Diamond Light Source:
Update on Facility and Diamond-II

Gianluigi Botton

on behalf of all Diamond Staff

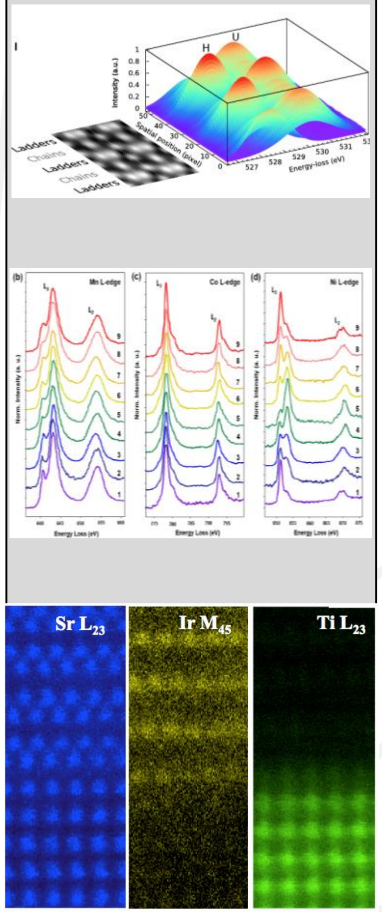
diamond

Outline

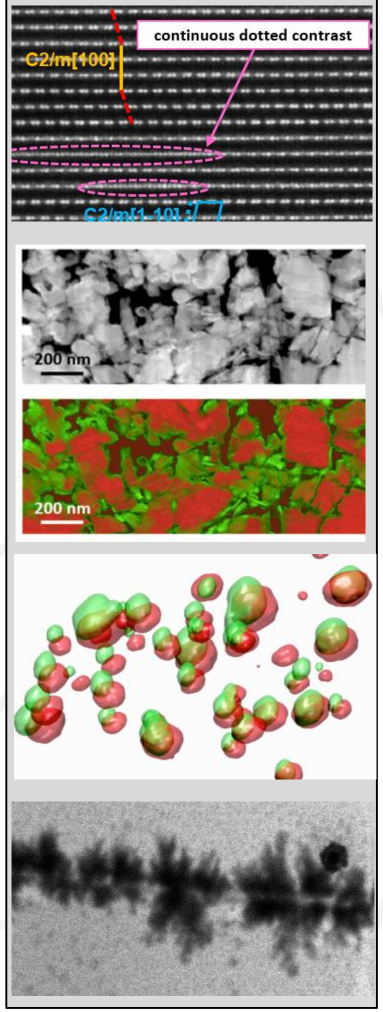
- Some updates on the Diamond facility
- Science/technical Case for Diamond-II
- Updates on the project

Some areas of my research

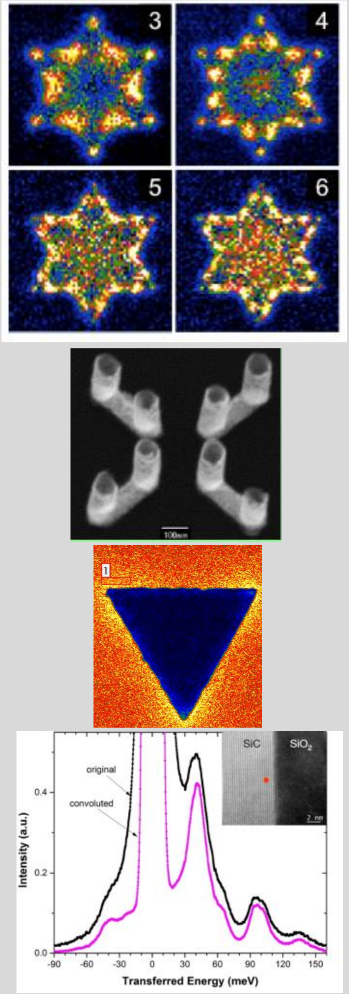
Functional Oxides



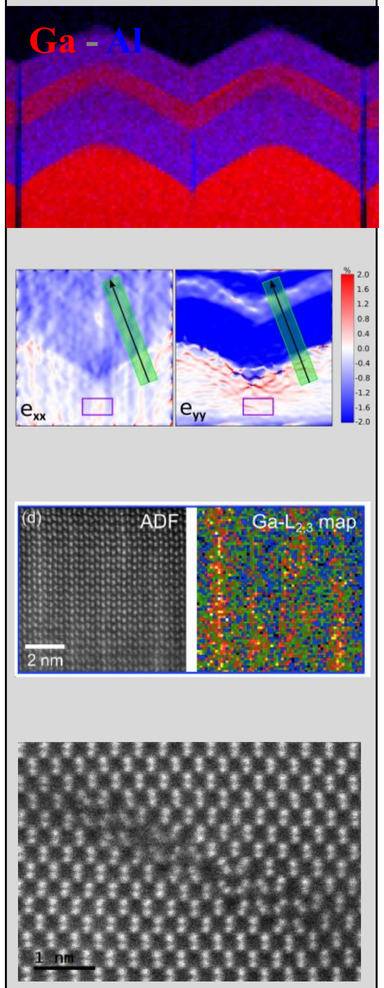
Energy Materials



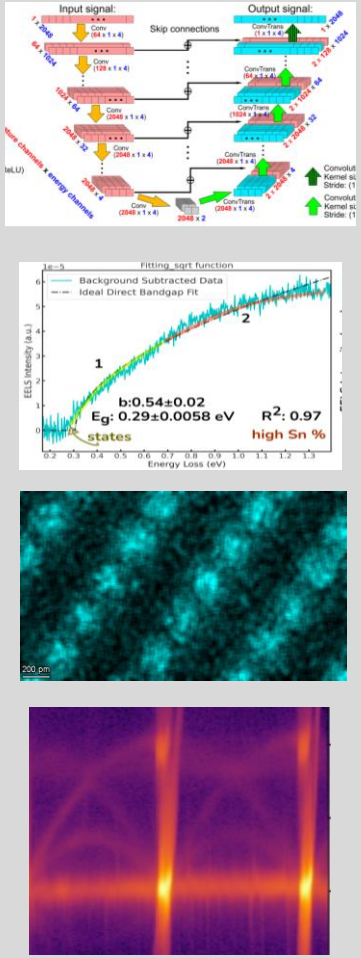
Plasmons/Phonons



Semiconductors



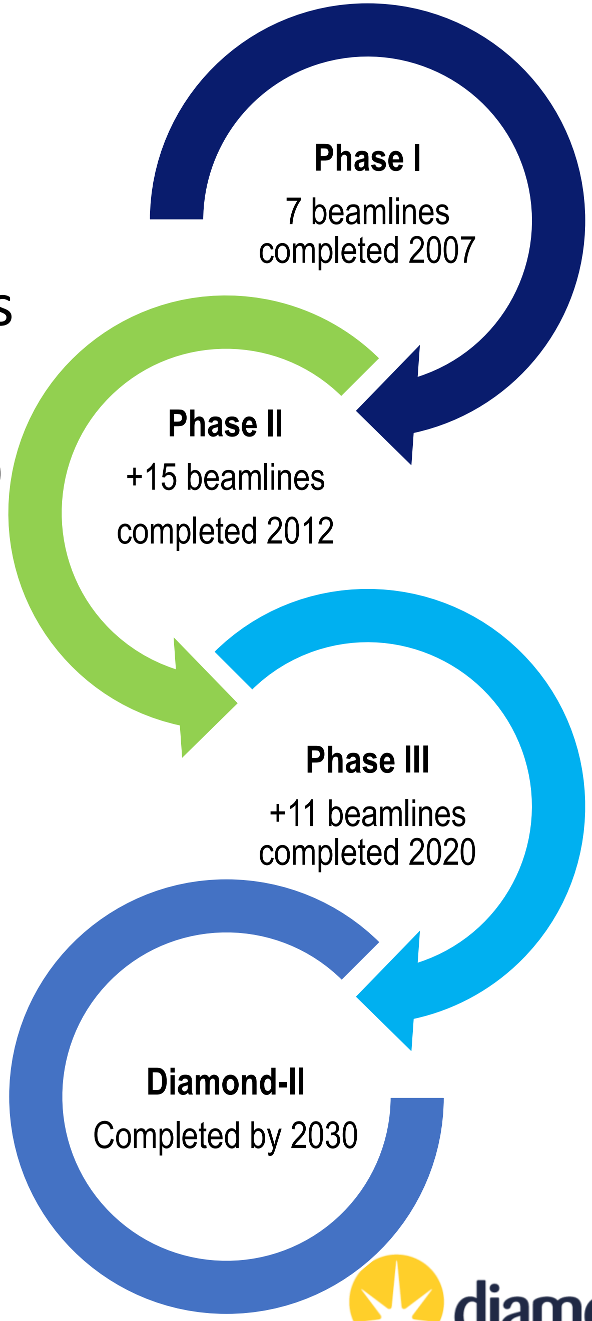
Recent work



Not just pretty pictures

Overview

- Largest scientific facility to be built in the UK over last 40 years
- Diamond is a private – not for profit – company, formed as a joint venture between UKRI's STFC (86%) and Wellcome (14%)
- 14,000 interested researchers with over 750 staff on the ground +140 more on Diamond-II and grants
- Located on the Harwell Campus, Oxfordshire
  - ✓£2+bn infrastructure
  - ✓250 organisations
  - ✓6,000 people
  - ✓710 acres

