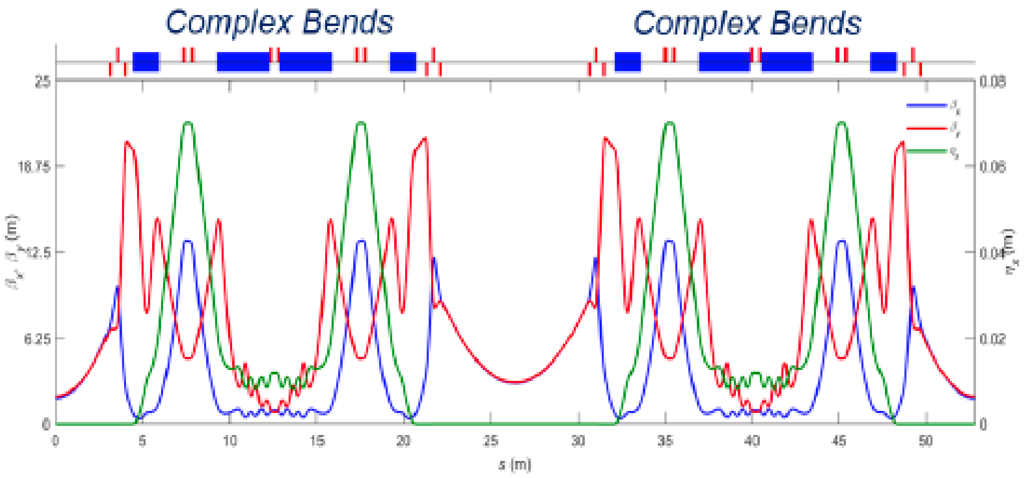
All are complex, multi-length and multi-time scale problems.
All require: world-leading brightness in the 1-10 keV photon energy range and multimodal capabilities

NSLS-II U Readiness

- NSLS-II U has a plan to deliver first beam to users eight years after a CD-0 decision
- Preserve present source locations to utilize existing beamlines
- Novel accelerator concept - a Triple Complex Bend Achromat (TCBA) lattice. – reduction in power use



- The science case for a medium energy storage ring, with world-leading brightness in the 1-10 keV range is **absolutely central**.
- Further evaluation of the accelerator concept by an expert panel is recommended as well as early engagement of the user community.



NSLS II NEXT III and NSLS II-U Recommendations

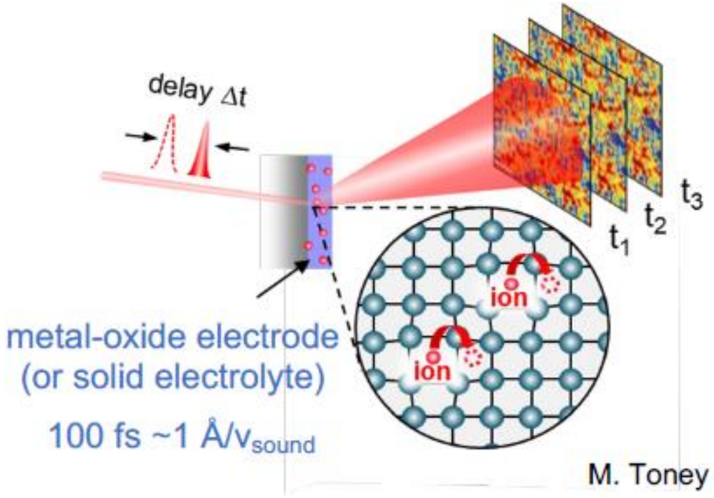
- **NEXT III** complements NSLS II existing beamline portfolio and could lead the way to multimodal, multiscale synchrotron with a fully integrated beamline suite and potential for impact in many areas of research
  - The science case is both **important** and **central** depending on the BL
  - NEXT III will be **ready for CD1** later this year; tech requirements need refining

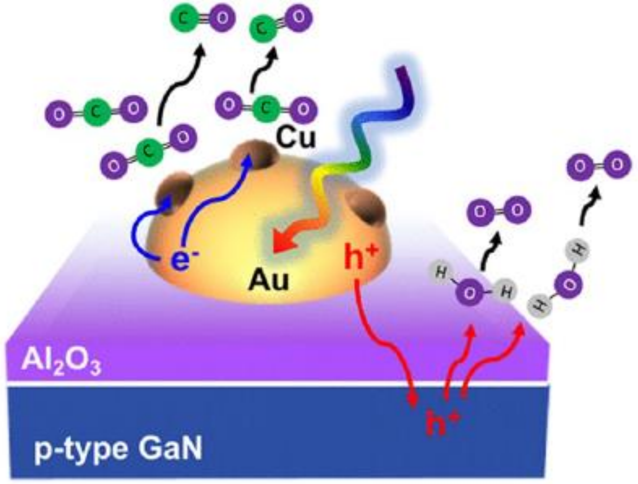
- **NSLS-II U** would be the World's brightest synchrotron source (10x APS-U and ALS-U for tender x-rays in the 1-10 keV range).
  - The science case is **absolutely central** for the US; novel accelerator concept – Triple Complex Bend Achromat; and new techniques (ghost imaging)
  - Recommend research on **engineering challenges** for the new accelerator concept, then proceed to CD0

Three LCLS projects for US Leadership in XFEL

Mike Dunn, SLAC

- **LCLS II-HE**: The World's first continuous-wave hard x-ray source
- **LEI**: High-energy extender for LCLS II-HE and for LCLS-X
- **LCLS-X**: Brings XFEL science into a SR-like era





