

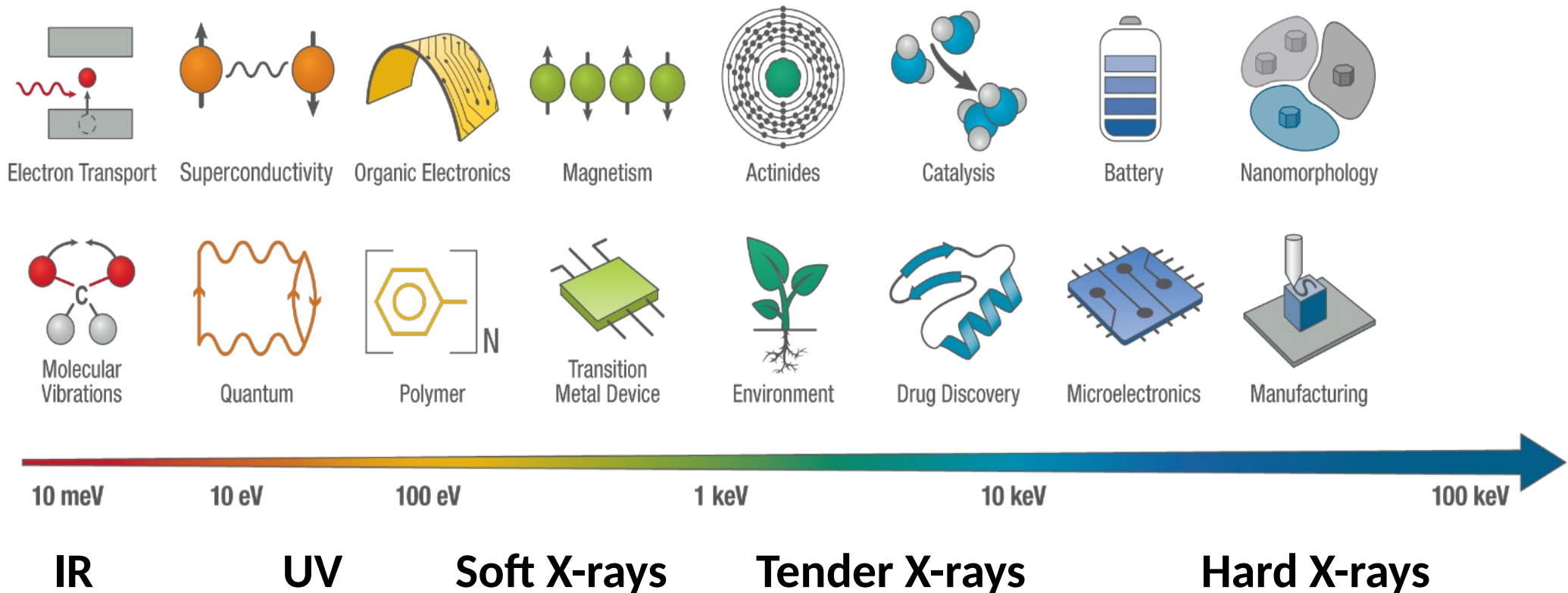
National Synchrotron Light Source-II, NSLS-II