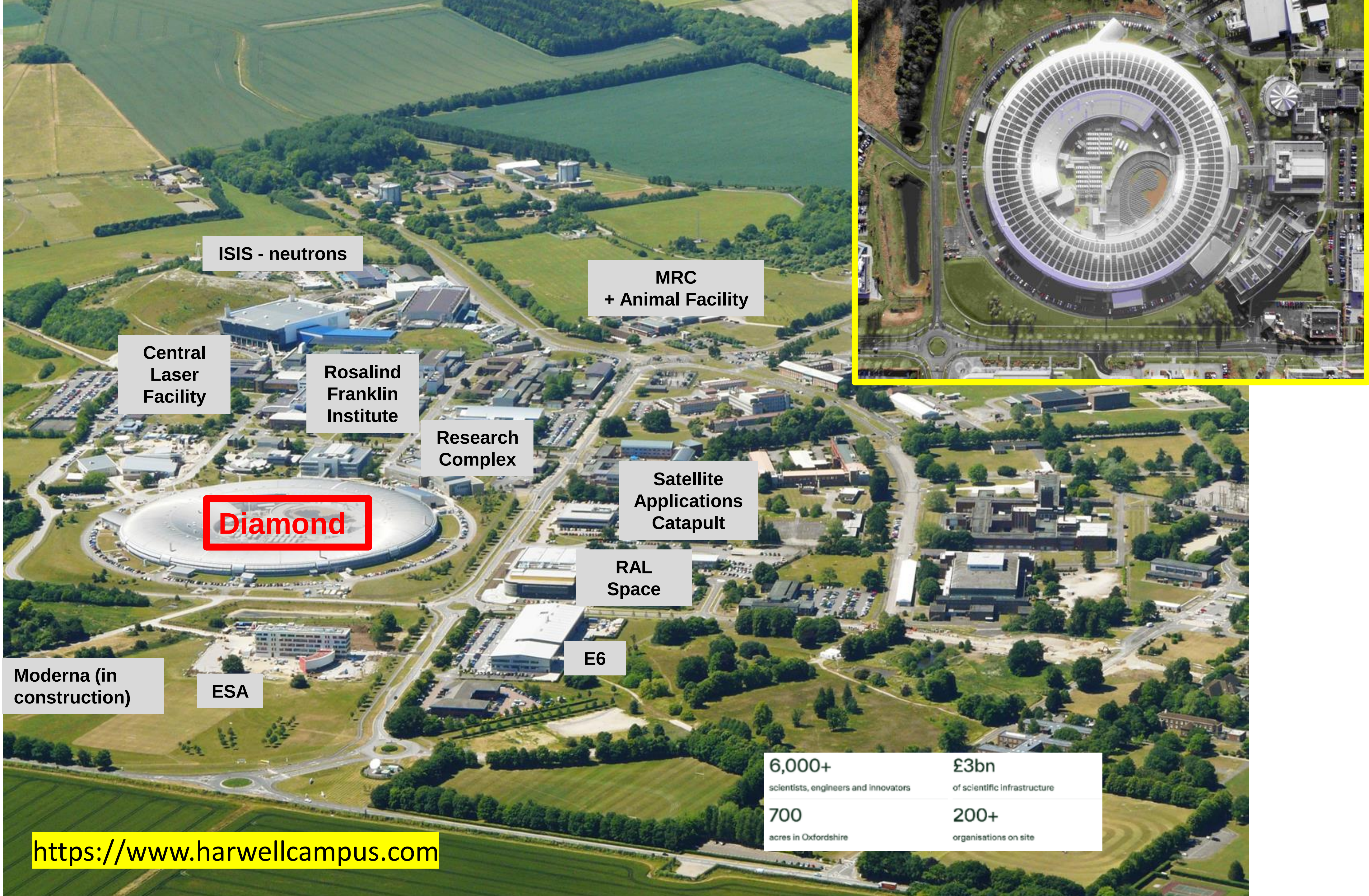


UKRI Science and Technology Facilities Council

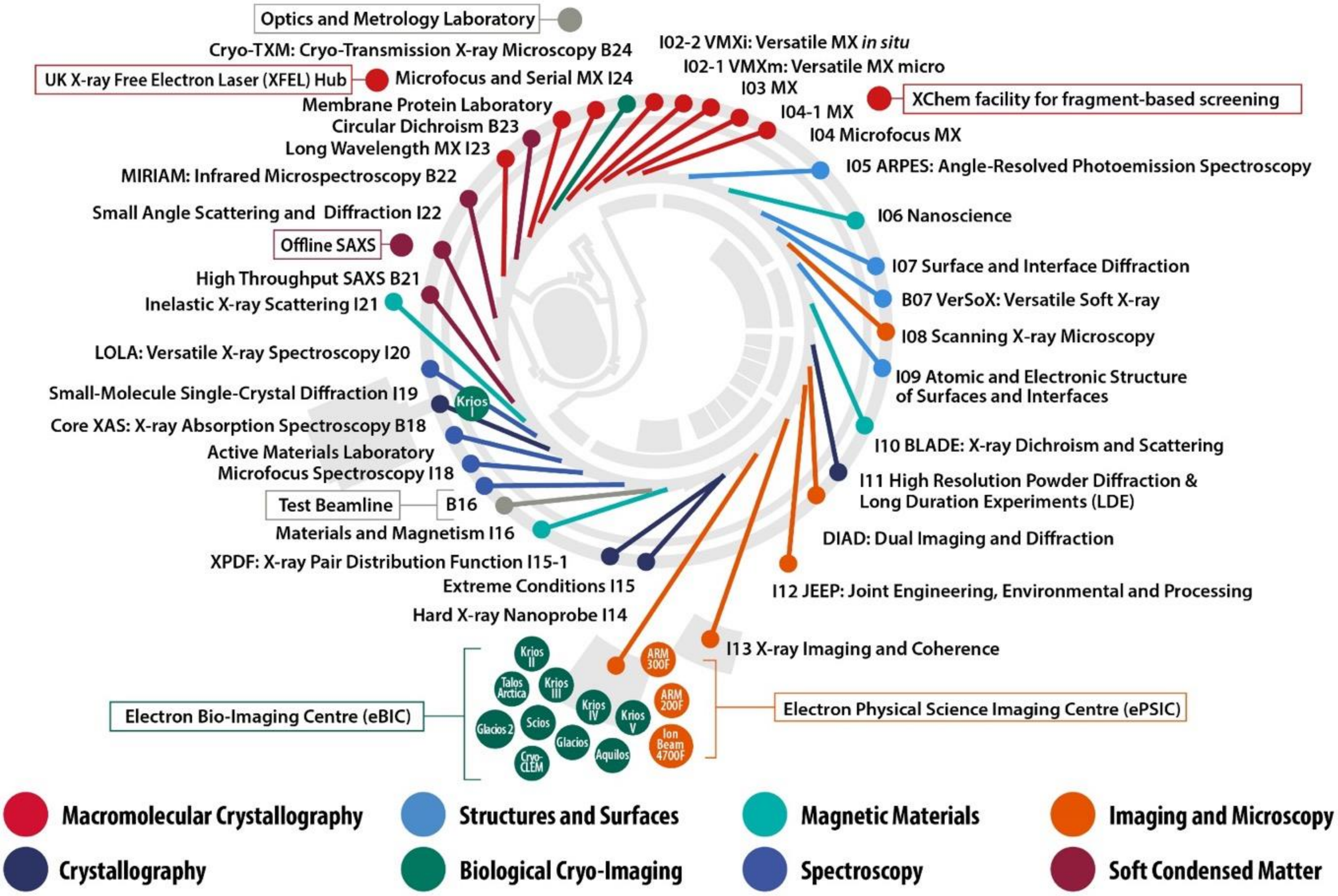
wellcome

All areas of science covered except military and tobacco research

diamond


ISIS - neutrons
MRC
+ Animal Facility
Central
Laser
Facility
Rosalind
Franklin
Institute
Research
Complex
Satellite
Applications
Catapult
Diamond
RAL
Space
E6
Moderna (in
construction)
ESA
6,000+
scientists, engineers and innovators
£3bn
of scientific infrastructure
700
acres in Oxfordshire
200+
organisations on site
https://www.harwellcampus.com

Instruments/beamlines



+Protein Membrane Laboratory, Crystallization Facility @ RCaH Active Materials Laboratory. Optics fabrication facility

34 Beamlines, + suite of EMs

Microscope	Main Capabilities
Titan Krios I	Cryo-EM, Cryo-ET
Titan Krios II	Cryo-EM, Cryo-ET
Titan Krios III	Cryo-EM, Cryo-ET
Titan Krios IV	Cryo-EM, Cryo-ET
Titan Krios V (Industrial)	Cryo-EM, Cryo-ET
Glacios (Industrial)	Cryo-EM, Cryo-ET
Aquilos 2	Cryo-SEM, Cryo-FIB
Leica cryo-CLEM	Cryo-CLEM
JEOL ARM200F	Atomic scale STEM imaging, EELS, EDX, electron diffraction
JEOL ARM300F	Atomic scale TEM and STEM imaging, electron diffraction, 4D-STEM, EDX
JEOL Ion Beam 4700F	SEM, FIB
Helios PFIB	HR-SEM + Plasma FIB

An enabling facility

Supporting 13 of the 17 SDG

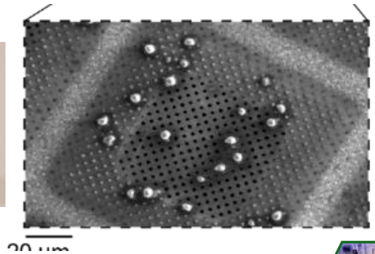
diamond

Some highlights

And recently completed capabilities

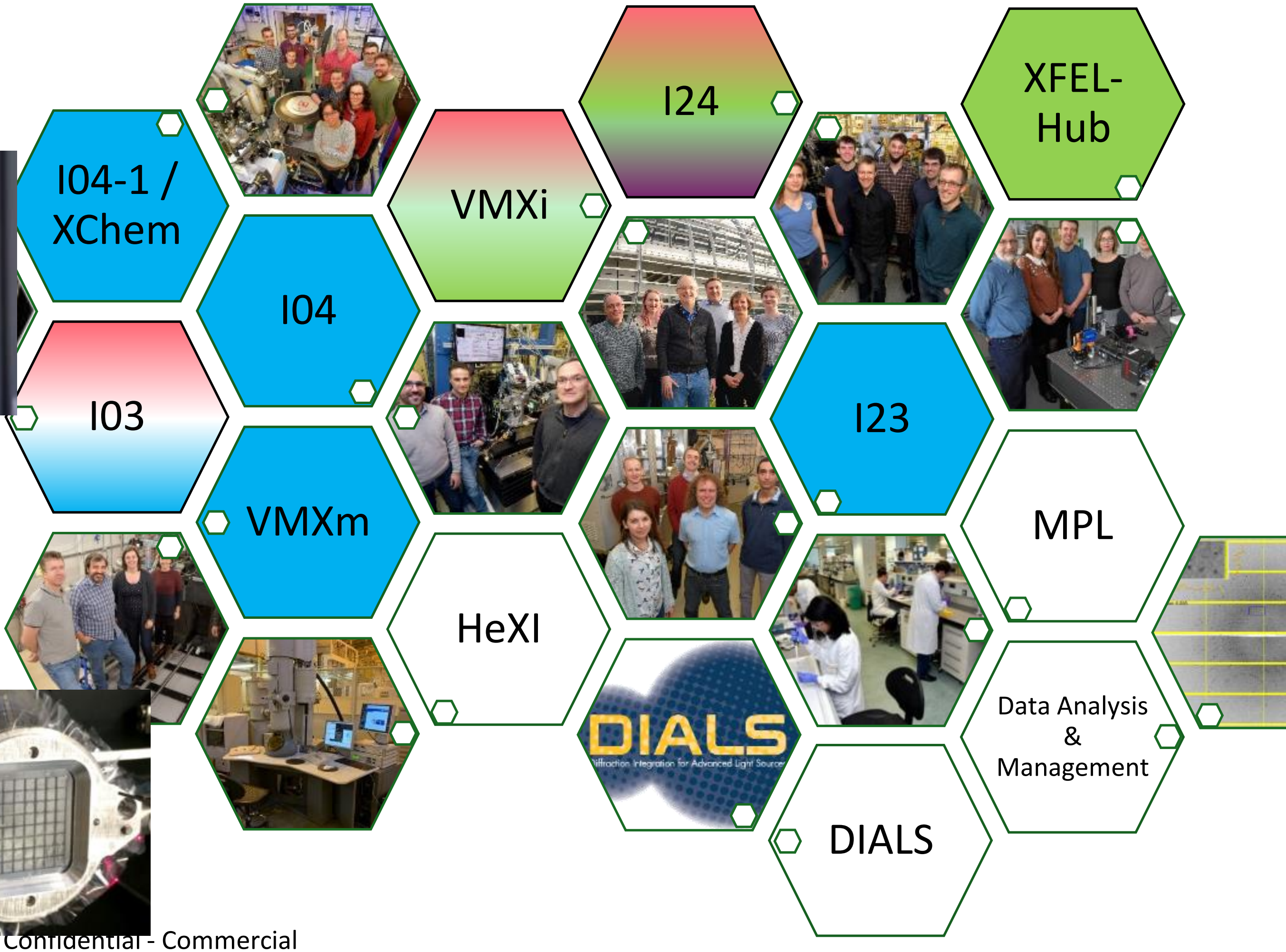
Cryo, Room Temperature & Serial Synchrotron Xtallography