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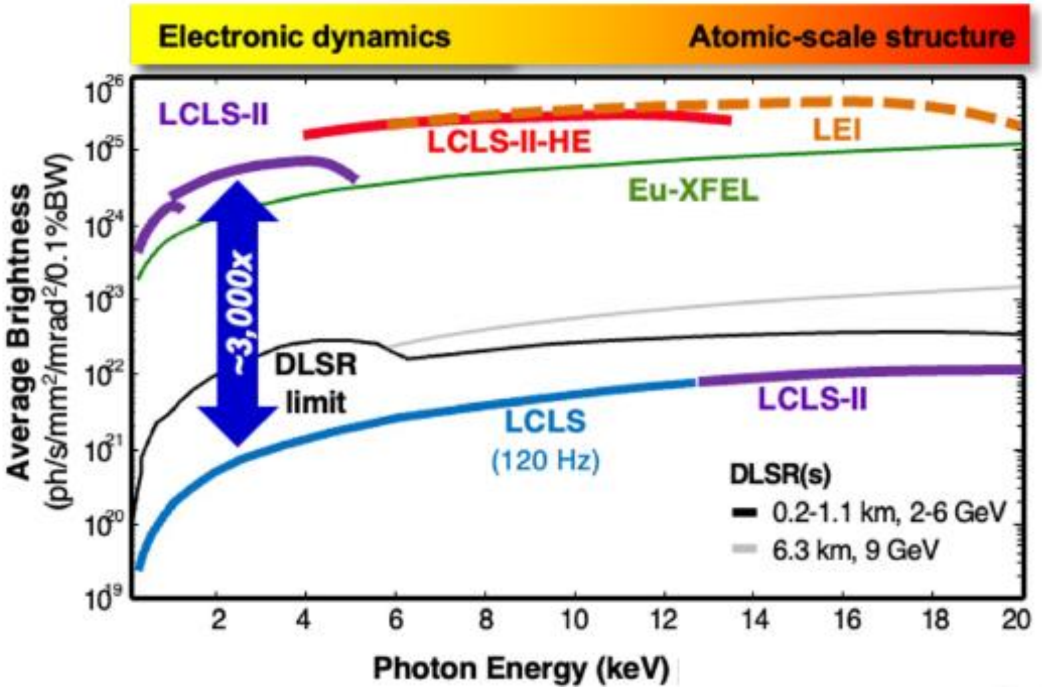
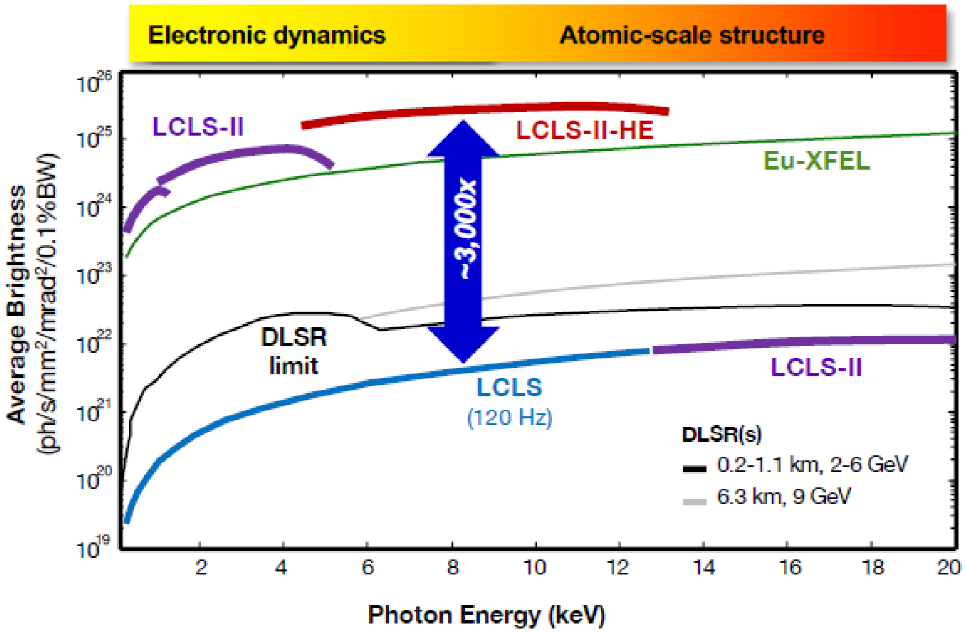


LCLS-II-HE (High Energy)

- The first continuous wave hard X-ray source in the world
- A scientifically essential extension that transforms LCLS-II, providing high repetition-rate in the critically important “hard X-ray” regime

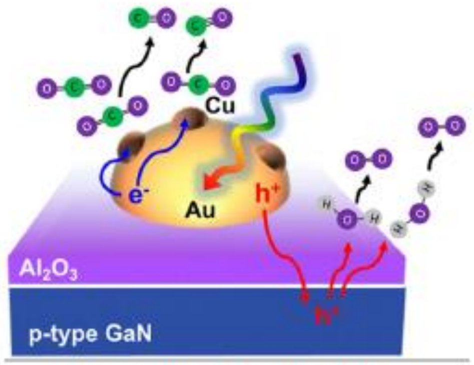


- Capabilities move far beyond the present generation of XFELs and the ultimate potential of storage rings, firmly maintaining the U.S. as the international leader in the science enabled by X-ray sources
- However, matching or exceeding capabilities may be available in China by the end of the 2020s, and at the European XFEL in the early 2030s

LCLS-II-HE Science Drivers

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

Design principles for cost-effective and sustainable chemical transformations



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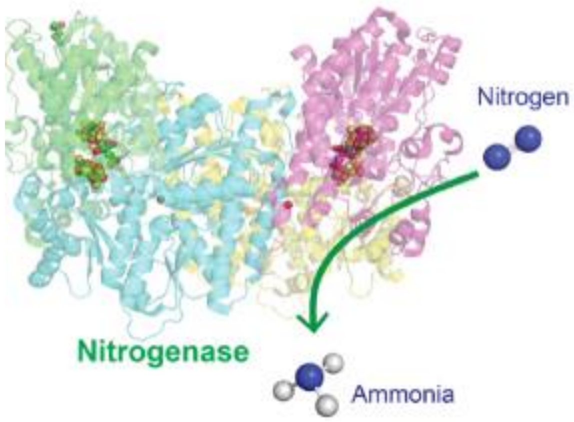
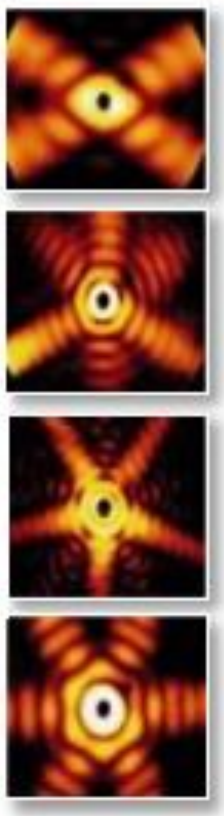
Directed design of nano-catalysts with tunable properties

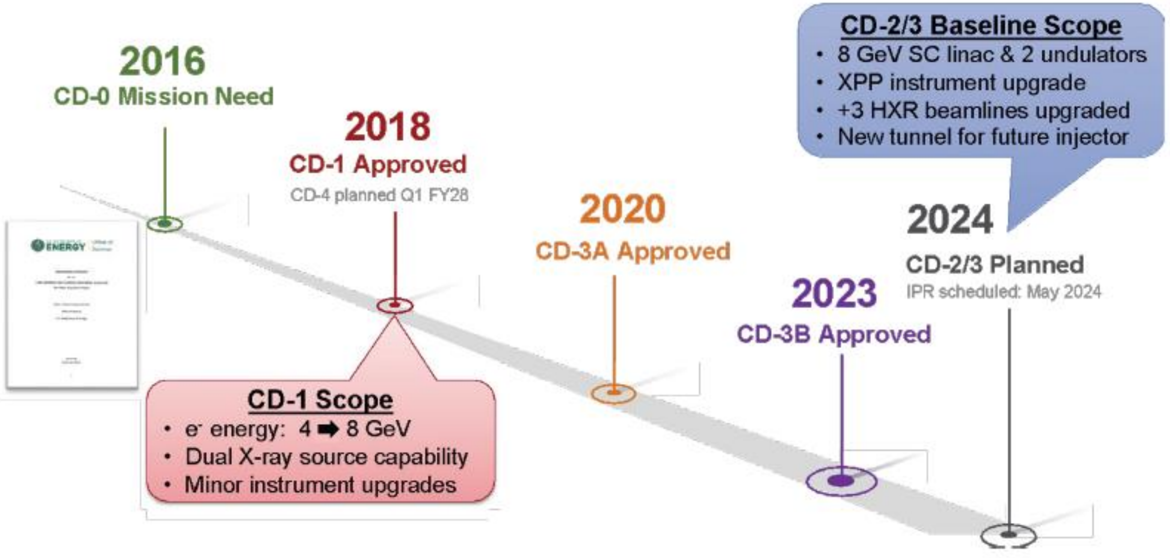


Imaging biological function in real time to underpin human health and bio-inspired clean energy solutions