Elke Arenholz
Director

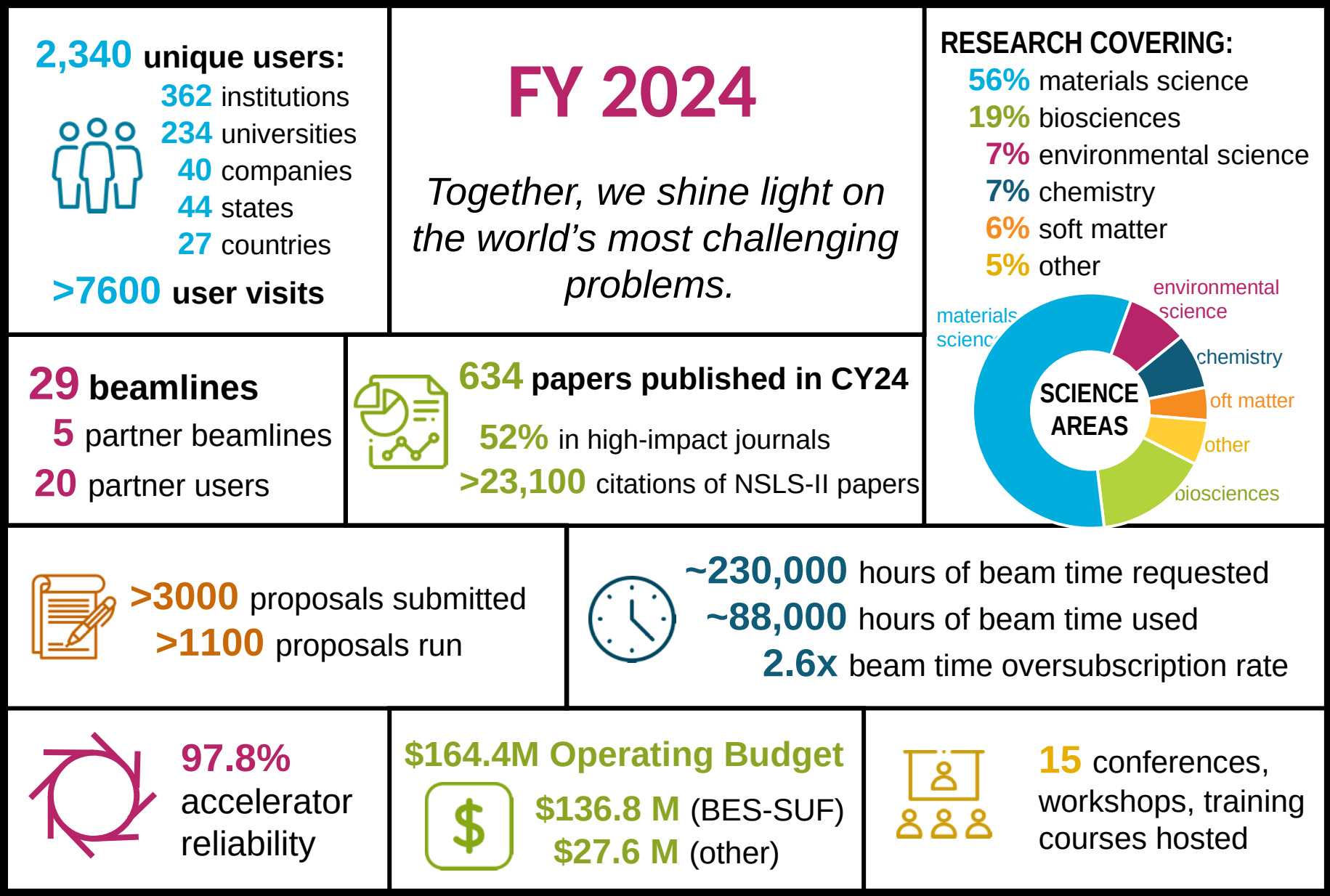


About NSLS-II

NSLS-II is a **DOE Office of Science user facility** that provides **high-brightness synchrotron radiation** from the **far infra-red (IR)** to the **hard x-ray regime** and **world-leading experimental capabilities** to enable high-impact science across disciplines.



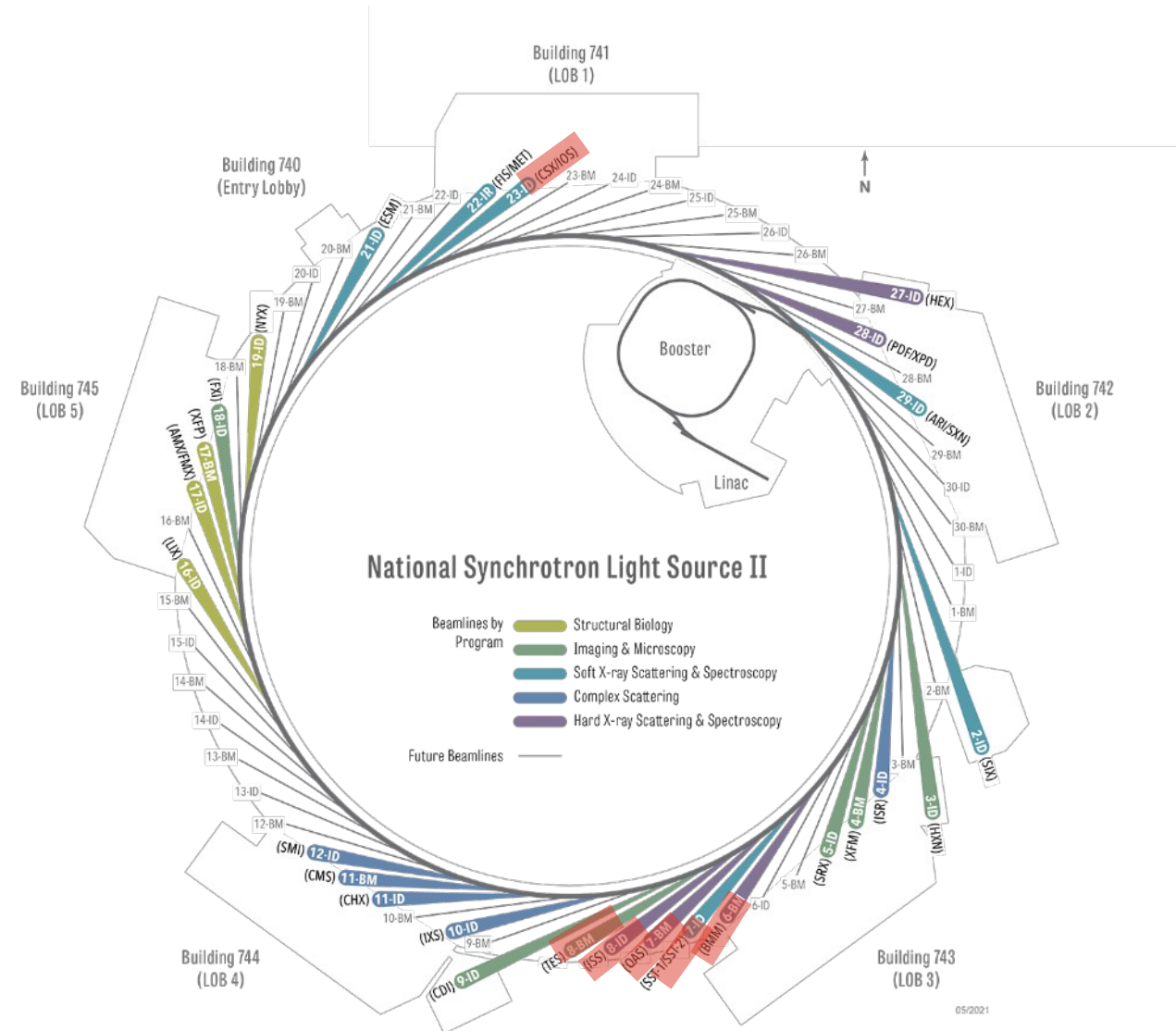
NSLS-II by the Numbers



X-ray spectroscopy program @NSLS-II

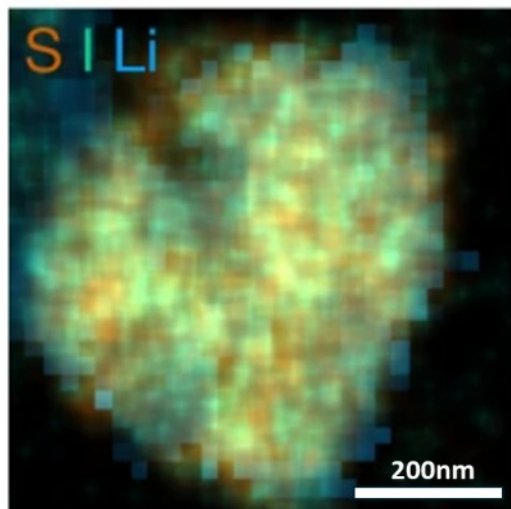
- Hard X-ray beamlines
 - Inner Shell Spectroscopy (ISS)
 - Quick Absorption and Scattering (QAS)
 - Beamline for Materials Measurements (BMM)*
- Tender X-ray beamlines
 - Tender Energy Spectroscopy (TES)
 - Spectroscopy Soft and Tender I/II (SST)*
- Soft X-ray beamlines
 - In situ and Operando Spectroscopy (IOS)
 - Spectroscopy Soft and Tender I/II (SST)*