- Cryo
  - standard SPINE pins
  - I23 specific holders
  - VMXm – EM grids



- Room temperature *in-situ*:
  - VMXi dedicated beamline
  - I03 for biological containment

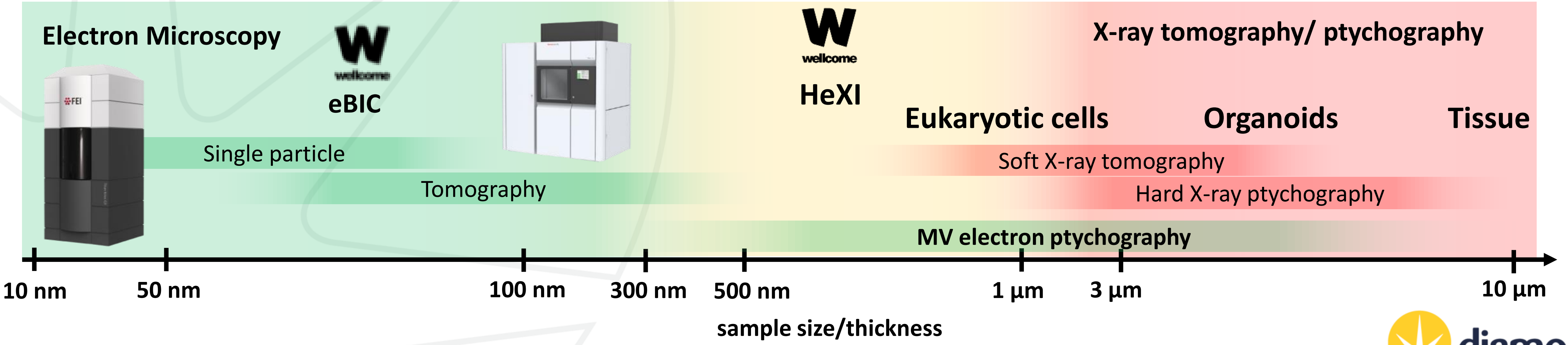
- SSX at I24, VMXi and XFEL Hub
  - Fixed targets
  - Thin films
  - Extruders
  - Acoustic drop ejection
  - Tape drives (in dev)



The new frontier

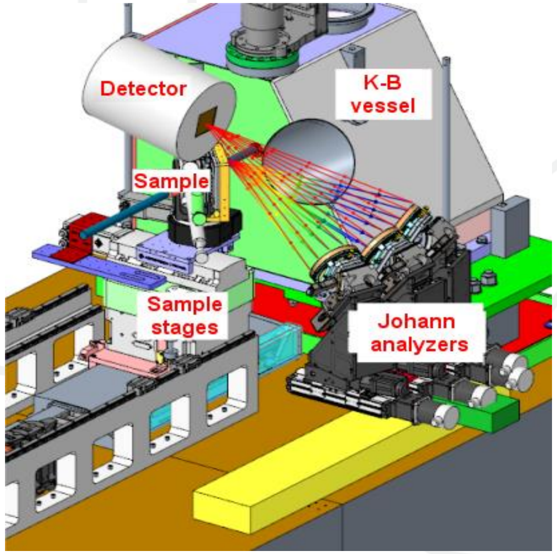
- Bridging single particle + MX structural biology with cell biology / tissues.

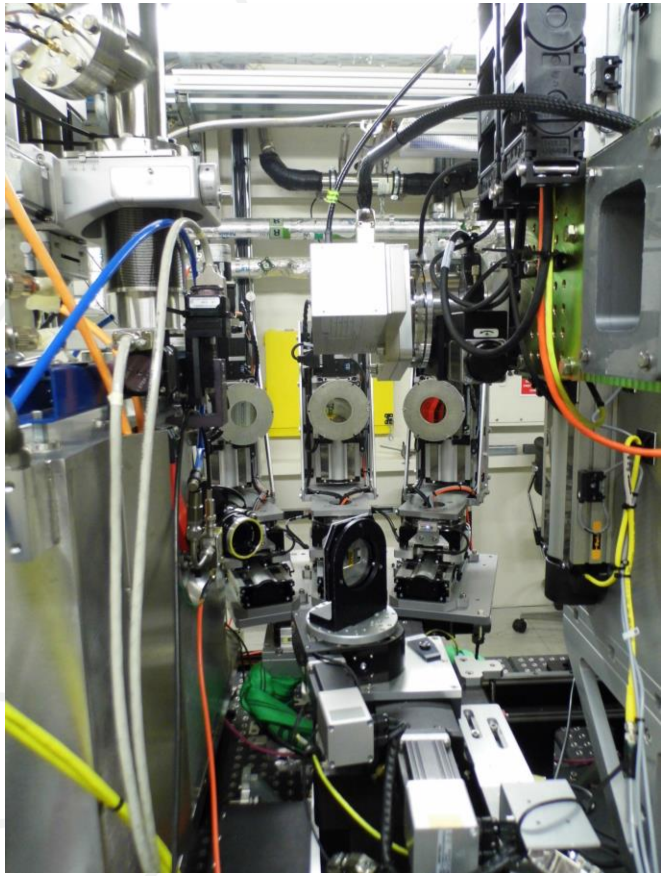
- – strong role for hard X-rays
  – multi-disciplinary, correlative, collaborative, eg Diamond / Rosalind Franklin Institute

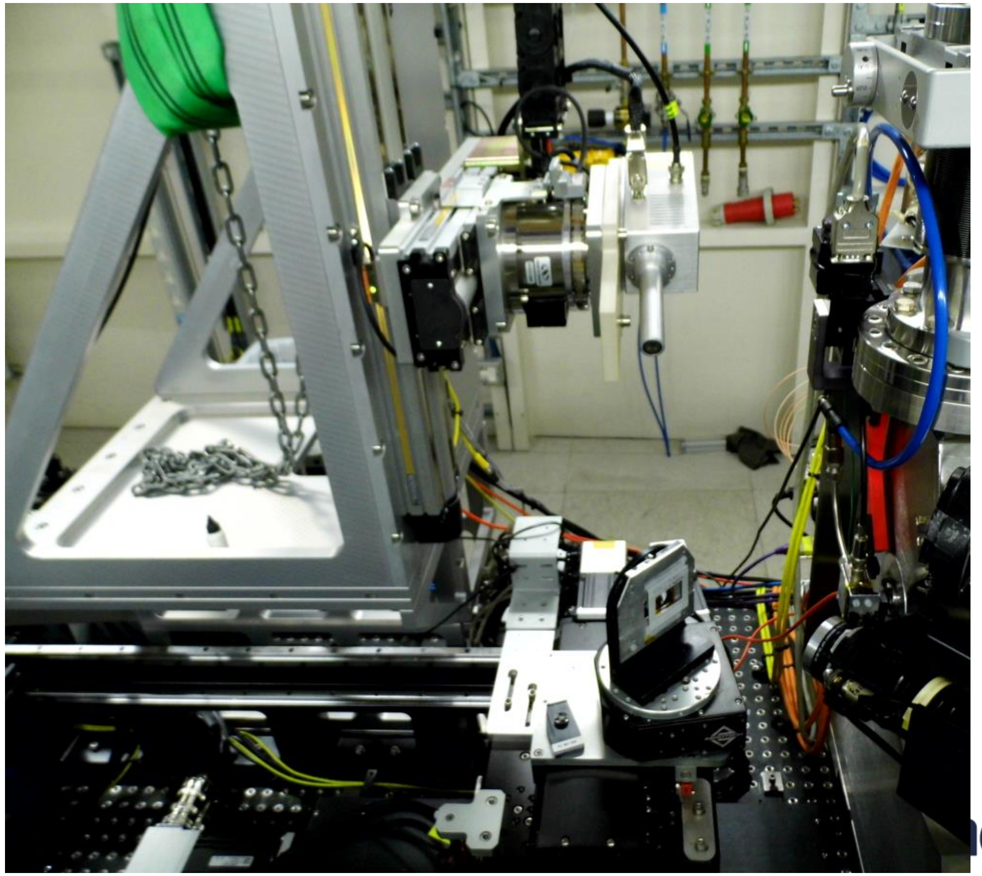


Recent new features: XES Spectrometer on I18

This spectrometer expand the capabilities of the Spectroscopy group in photon-in/photon-out spectroscopy to the tender X-ray regime. It will also enable spatially resolved XES measurements, taking advantage of the small beam available in I18. The spectrometer is a modular system, formed by three-crystal analyzers in a 0.5m Rowland circle geometry, working in the vertical plane following the Johann configuration.