LCLS-II-HE Readiness

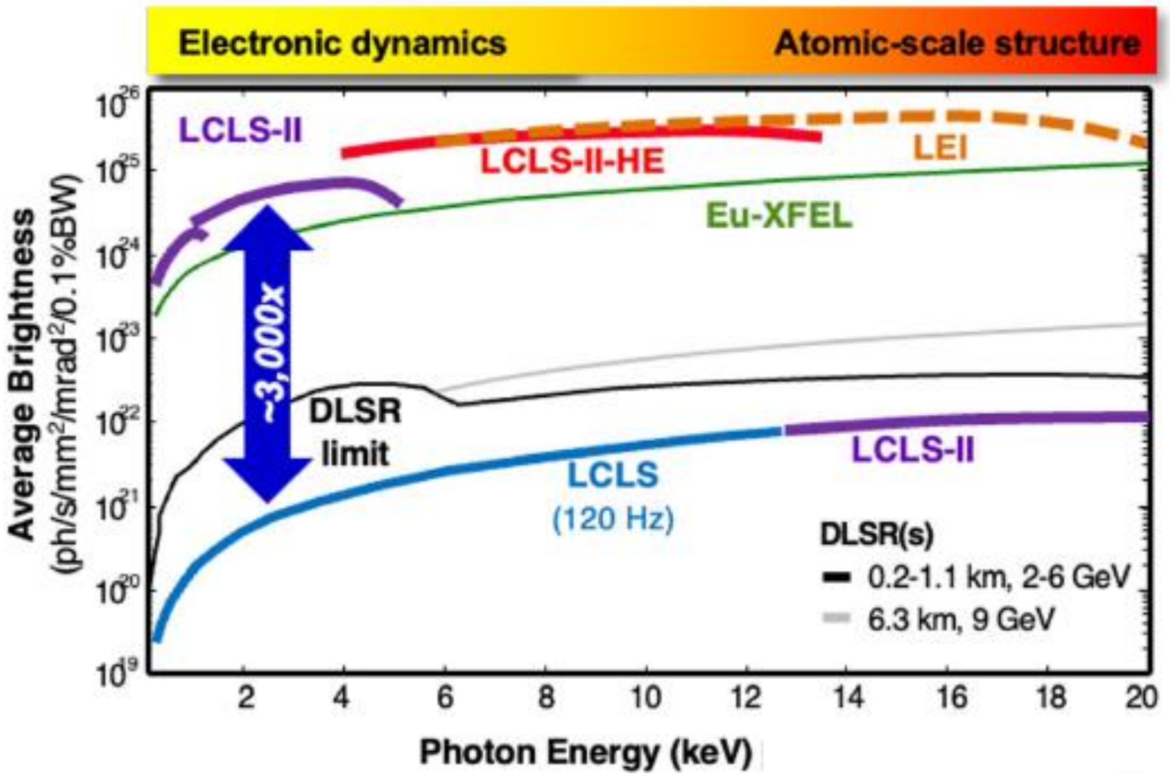
- The project has completed 90% of the facility design
- The suite of high-performance cryomodules in an advanced state of delivery
- **Ready for CD-2/3** May 2024
- Major construction activities are planned to begin in summer 2025, with a projected early finish date of readiness for CD-4 by the end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



- 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
- Programs have been launched and progressing well, but regular progress assessments to be performed

Low Emittance Injector (LEI)

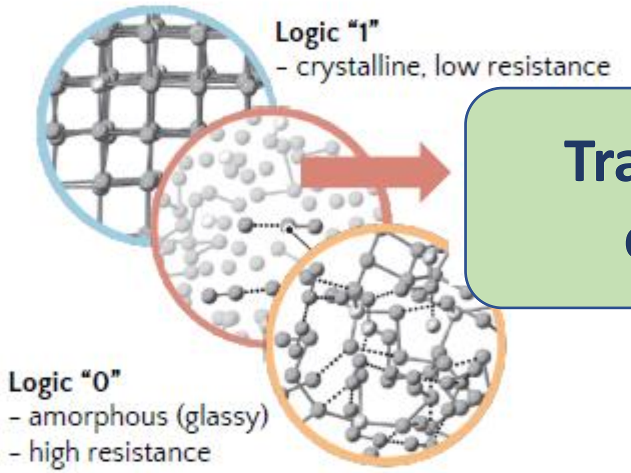
- Low Emittance Injector upgrade to LCLS-II-HE
- Scientifically essential extension to LCLS-II-HE, covering need for sub-Å ultrafast X-rays at high repetition rates
- Provides essential operational redundancy
- Protects availability of superconducting RF (SRF) operations for user science
- Sustains US leadership via ongoing injector improvements



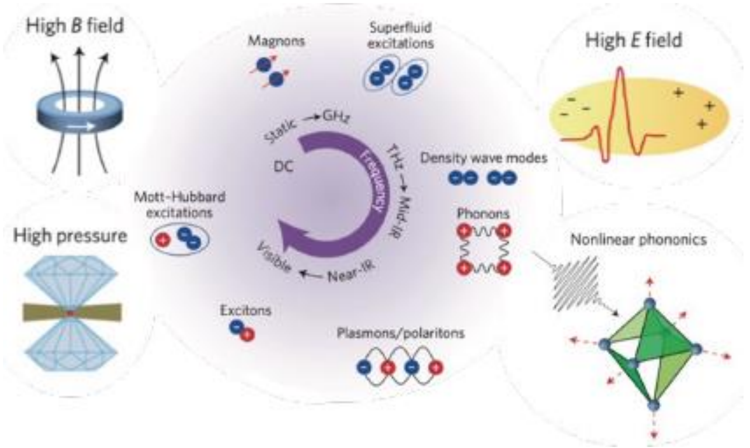
- Internationally, active development of highly competitive XFEL facilities, with performance that will exceed LCLS-II-HE & LEI
- LEI is needed in order to remain internationally competitive

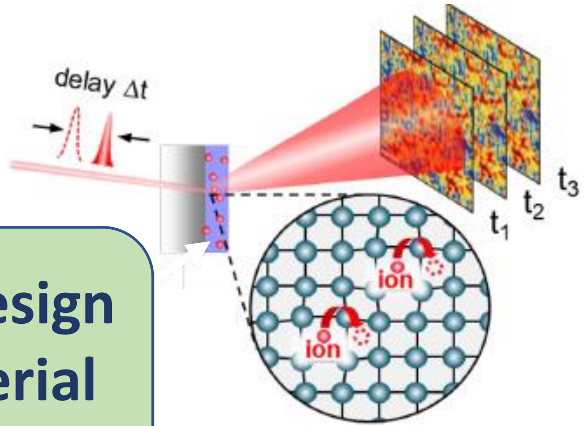
LEI Science Drivers

The world's brightest X-ray laser for model-free structural dynamics and insights into complex energy systems and quantum materials