*operated by National Institute of Standards and Technology



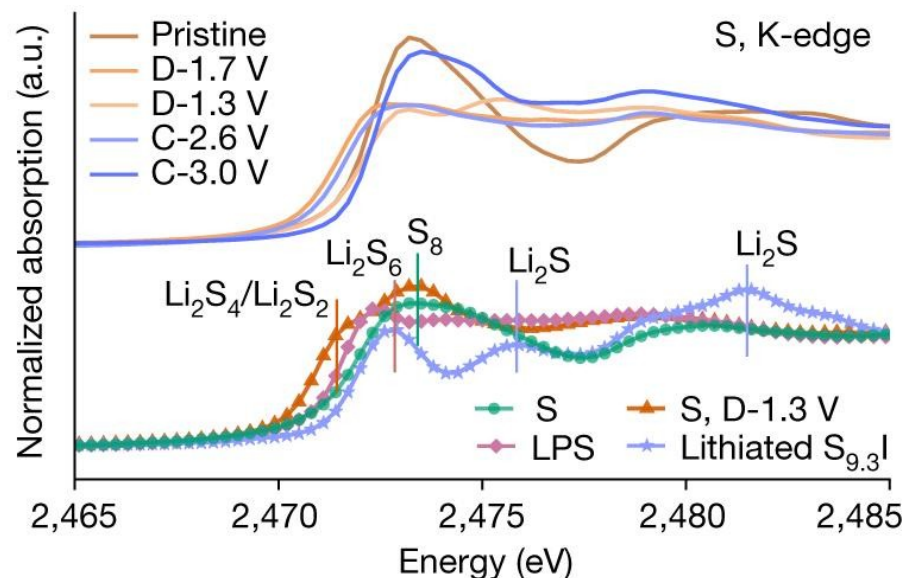
Sulfur Iodide Paves the Way for Cheaper, “Healable” Vehicle Batteries

7- μ B —M— OAS	8- μ B —M— TES	28- μ ID — μ 2— XPD
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TEM EDX, and
EELS mapping
images of $S_{9.3}I$.

J. Zhou, et al.,
Nature **627**, 301 (2024)



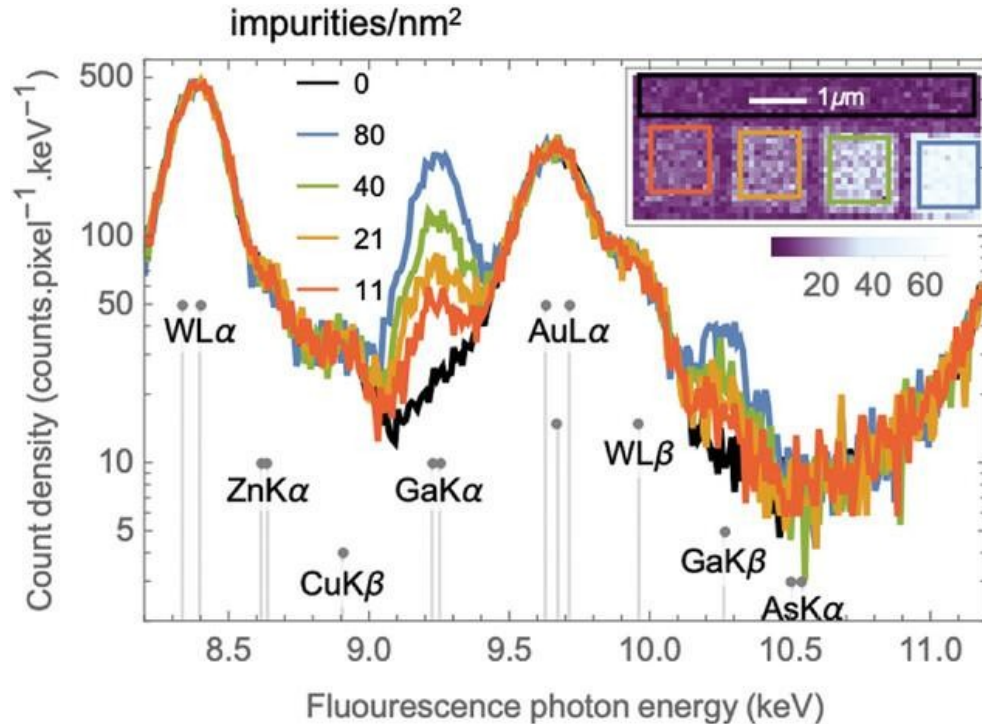
Scientific Achievement

- **Adding iodine (I)** to a solid-state lithium sulfur (Li-S) battery (SSLSB), yielded **vastly improved conductivity**.
- Observing charging (C) and discharging (D) mechanisms of $S_{9.3}I$ via X-ray absorption spectroscopy confirm the formation of LiS chains upon discharge and recovery of S_8 ring upon charging.
- The **low melting point** of $Li-S_{9.3}I$ promotes **self-repair** of interfaces increasing the number of charging cycles the battery can sustain. The impact of melting on the battery process was confirmed, in part, via **in situ X-ray diffraction** at NSLS-II's XPD beamline.

Significance

- The results may help realize SSLSBs as a **viable option for cost-effective and robust electric vehicle batteries**.

Imaging hidden impurities in crystals



XRF spectra and image for different implant densities using commercial three-channel silicon drift detector (Vortex, Hitachi) and the Multi-Layer Laue (MLL) optics for nano-focusing at NSLS-II's HXN beamline.

Scientific Achievement

- **X-ray fluorescence (XRF) microscopy** at the Hard X-ray Nanoprobe (HXN) beamline allowed detecting tiny gallium clusters implanted in silicon.
- **Isolated features of 3000 Ga and 650 Ga atoms** can be detected with 1s and 25s single pixel integration time, respectively.
- With further increased X-ray brightness “**few-atom**” sensitivity could be achieved.