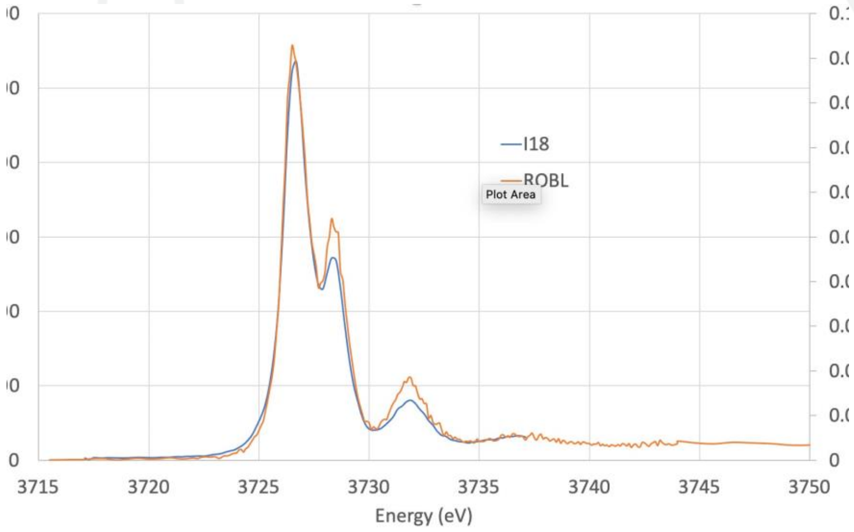




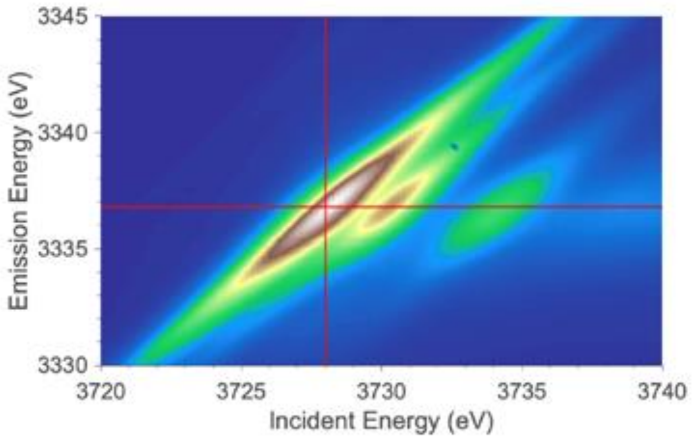


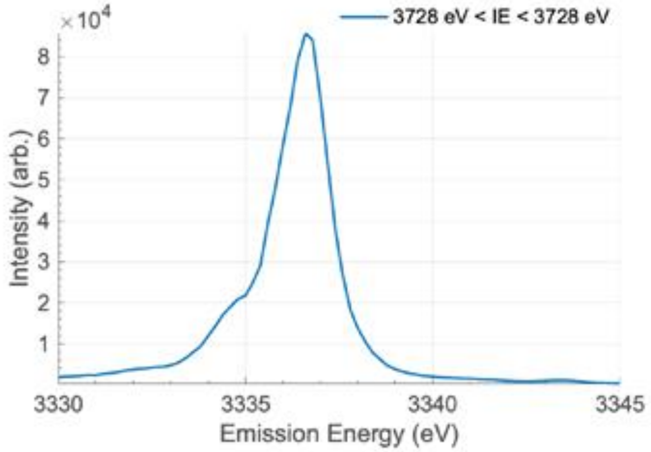
Recent new features: XES Spectrometer on I18

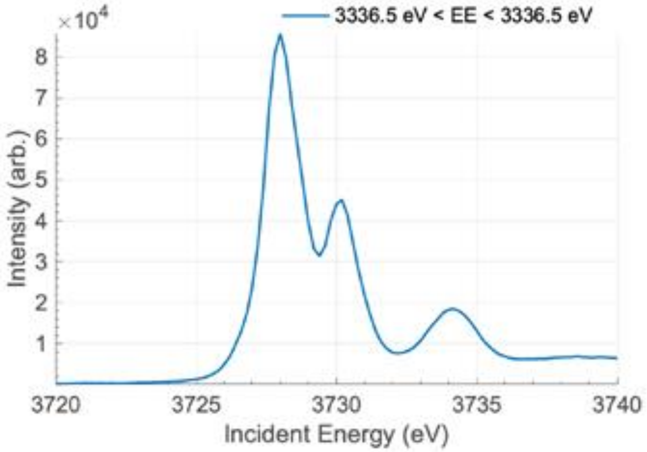
First experiment with users scheduled on the 18th of January.
The sample measured was grimselite, an uranium containing mineral. They measured the M4 absorption edge (3d3/2 to 5f5/2) recording the Mb emission line (4f5/2 to 3d3/2).



Comparison of the HERFD-XANES spectra on grimselite measured in I18 (blue line – three analyzer crystals) and the ROBL beamline at the ESRF (orange line – one analyzer crystal).



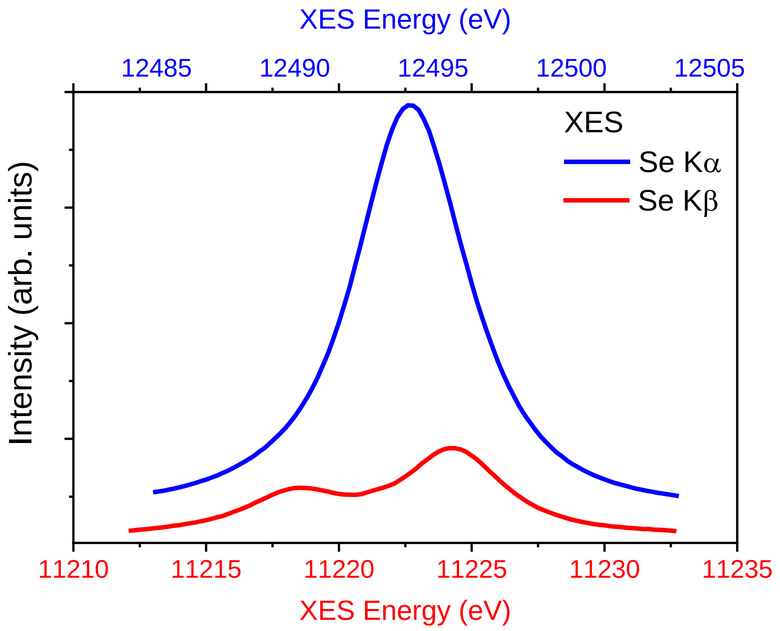


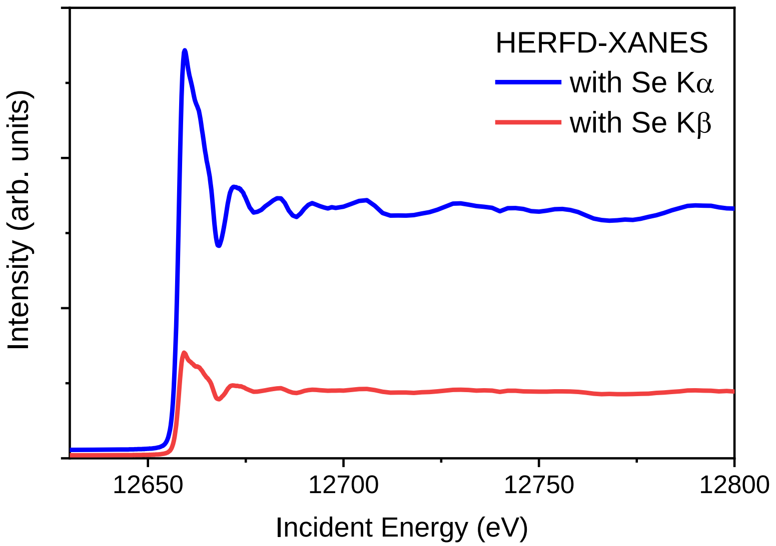


RXES map for the grimselite sample. The horizontal cut corresponds to the HERFD-XANES spectrum, while the vertical cut is the emission spectrum.

I20-Scanning; XES end-station

- New fourteen spectrometer was successfully installed and commissioned in Run 1-2023.
- 14 user experiments have been conducted, including two-colour HERFD-XANES experiments.
- On-going reliability improvements to make sure over 60 motorised axes can work seamlessly.





Example of the two-colour measurements enabled by the new spectrometer. XES and HERFD-XANES were taken simultaneously at the Se Kα and Kβ emission lines.

diamond

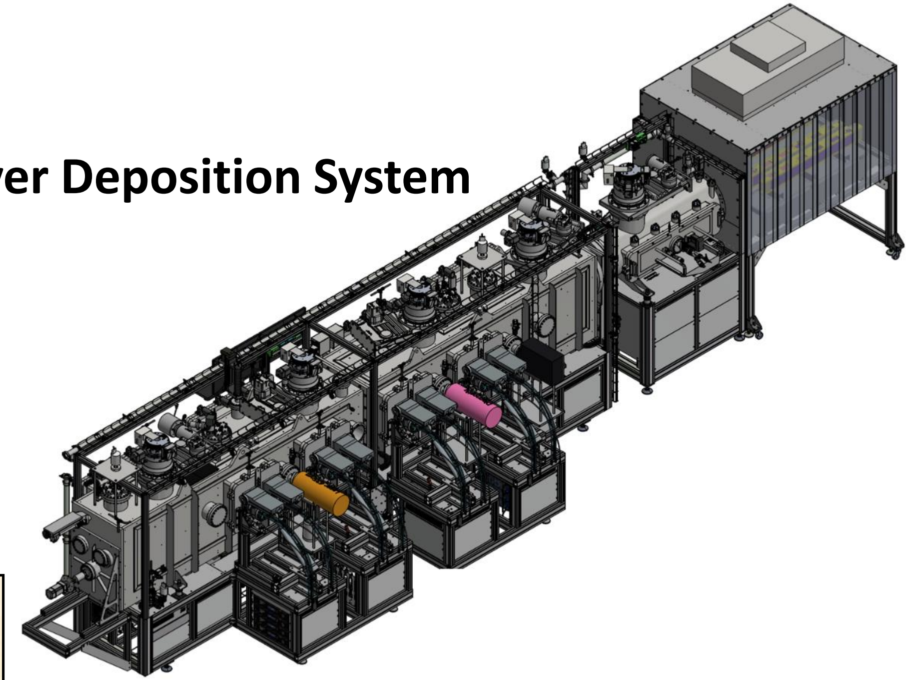
Multilayer Fabrication Facility (MFF)