Transforming our understanding of complex, disordered materials





Understanding & controlling emergent phenomena in quantum materials

Energy Storage Materials – predictive design to enhance energy density, safety, material compatibility, and longevity

LEI Potential

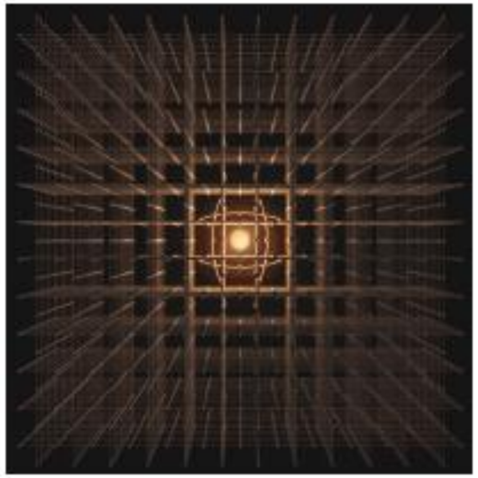
Existing facilities today outperform capabilities in the US, in particular in some strategic scientific areas

EXAMPLE: Characterization of dynamic heterogeneity on complex materials for energy and computing which lack long-range order and where and subtle atomic distortions underpin important properties, e.g.:

- Inorganic perovskite solar cells (polaron dynamics)
- Phase-change computer memory (liquid-liquid transition)

Requirements:

- sub-atomic spatial scale (large q-space volume) and natural timescales
- penetration depth for tailored sample environments (Pressure, E/B fields, …)

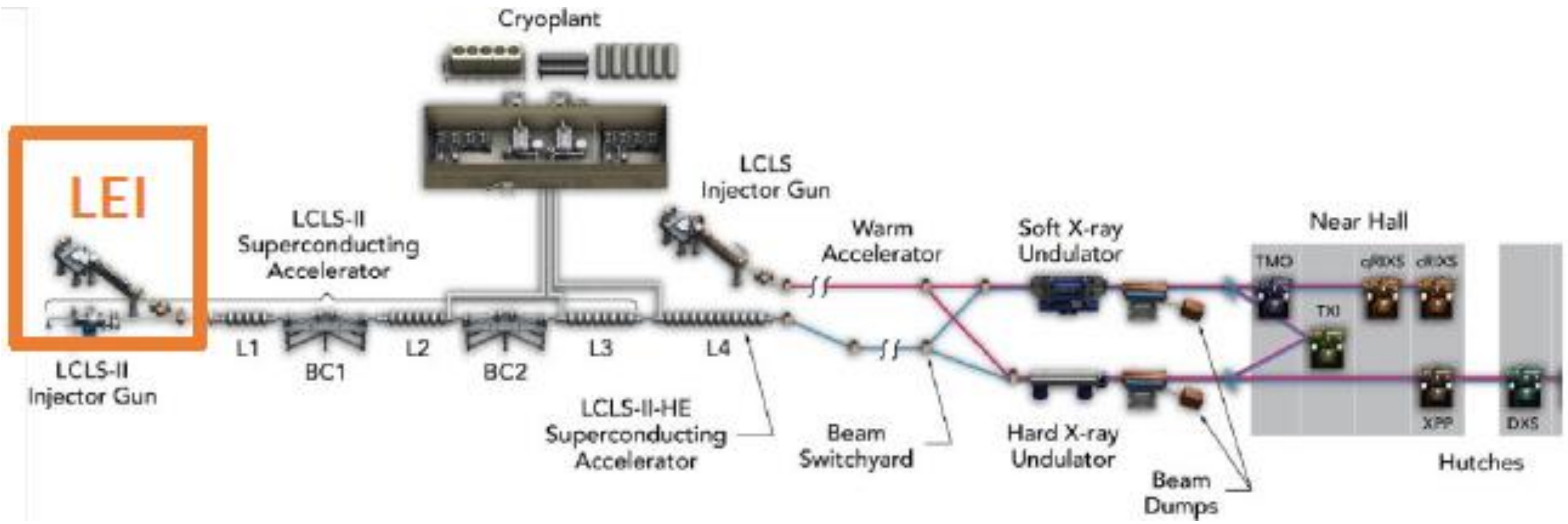


B. Guzelturk *et al.*, *Nature Materials*, **20**, 618 (2021)

- LEI will provide world-leading capabilities exceeding any SR or XFEL operating today in terms of average brilliance for sub-atomic scale investigations
- LEI is an **absolutely critical** step for the U.S. to maintain leadership in the fundamental science that underpins complex matter

LEI Readiness

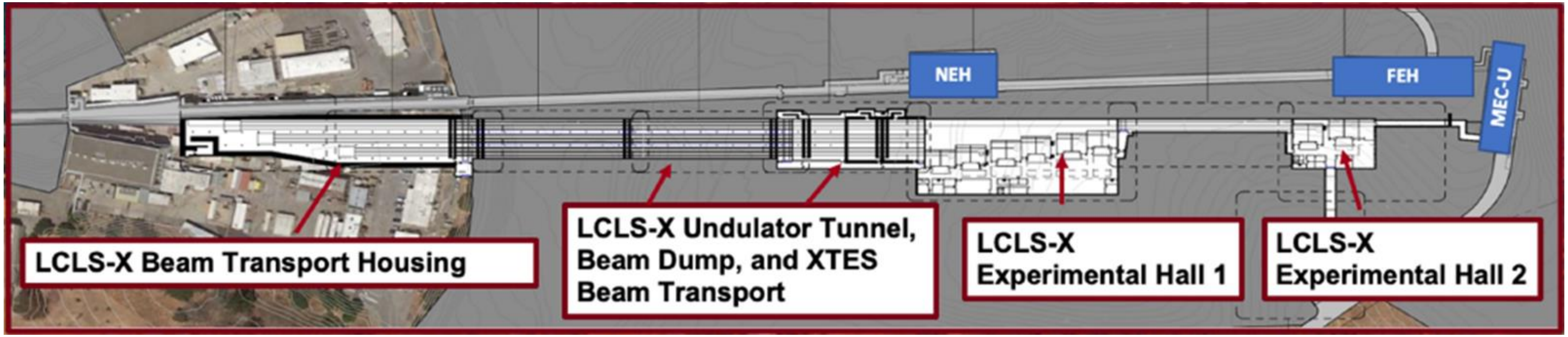
- **LEI is in an advanced state of readiness-to-construct with essential R&D underway**
- **The design of the injector is largely complete, with modeling showing the required emittance can be reached**



- A more detailed assessment of **readiness** of LEI will presents something of an **engineering challenge**, but will be enabled after RF gun prototype tests, planned for 2025