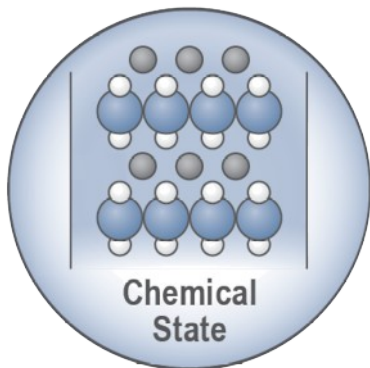
Significance

- Features created through **nanoscale semiconductor doping** allow constructing electrical contacts in quantum technology devices.
- **Single atom impurities in insulators** can be used for quantum sensors and single photon sources

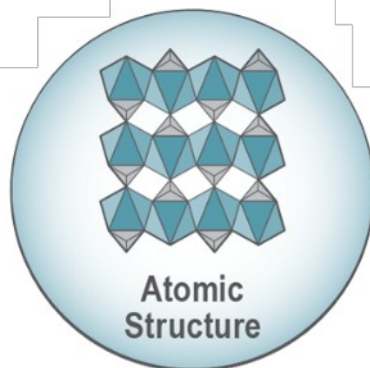
Multimodal Experiments at NSLS-II

Multimodal experiments combining spectroscopy, scattering and imaging techniques provide complementary and detailed **information on complex systems and processes.**

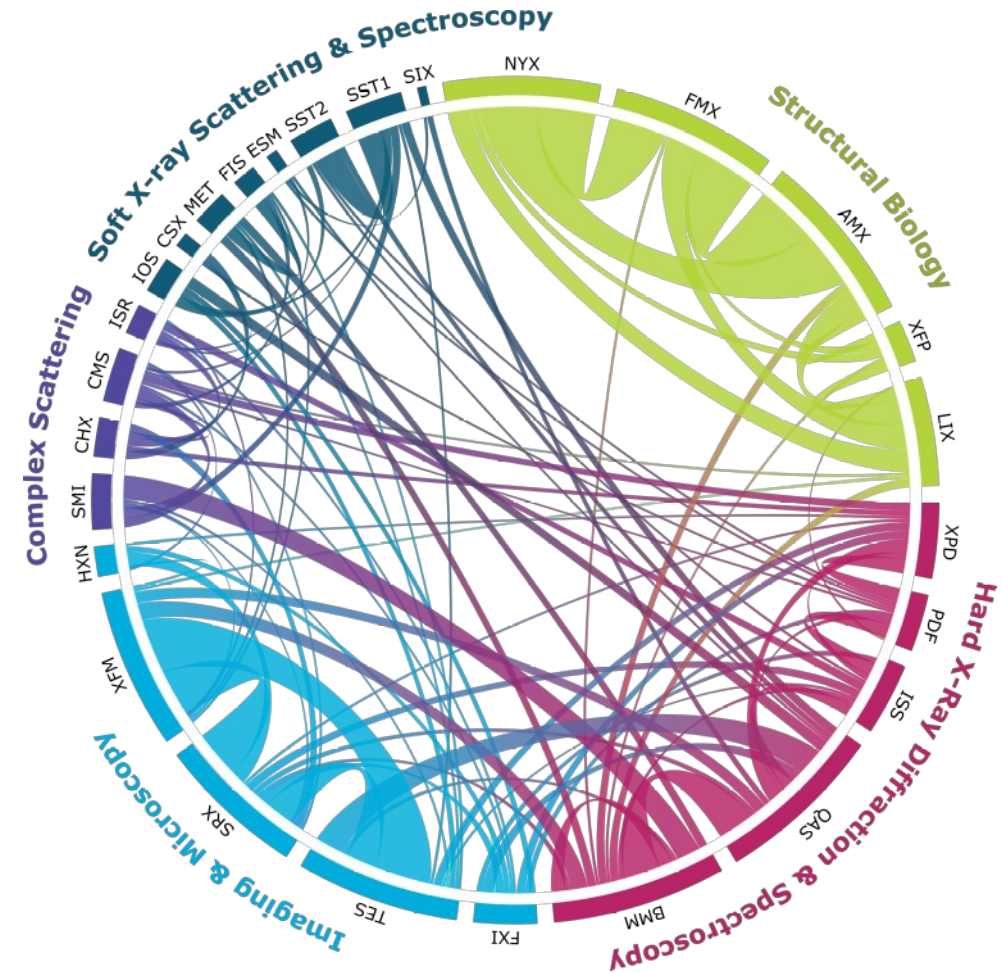
X-ray Absorption Spectroscopy



X-ray Diffraction

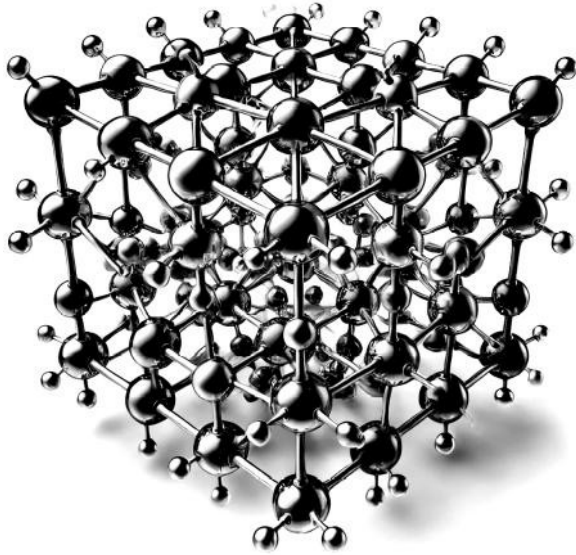


Full-field and Scanning Microscopy



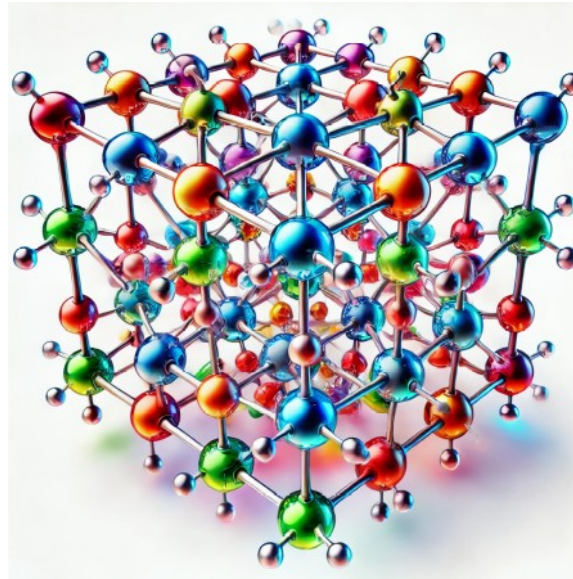
Lines connect beamlines that carry out multimodal experiments. The thickness of the lines is the number of proposals that ran on the 2 beamlines.