- An in-house Multilayer Fabrication Facility has been setup
- Optics Fabrication building (OFB) built
- Multilayer deposition system
  - can coat up to 1m long substrates
- Several supporting instruments
  - ML characterization (XRD)
  - Roughness and stress measurements (AFM & MOS)
  - Coating removal, substrate cleaning

➢ *Will enable reliable availability of ML optics for Diamond beamlines, especially niche optics*

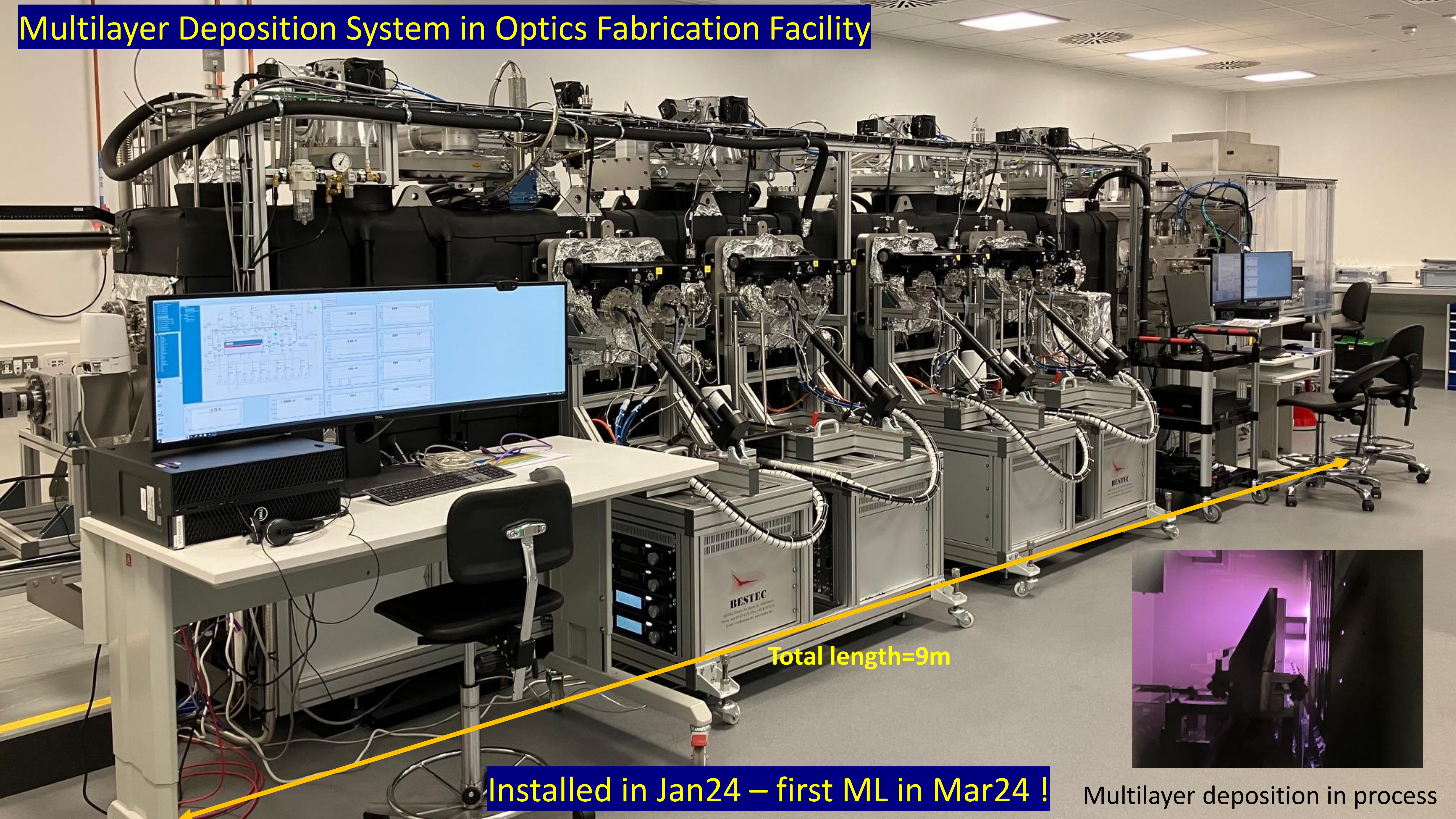
Optics Fabrication Building

Multilayer Deposition System



❖ Development of an advanced in-line multilayer deposition system at Diamond Light Source, H Wang, A Majhi, W J Tan, W Singhapong, C Morawe, K Sawhney, ***J. Synchrotron Rad.***, *31 (2024)*

Multilayer Deposition System in Optics Fabrication Facility



Multilayer deposition in process

Installed in Jan24 – first ML in Mar24 !

Ion-Beam Figuring (IBF)

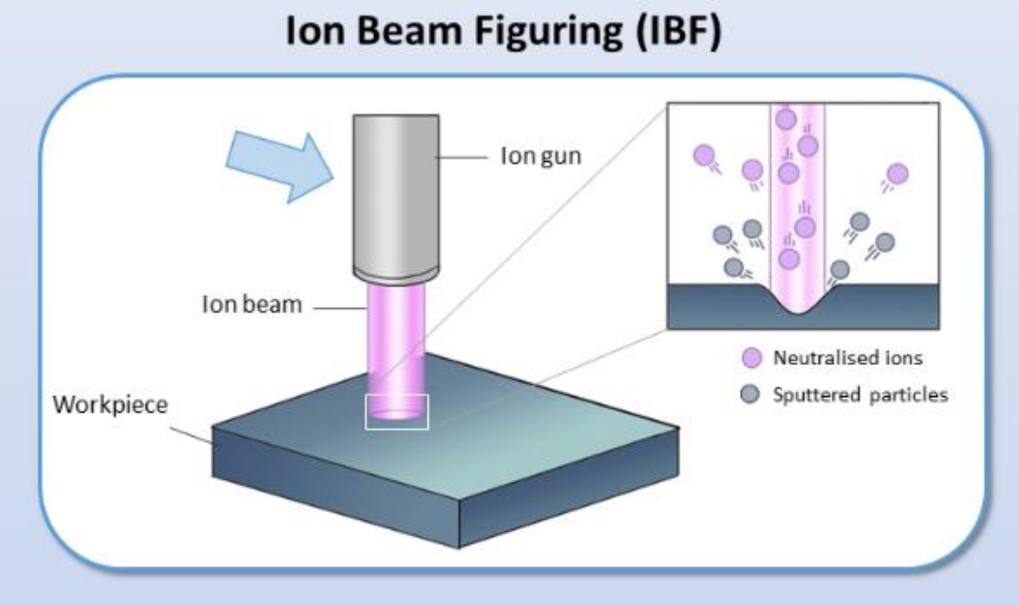
— for deterministic polishing of mirrors

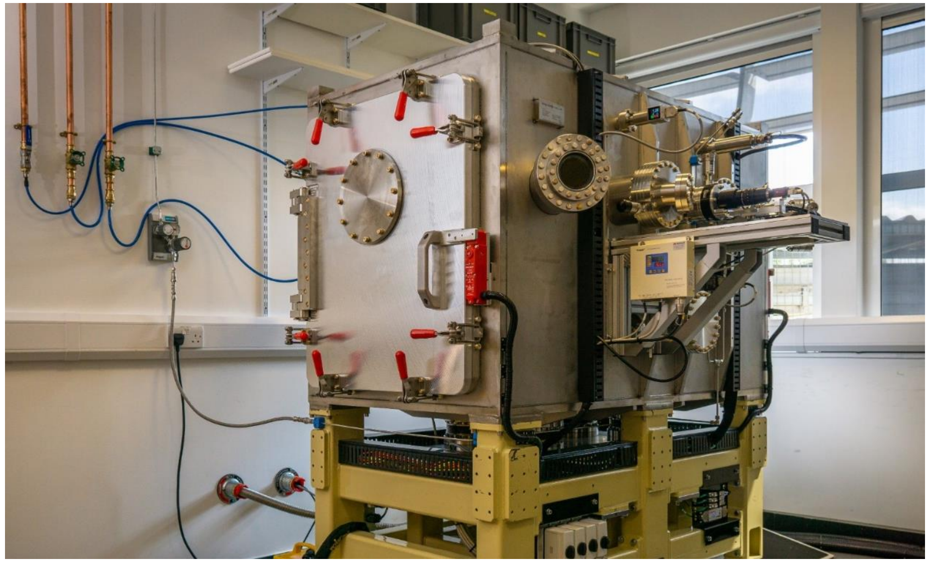
- Developed in-house at Diamond
- Uses a beam of ions to ***selectively remove*** material from a mirror surface at a rate of ~1 nm/s
- A ***high-precision technique*** for mirror shaping and figure (slope) error correction
- Creating next-generation optics and novel custom-shaped optics

- Results: height errors 1.6nm →**0.18 nm** (rms) , slope errors: 112nrad → ***29 nrad*** *rms*

Comparable / Better than the best available from industry

❖ Sub-nanometre quality X-ray mirrors created using ion beam figuring, A Majhi, R Shurvinton, PC Pradhan, M Hand, WG Gu, H Wang, K Sawhney, ***J. Synchrotron Rad.,*** *31 (2024)*