LCLS-X

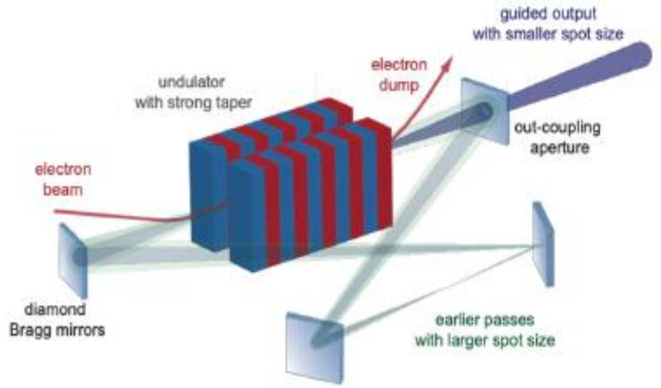
- **The world's first 3rd Generation X-ray Free Electron Laser**
- **Brings XFEL science into a SR-like era, supporting a broad critical mass of the science community, and with an associated order-of-magnitude change in cost per experiment, scientific throughput and impact**



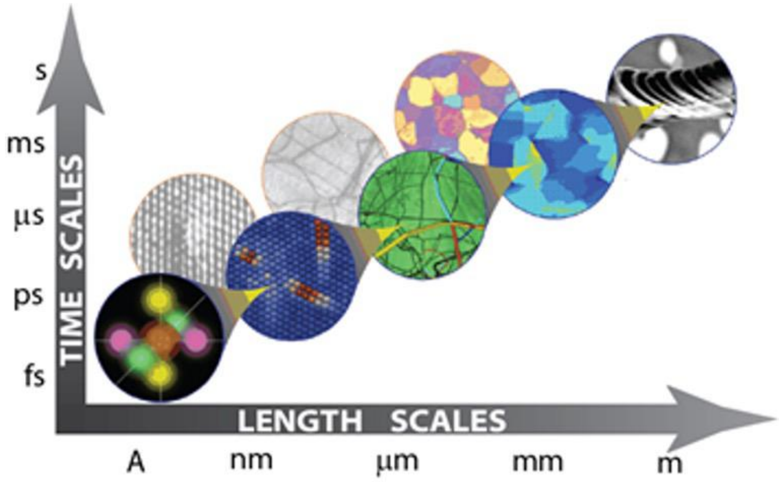
- Internationally, no similar plan yet
- But US is lagging behind Europe and Asia in the number of optimized XFEL sources, beamlines and instruments.

LCLS-X Science Drivers - I

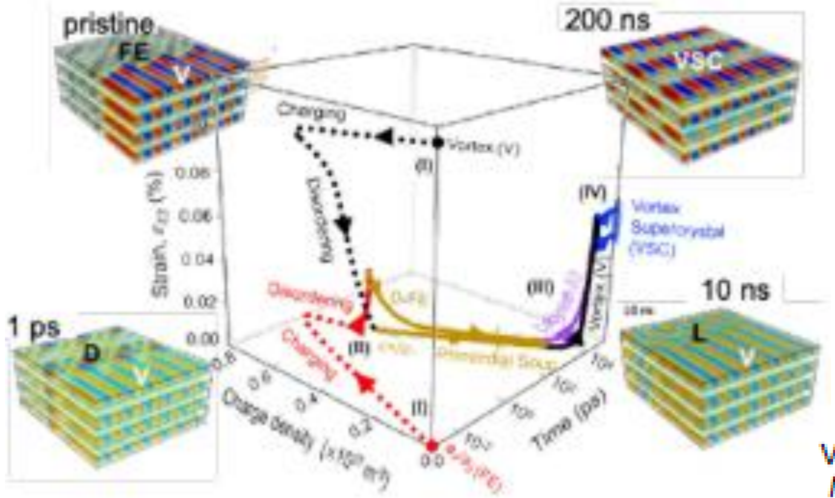
- Dedicated, custom-designed instruments, with tailored infrastructure for each operating environment
- Ability to host new types of source (cavity FELs, SCU, …), with dedicated setups for each source



EXAMPLE: Reveal "microstructural black swan events" in operating devices - to detect initial steps in materials degradation and failure



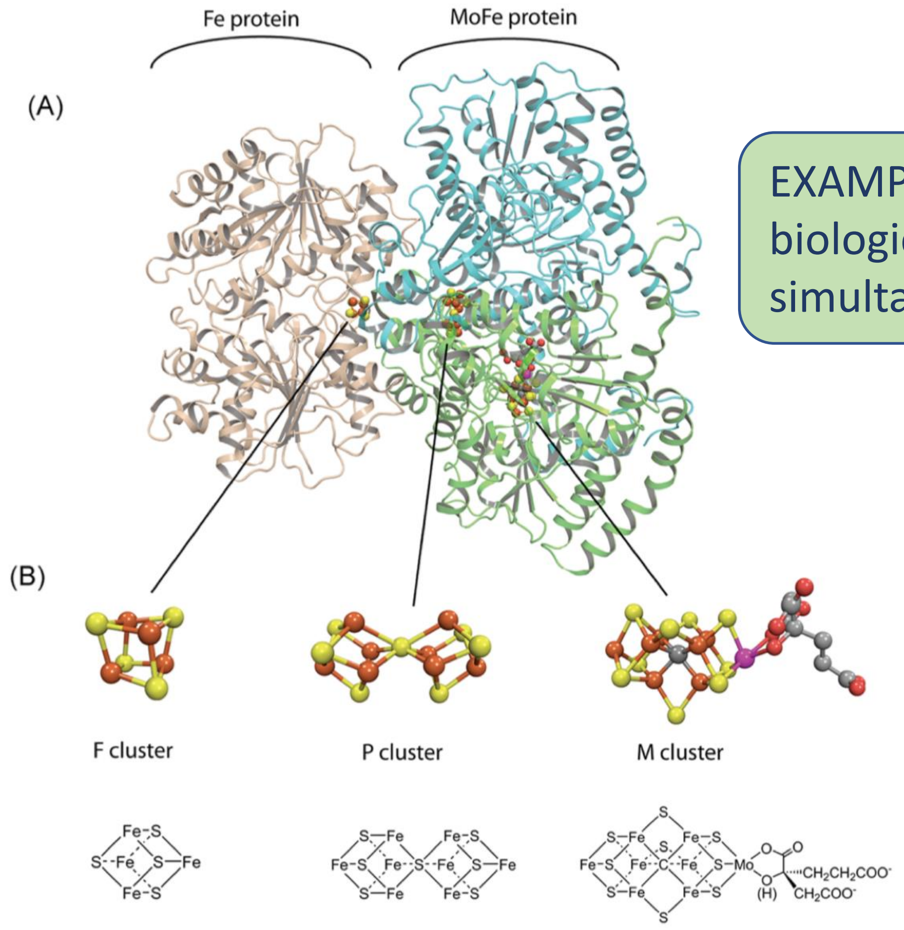
EXAMPLE: New insights into intertwined order parameters to inform the control of quantum materials through coherent light-matter interaction