Real-time Multimodal Measurements at NSLS-II



X-ray Diffraction, XRD

- Provides atomic scale structural information
- No chemistry-specific information



**Combination of
XRD and XAFS**
provide **comprehensive
information** on new
materials

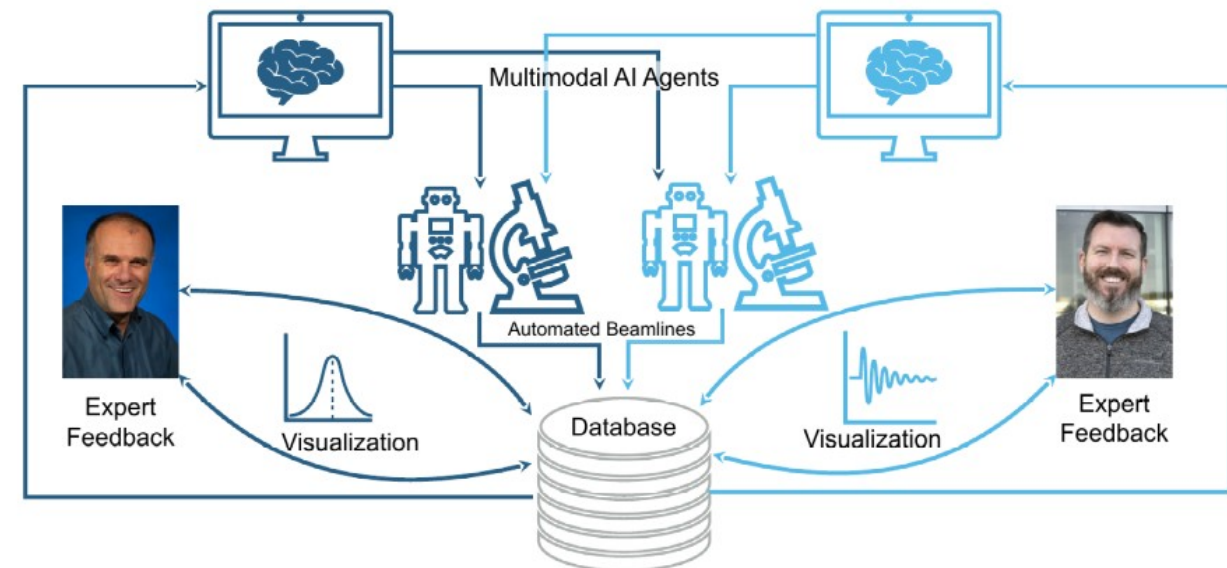
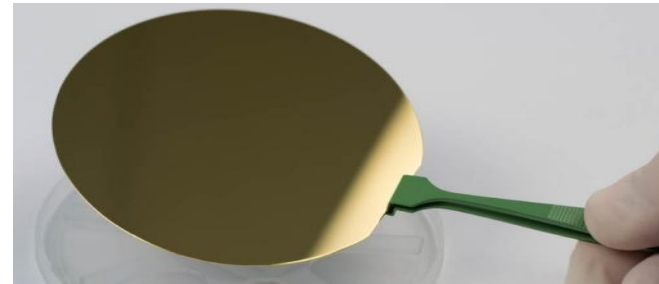
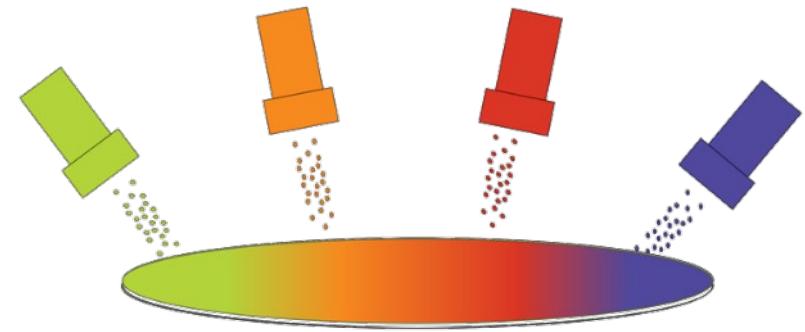


X-ray Absorption Fine Structure, XAFS

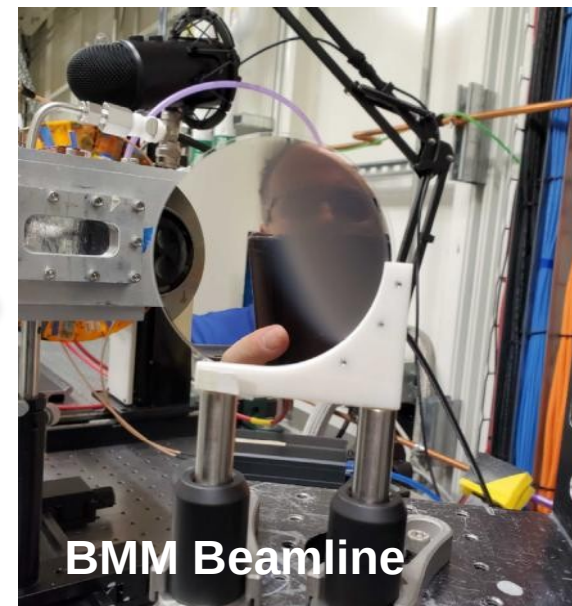
- Specific chemistry information
- Precise details of short-range chemical species (nearest neighbors)
- No long-range structure information