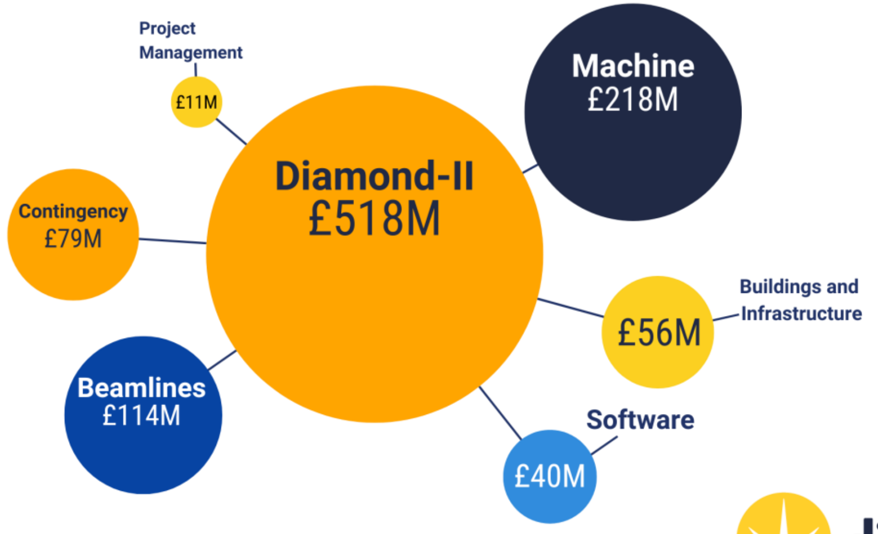


Drivers to Keep Diamond Competitive

Acknowledgements to get the project under way

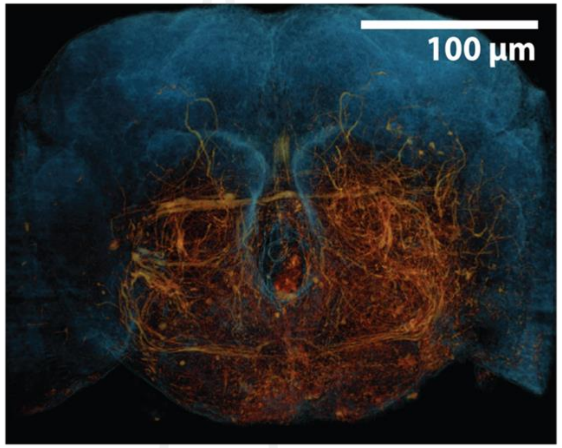
- Laurent Chapon (Science Director @ Diamond, now APS)
- Richard Walker (Technical Director)
- Andy Dent (Beamline Pillar Lead)
- Isabelle Boscaro-Clarke (Comms, Engagement, Impact)
- Andrea Ward (Finance Director)
- And all staff at Diamond

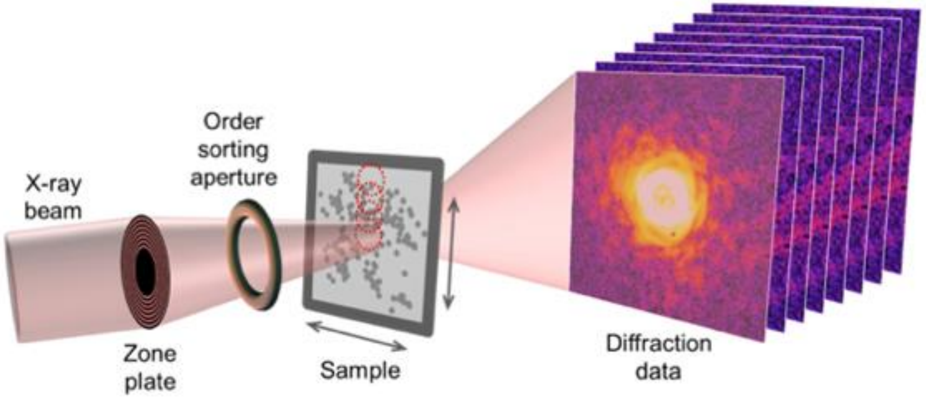
- Funding:
  - 86% from UK government
  - 14% from Wellcome Trust



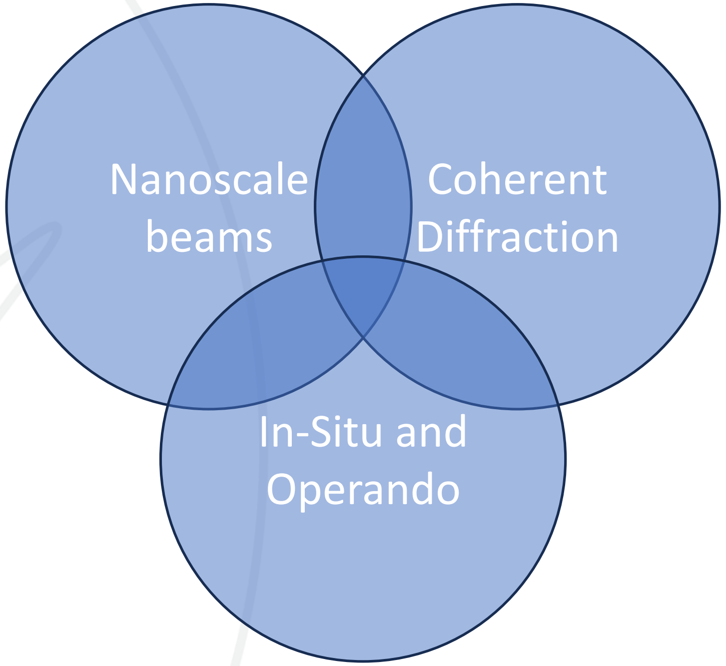
diamond

Science Drivers from Users' Community



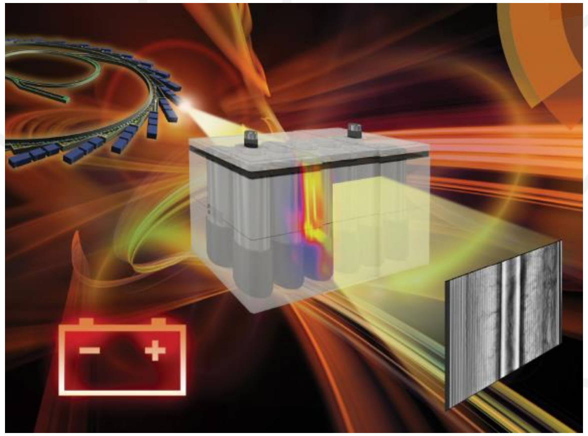


Diffraction



Imaging

Spectroscopy



More complex/heterogeneous
Materials, realistic environments

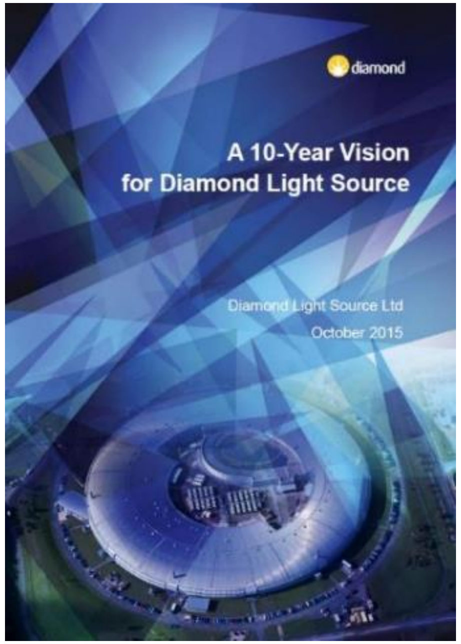
Diamond-II upgrade to machine and beamlines

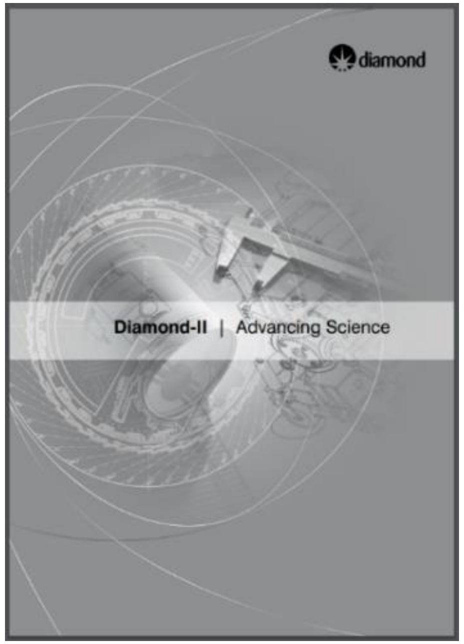
diamond

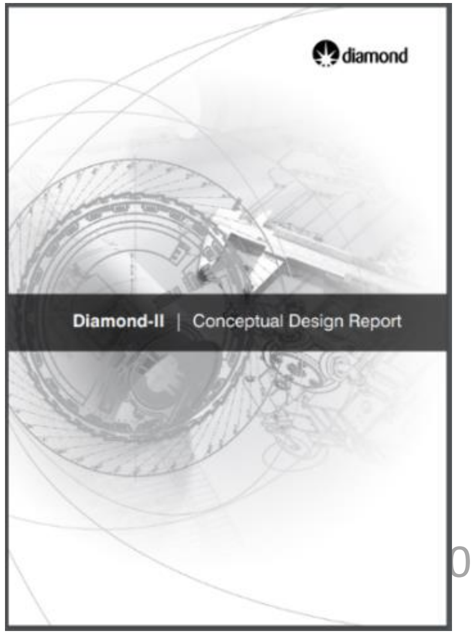
Background to Diamond-II

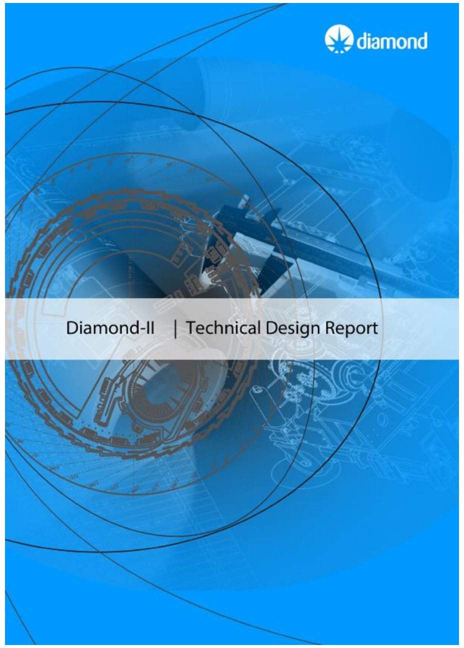
- 10-Year Vision, October 2015
  included a major upgrade: Diamond-II
- Diamond Science Advisory Committee, April 2016

  "SAC agree … that a major upgrade of DIAMOND Light Source, to achieve a source of radiation of much higher brightness, is required in order to maintain the excellence of the facility …."
- Science case endorsed by Science Advisory Committee, November 2018
- Conceptual Design Report endorsed by international review committee, April 2019
- Diamond Board approved proceeding to the Technical Design Report (TDR) phase, June 2019
- **Start of the funding application process: April 2021**
- **Confirmation of funding: July 2023**