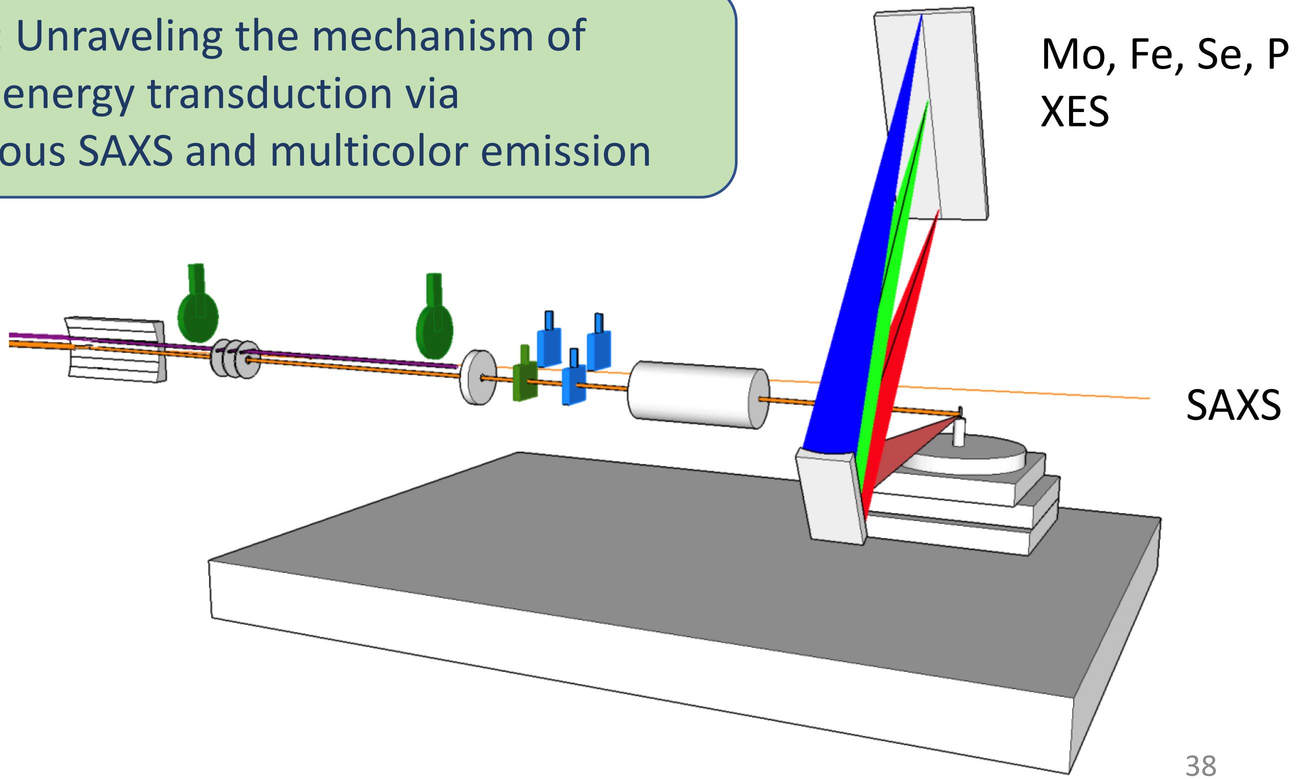
V. Gopalan *et al.*, *Nature* (2021)

LCLS-X Science Drivers - II

Ability to conduct multimodal experiments simultaneously to reveal long range and atomic level changes with femtosecond temporal resolution



EXAMPLE: Unraveling the mechanism of biological energy transduction via simultaneous SAXS and multicolor emission



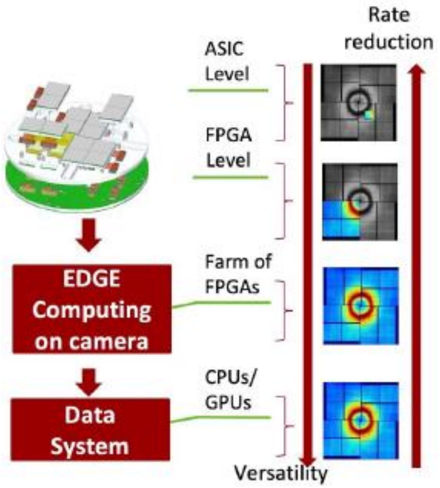
LCLS-X Potential

- LCLS-X is **absolutely central** to US science leadership, if approached with urgency
- The scientific output of existing XFEL facilities around the world is critically hampered by their efficiency and limited amount of end-stations
- This context hinders the production of a critical mass of publications in any specific science area, a necessary condition to have real impact
- LCLS-X overcomes this by supporting a suite of XFEL sources and instruments optimized for critical science areas.

- LCLS-X is has the potential to project the relevance and the impact of XFEL science to similar levels reached today by SR.
- The US has a unique opportunity today to lead this XFEL science revolution.

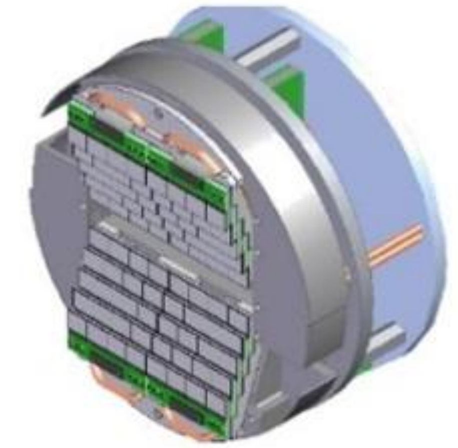
LCLS-X Readiness

- The existing LCLS-II-HE accelerator should be sufficiently powerful to feed 10 XFEL undulators.
- Data science integration is at the heart of LCLS-X design
- Phased delivery of end stations and instruments to allow staged growth, responsive to new discoveries and emerging national priorities.



Intelligent Data Extraction

Massive Scale Training Data for ML models



- Revolutionary advances in data science and the development of a new generation of detectors are needed to fulfill the scientific potential of LCLS-X
- Programs have been launched and progressing well, but regular progress assessments to be performed

LCLS II Recommendations

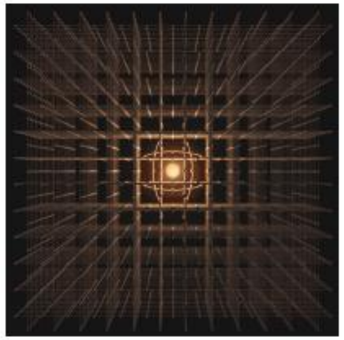
- LCLS II-HE - world's first continuous-wave hard x-ray source, with potential impact significantly beyond current x-ray facilities (EU XFEL, SHINE)
  - The science case is **absolutely central**
  - Ready for CD 2/3 in May 2024
  - Advances in data science and next generation detectors needed

- Low Emittance Injector – World-leading capabilities in terms of average brilliance for sub-atomic scale investigations
  - The science case is deemed as **absolutely central**
  - A more detailed assessment of readiness of LEI will be enabled after RF gun prototype tests, planned for 2025

- LCLS-X – World leading opportunity to advance the capabilities of XFEL science and to similar capacity levels reached today by synchrotrons
  - An unchallenged potential to advance fundamental scientific discovery and translate to address pressing national challenges - **absolutely central**
  - Readiness assessed after addressing engineering challenges