Combinatorial Materials

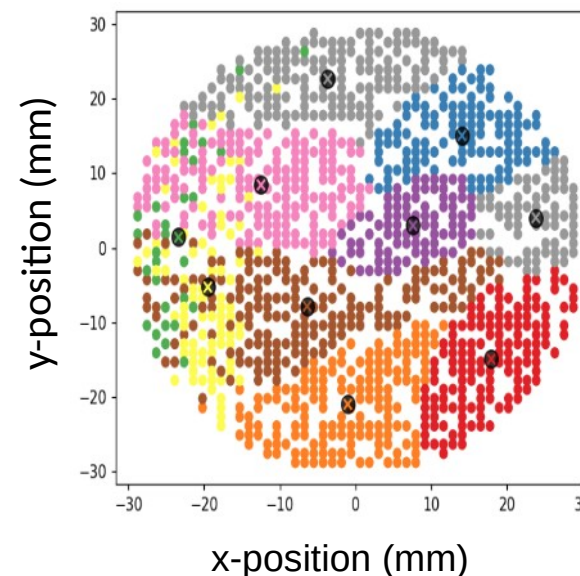
- Many new materials are studied in **combinatorial compositions prepared simultaneously on wafers** resulting in a spatial variation of composition, structure, phases and mixtures of phases.
- To fully characterize a wafer with XRD and XAFS:
 - Total number of measurements: \approx **18,000**
(Given by the X-ray spot size)
 - XRD at PDF beamline:** \approx 10 s / each
Time to measure fully: **2 days**
 - XAFS at BMM beamline:** \approx 10 min. / each:
Time to measure fully: **4 months**
- Enter AI/ML: Autonomously and simultaneously drive two beamlines** measuring two identical samples while continuously **leveraging all information possible**.



AI-Driven, Realtime, Multimodal Experiments

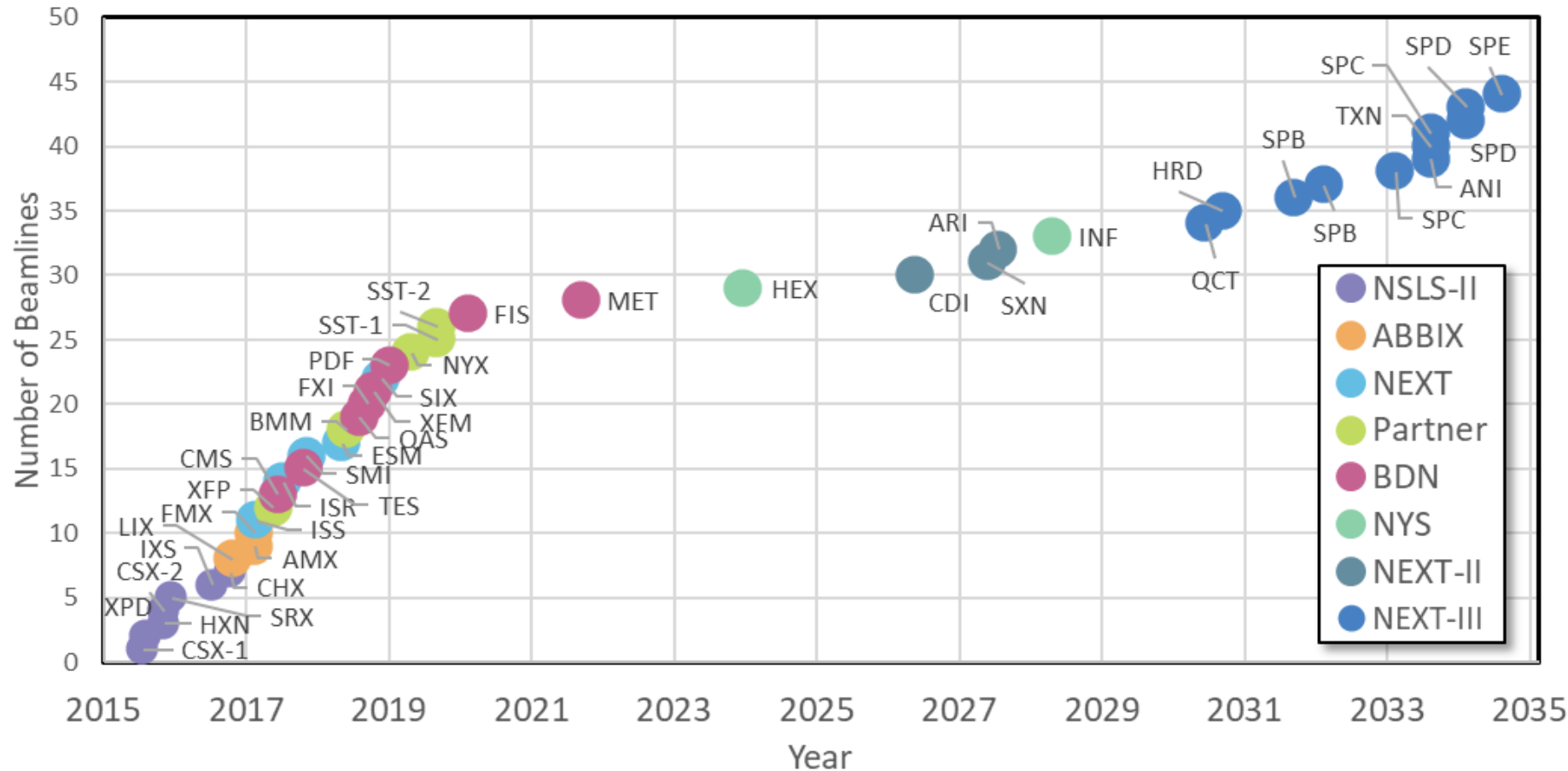


- The **AI agent** chooses the **next XRD experiment (fast)** at the PDF beamline based on **all previous XRD and XAFS data** and **maximum variation/uncertainty**.
- The AI agent dictates the **next XAFS experiments (slow)** at the BMM beamline for further characterization the identified regions of interest.
- **This approach allowed identifying areas with distinct materials characteristics in 8 hours.**



NEXT-III Project Schedule (Notional)