Engagement

Diamond-II - supported by the user community

1,561 statements of support submitted

1,400 attendees across 13 community engagement webinars

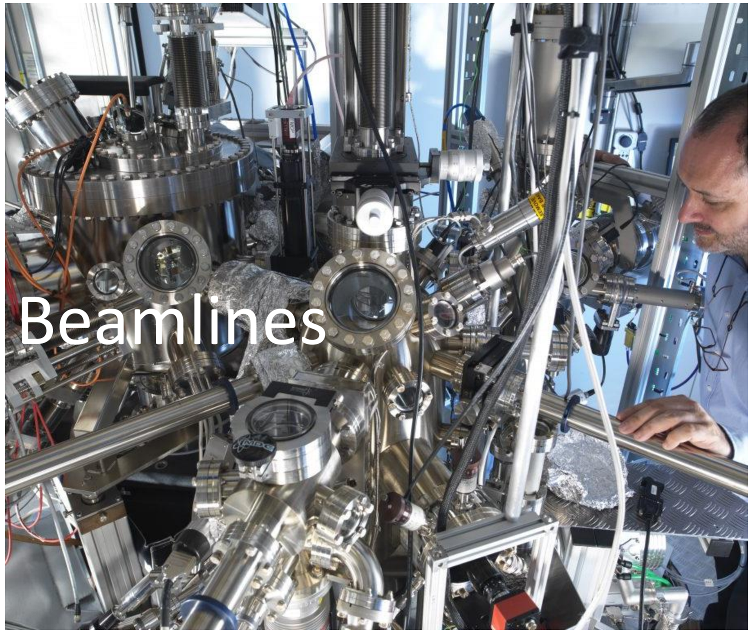
393 attendees across 7 user engagement workshops

Science Case

Conceptual Design Report

Technical Design Report

diamond



An integrated programme

transforming radically Diamond but reusing as much as possible

The Diamond-II lattice to achieve the science

160pm.rad

2.7nm.rad

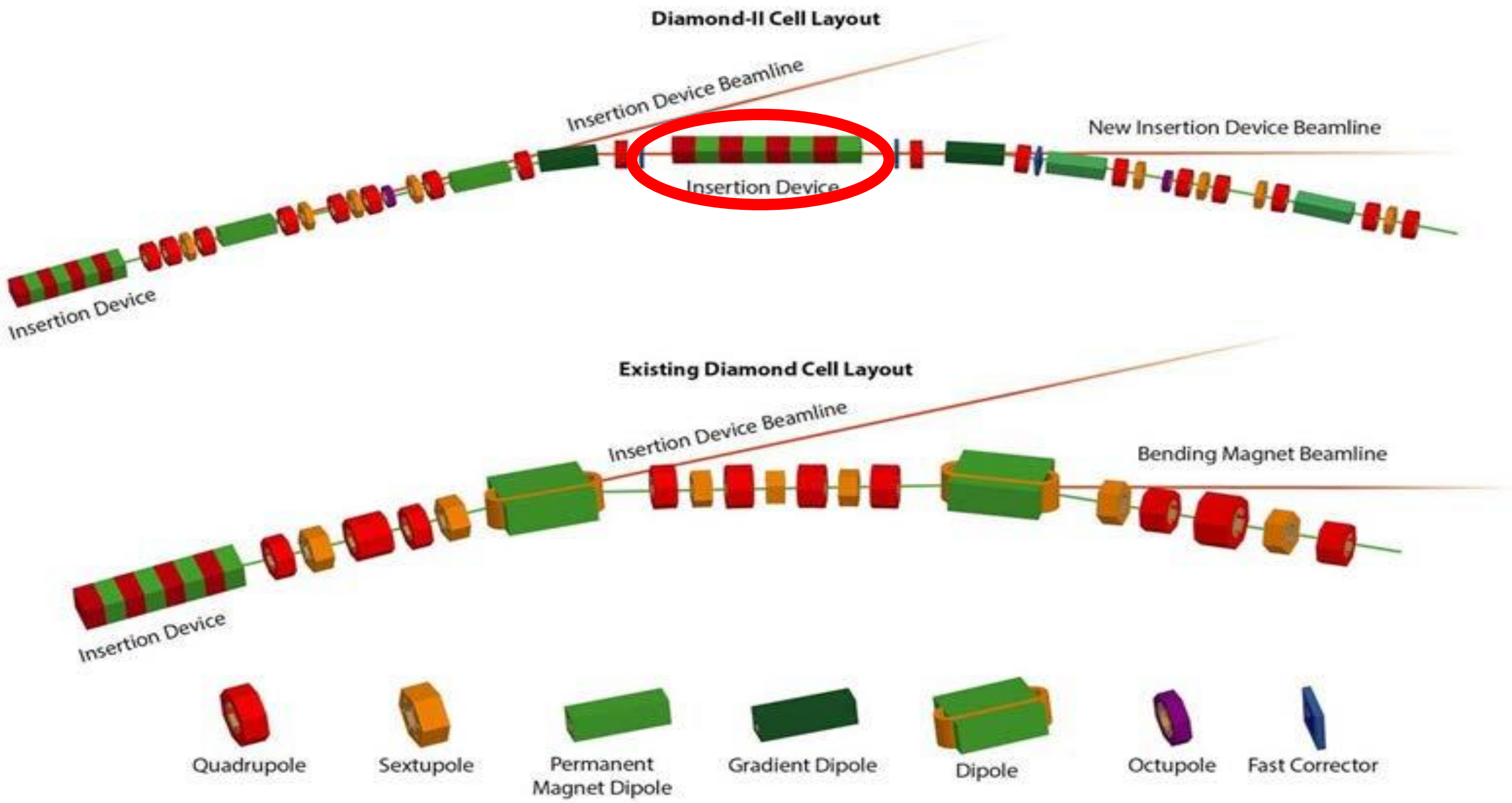


Figure 1-1 : Schematic of the current Diamond DBA (Double Bend Achromat) lattice (bottom), and the proposed design of a DTBA (Double Triple Bend Achromat) lattice for Diamond-II (top).

1) Lower emittance,
2) Increased capacity,
3) Higher energies

Go to higher energies 3.5GeV

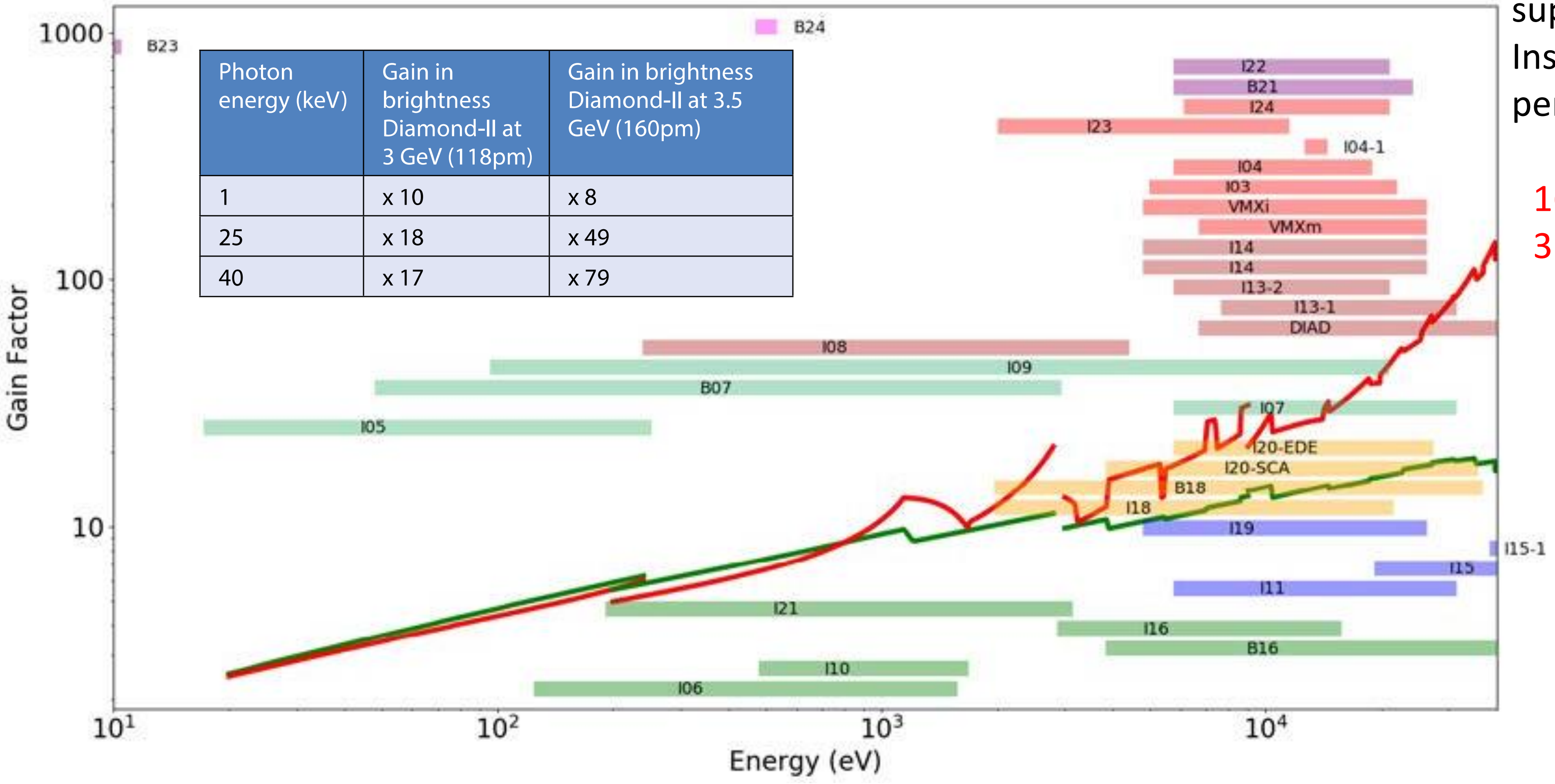
Design and changes in energy reduce the emittance by a factor of 20

One dipole replaced by 6 dipoles (modified hybrid 6BA) => lower emittance.