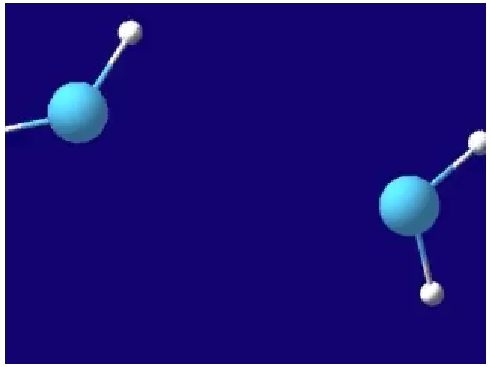
Future Light Source(s) (FLS)

- Science case is in a preliminary stage
- Choice of facility layout, accelerators, sources, and instruments will depend on science case and potential future user communities
- Unique opportunity for a completely integrated, multimodal user facility



Formation and evolution of polaronic strain fields in hybrid perovskites

B. Guzelturk *et al.*, *Nature Materials*, **20**, 618 (2021)



FLS Expert Panel

Paul McIntyre
Ass. Lab Director SLAC
SSRL

Panel Members

Erica Ollmann Saphire,
Professor, La Jolla Institute for Immunology

Agostino Marinelli
Assistant Professor of Photon Science and of Particle Physics and Astrophysics, SLAC National Accelerator Laboratory

Zhi-Xun Shen
Paul Pigott Professor of Physical Sciences, Stanford University

David Robin
ALS-U Project Director
Lawrence Berkeley National Laboratory

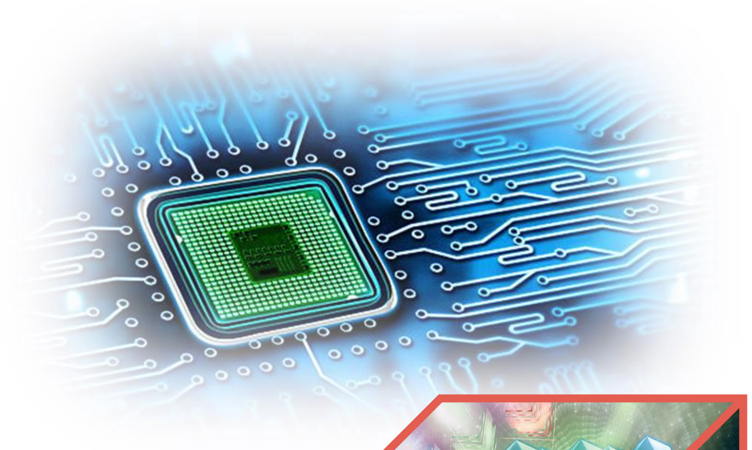
Jingguang Chen
Thayer Lindsley Professor of Chemical Engineering, Columbia University

James Benjamin Rosenzweig
Distinguished Professor of Physics, University of California, Los Angeles

Science Drivers

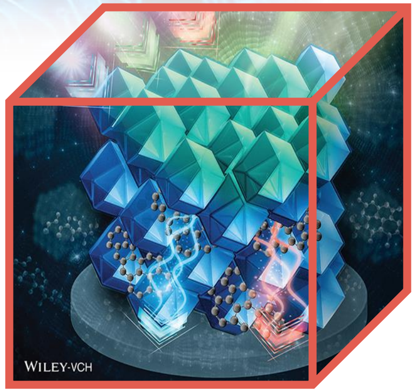
Precision data at the atomic/attosecond scale

- Quantum control of matter and energy
- Materials at extreme conditions
- Crystallography and control of complex/disordered matter



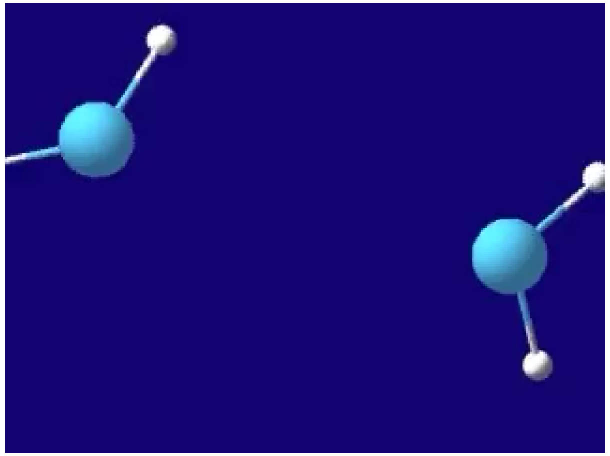
Bio/Soft Materials & Biomedical Science Drivers

- Low-dose 4D X-ray imaging at sub-nm resolution
- Massive image screening of cells to organs
- Biology meets water, attosecond biochemistry



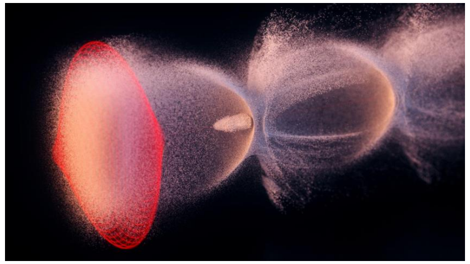
Atto second chemistry

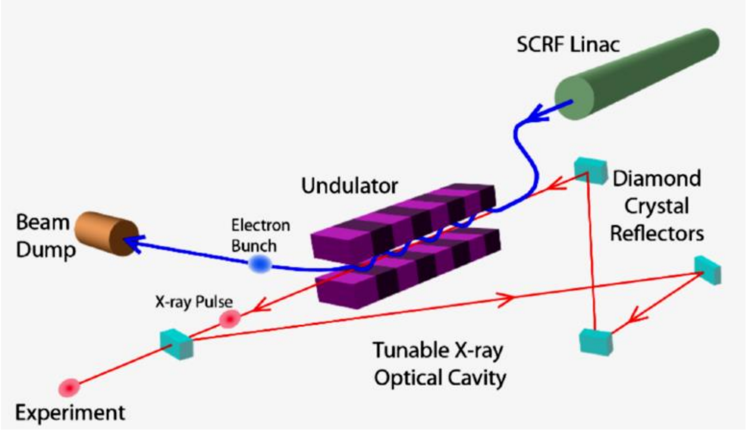
- Movies of making and braking bonds in solution, solvated matter - transients
- Quantum mechanics in action

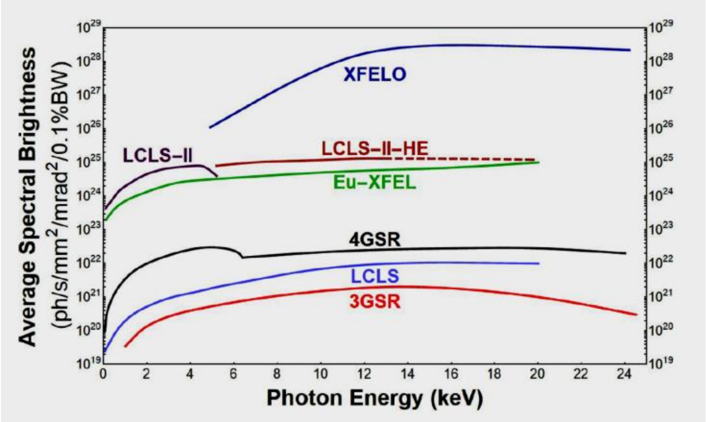


Facility Options

The technology and layout of the facility are inextricably linked with the science case