Beamlines in Service by Project and General User Start Date



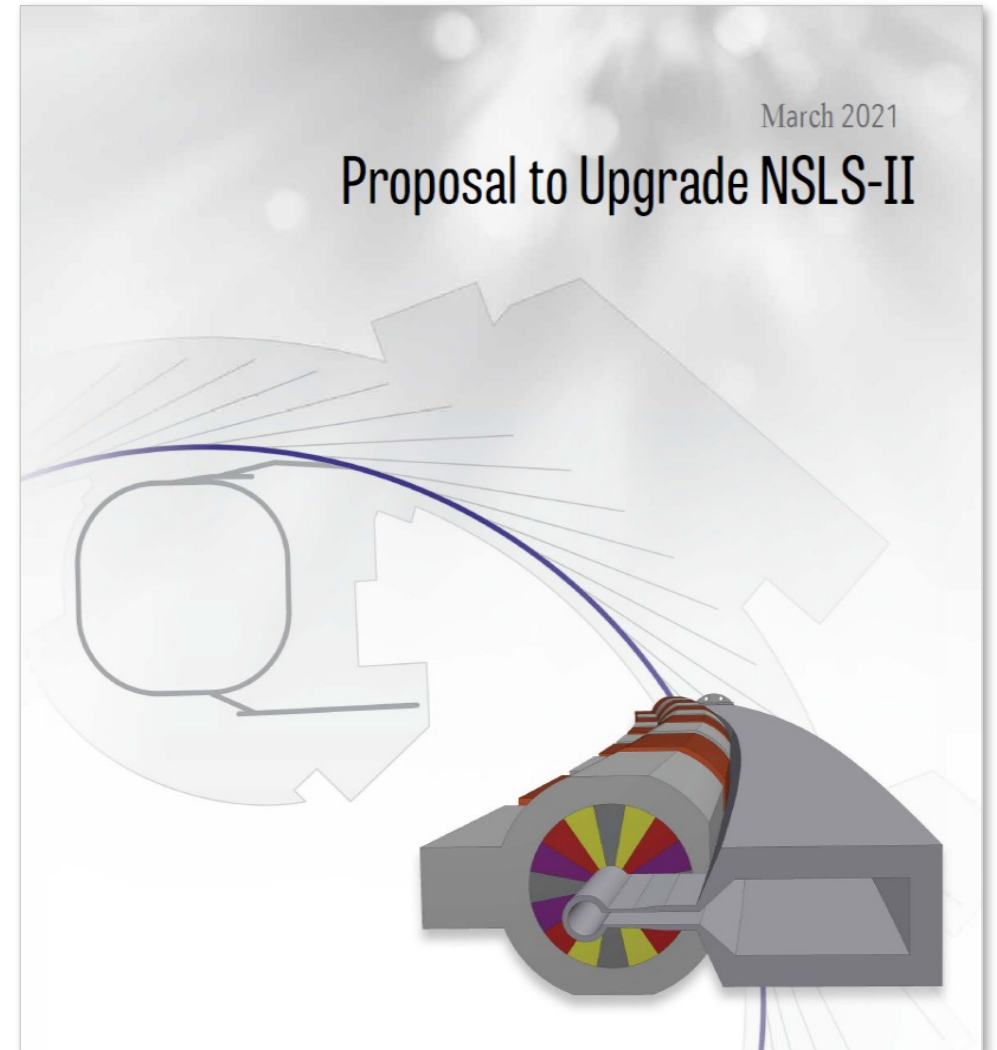
- NEXT-III beamlines will be identified over the course of the project in collaboration with the user community.
- NEXT-III beamlines will be designed to **take advantage of AI/ML** from the start.

NSLS-IIU: The world-leading multimodal source

Future science requires a light source

- Equipped with a **portfolio of world class scattering, imaging, and spectroscopy beamlines optimized for multimodal experiments**
- Providing **highest brightness between 1 keV and 10 keV** as well as **high brightness in the extended soft and hard x-ray range.**
- Providing **advanced data handling, processing and analysis capabilities** so that user take home results, not “just” data.

To address future science needs we proposed the NSLS-II upgrade project, NSLS-IIU.



NSLS-IIU: The “whole-facility” upgrade

Source

>10x improvement in number of useful photons generated at the source by reducing beam emittance, increase electron energy, and further optimize insertion devices

Optics

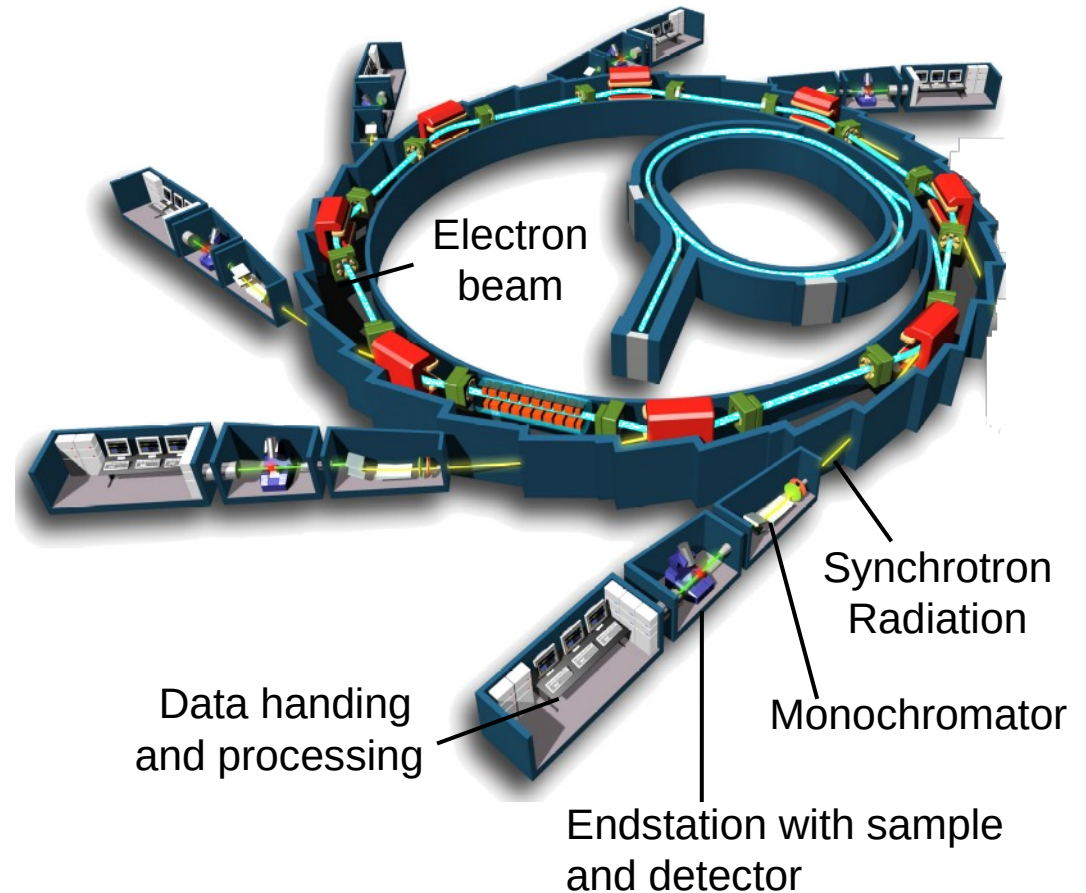
Improve efficiency of transmitting useful photons from the source to sample and maintain coherent wavefront

Detection of photon/secondary particles samples

Increase detection efficiency by optimizing solid angle coverage, frame rate as well as spatial, time, and energy resolution

Data handing and processing:

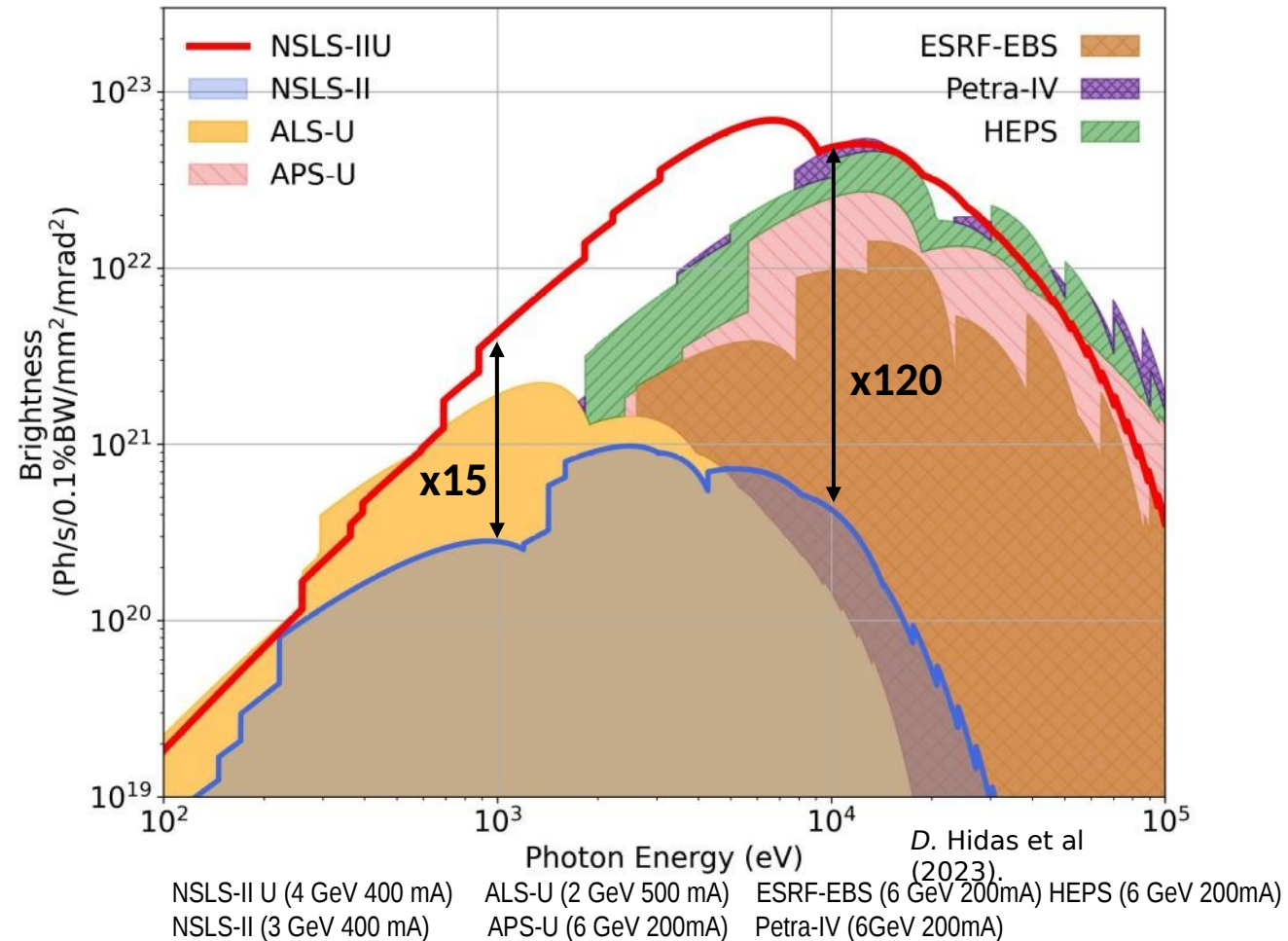
>10x reduction in time from data acquisition to results through optimized analysis workflows and AI/ML




NSLS-IIU: The world-leading multimodal source

The NSLS-IIU storage ring design will deliver an **internationally competitive light source**:

- **Lattice design** optimized for world-leading brightness in the 1-10 keV range and competitive in the soft and hard X-ray ranges.
- The **draft schedule** projects first light to users 8 years after CD-0.
- **Beamlines developed and constructed through NEXT-III** will be optimized to take full advantage of the increased brightness. Additional flagship beamlines will be constructed through NSLS-IIU.
- Beamlines will be designed to take **advantage of AI/ML from the start**.





National Synchrotron Light Source-II, NSLS-II

*10 years shining light on the world's most challenging
science problems and a bright future ahead.*



NSLS-II
FIRST LIGHT
10TH ANNIVERSARY

CELEBRATING 10 YEARS SINCE FIRST LIGHT