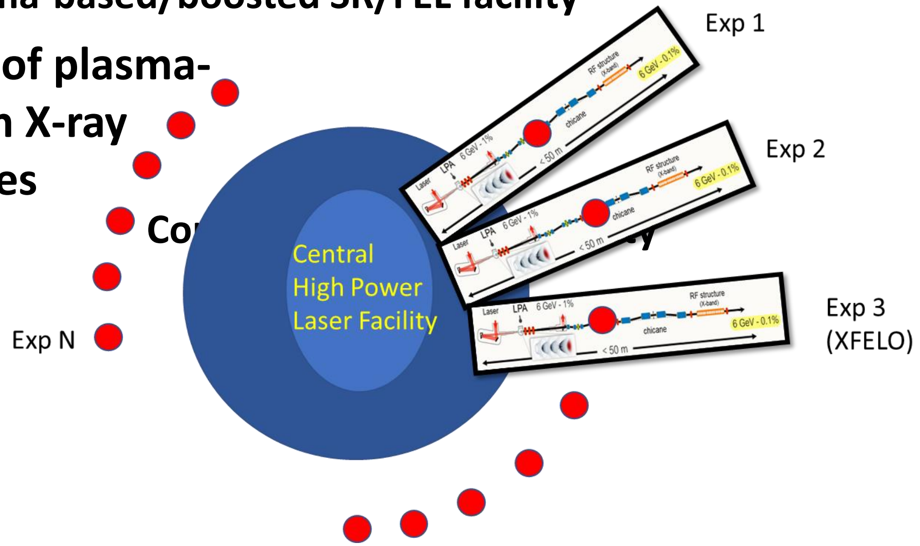


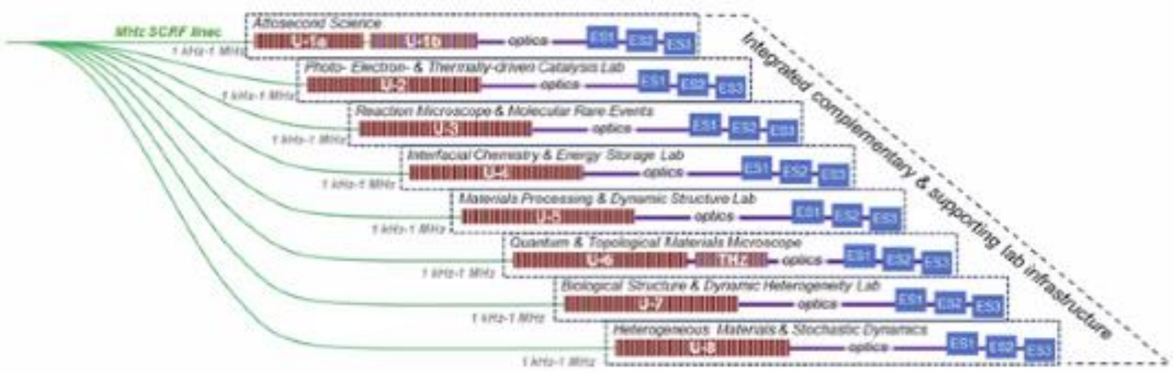
XFEL-Oscillator (XFELO):
Could be combined with ERL

Distributed layouts:
1. Compact XFEL
2. Compact synchrotrons
3. Multiple data centers
4. Combined with other facilities (nano, bio, materials, cyro-EM….)

Plasma-based/boosted SR/FEL facility

Plant of plasma-driven X-ray sources





Massively multiplexed XFEL supporting dedicated endstations

Accelerated Discovery, New Modalities

Transform user access and enhance productivity

Intelligent automation

- Intelligent automation (AI/ML/VR): complete digitalization and modeling of data and experimental processes in real-time
- Facility digital twin: facility training and efficient use, supports non-expert users and remote access
- Portfolio of remote and hybrid access modes and VR user experiences with precision robotics and high throughput
- Rolling (continuous) access
  → Fast access to single or multiple BLs, modes & techniques
- Engage new communities: Excitement in scientific communities for new characterization and visualization methods.

Future Light Source Observations and Recommendations

Observations and Recommendations

- FLS is **absolutely central** for the future of US-based light source science and global competitiveness
- This is a good start: The FLS science **mission and facility layout need to be iterated with the science case**.
- Opportunity to fully Integrate instruments with AI/ML/data/VR/facility twins
- Need to balance transformational capabilities with capacity for impact across research topics and research communities; single FLS vs. distributed sources
- Launch process in 2024+ with expert panels, workshops to anticipate science and user needs in the next 10-15 years
- Initiate pilot projects like ghost imaging, autonomous operation, robotics, and AI/ML concepts at existing facilities

Overall Facilities Observations

- All eight proposed x-ray and neutron facilities address the DOE BES mission
  - The Nation's top scientific and technological challenges in new materials, physics, chemistry, biology, environmental science, energy technologies, water and sustainability of Earth's ecosystems; and the capacity for transformational discovery.
- Each facility is in a different state of developing their science case and layouts
- Essential for BES to continue to balance funding core programs and facilities
- It is natural that there will be scientific complementarity and overlap among the facilities. However, while the facilities layouts are quite distinctive, the subcommittee would like to see better distinction among the science cases.

Recommendations: Science Case

- The Subcommittee encourages each facility to identify a few crisp, distinct and compelling targets for grand challenge science (e.g., that utilize the first instrument suite)
- BES should consider coordinating an effort with the 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 inform facility and instrument capabilities, and engage and build new user communities
- BES should continue their effective strategy of balancing funding for major user facilities and research

Recommendations: Readiness

Though each facility is in a different state of readiness, as per the subcommittee recommendations, global competition in the EU and China is creative, energized and getting funds

Encourage **urgency** to ensure future US leadership in scientific discovery

Recommendations: Partnerships

- BES should oversee a proactive effort with each facility to engage with other SC programs as needed.
  - ASCR could partner on major advances for BES facilities in digital/data, including large-scale data storage, machine learning, virtual reality, beamline twins, etc.
  - Also consider BER (bio and enviro), NP/HEP (accelerator concepts), FES (extreme materials); EERE and NNSA; other agencies - NSF, NIH, EPA, NOAA and NASA
  - Note: each of the SC Directorates advisory committees are also considering their strategies for future facilities. Example: BES and ASCR have strong mutual interests in semiconductor and quantum devices
- BES partnerships with international neutron and x-ray sources are a very good current practice, especially transatlantic cooperation. This is strongly encouraged.

Recommendations: Users

- Users are ‘**absolutely central’** for facility design and modalities
- Articulation of potential future research topics will be important to support efforts to support existing users, and to identify new user communities that will be ready for CD4 and beyon.
- Need to provide approaches for accommodating current users and training new user communities and develop most effective new modalities

Thank you

BESAC (Cynthia Friend, chair) for the opportunity to delve

BES team (Kerry, Adam, Linda, Andrew, ..) for advice and support

DOE National Laboratories and their facilities teams for thoughtful concepts, excellent presentations, and rapid responses

BESAC Facilities Subcommittee members for their perspicacity and rapid turnaround of materials for our report

Discussion