Diamond-II Design Goals and Main Features

❖ Increased brightness and coherence	→ low emittance MBA lattice → increase in energy from 3 GeV to 3.5 GeV
❖ Increased capacity for insertion devices	→ inclusion of ‘mid straights’ in a 6BA lattice
❖ Maintain ID source points where possible	→ adjustment of straight section lengths
❖ Minimise downtime	→ detailed planning → do what is possible before the dark period *many activities already underway*

Decisions to Achieve the Science at Diamond-II



Photon energy (keV)	Gain in brightness Diamond-II at 3 GeV (118pm)	Gain in brightness Diamond-II at 3.5 GeV (160pm)
1	x 10	x 8
25	x 18	x 49
40	x 17	x 79

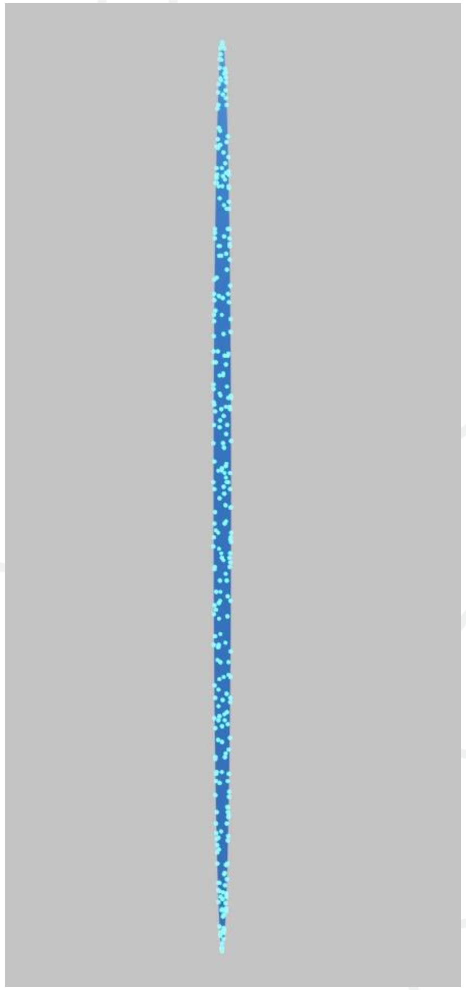
Replace current superconducting Insertion devices with permanent magnets

160 pm.rad
3.5GeV

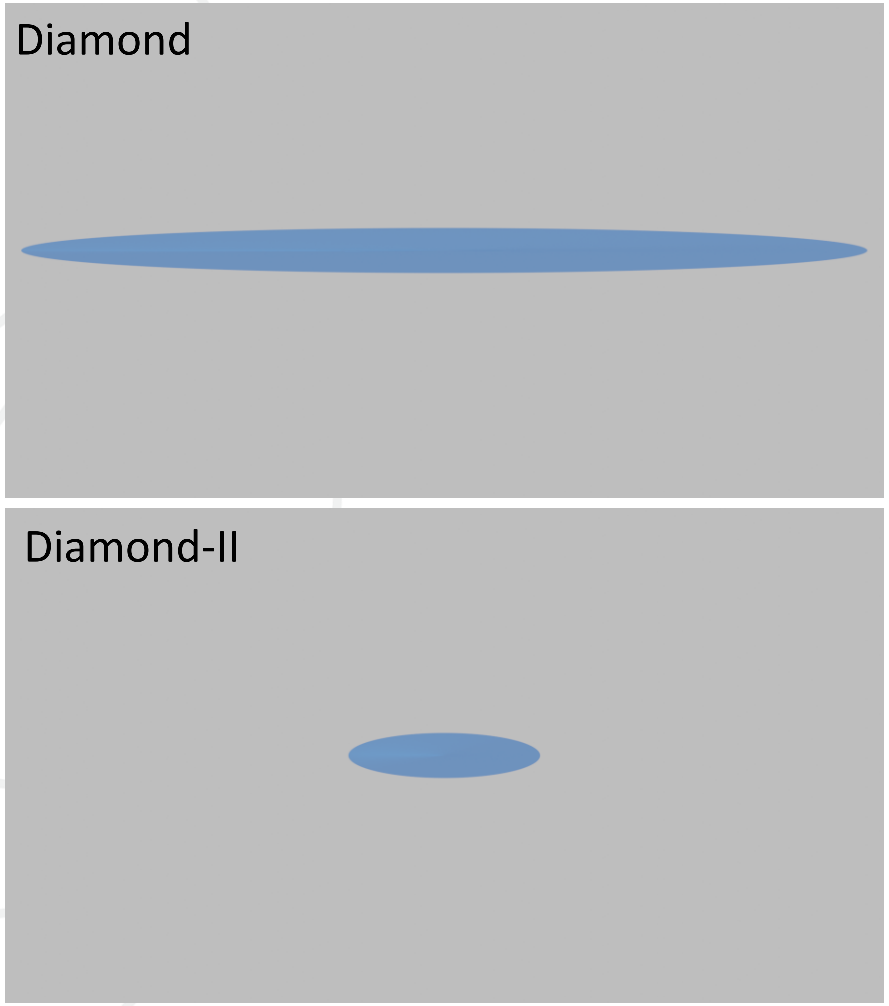
118 pm.rad
3.0GeV

‘Squeezing’ the electron beam

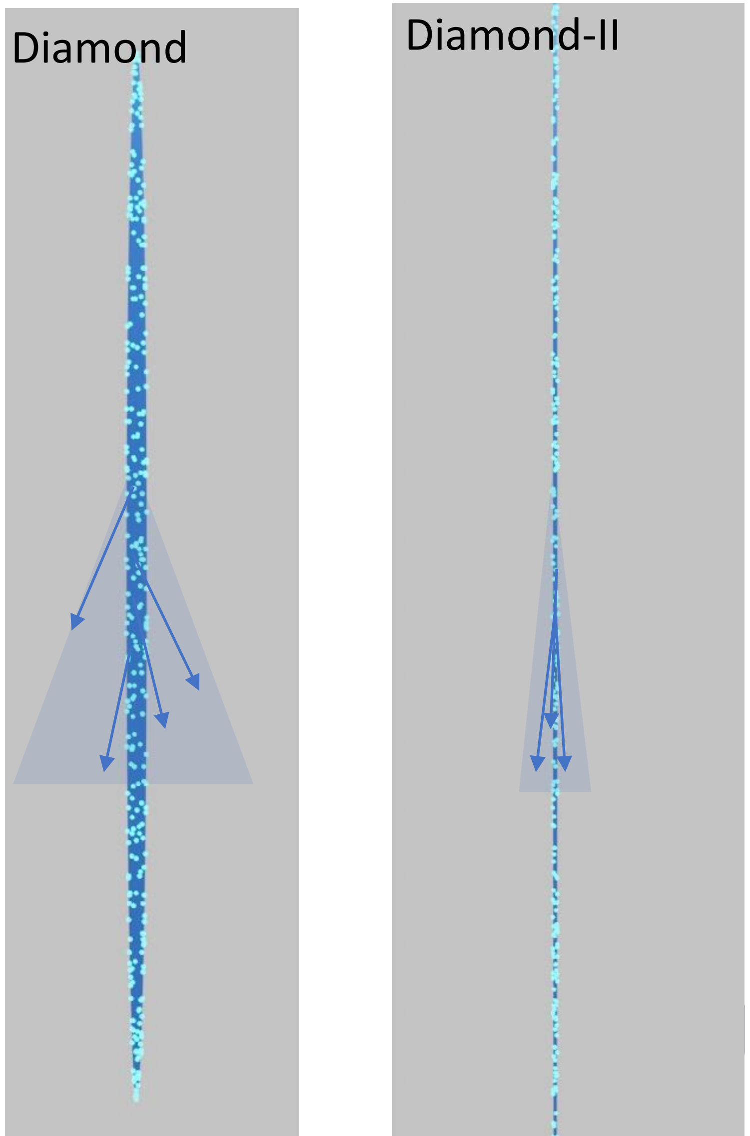
Packing a few billion electrons in a very small volume, typically 1 cm long but not much thicker than a hair



Diamond-II : compressing the lateral size of the beam by a factor ~5.



Diamond-II : the beam is also better collimated by a factor ~5



Improvements

Brightness

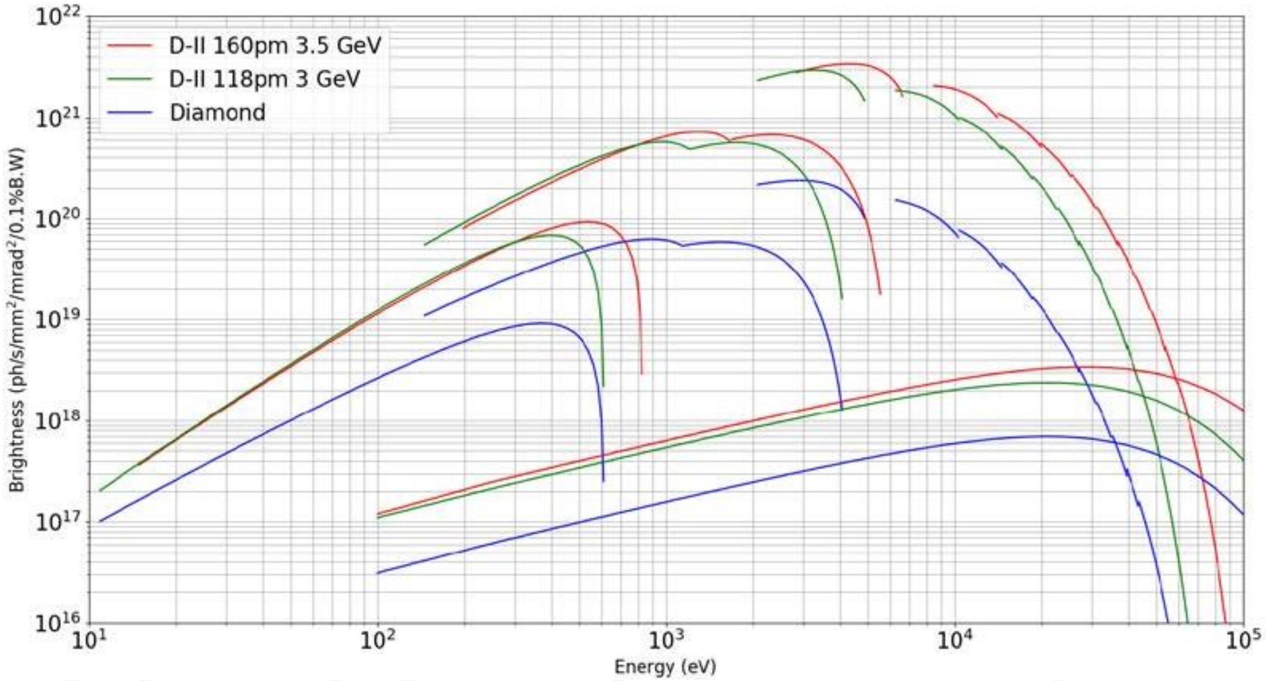


Figure 1-2 : Brightness for a set of selected sources at Diamond (blue curves), Diamond-II at 3 GeV (green curves) and Diamond-II at 3.5 GeV (red curves). In the UV regime, soft X-ray regime and hard X-ray, the brightness curves are shown respectively for the I05, I21, the future CPMU 15.6 mm period (to be installed on I11 and VMXm), and for the superconducting wiggler on I12 (JEEP). All calculations have been made with Spectra 9 using the Wigner function. A phase error of 3° for the undulators has been taken into account analytically.

Coherent Fraction

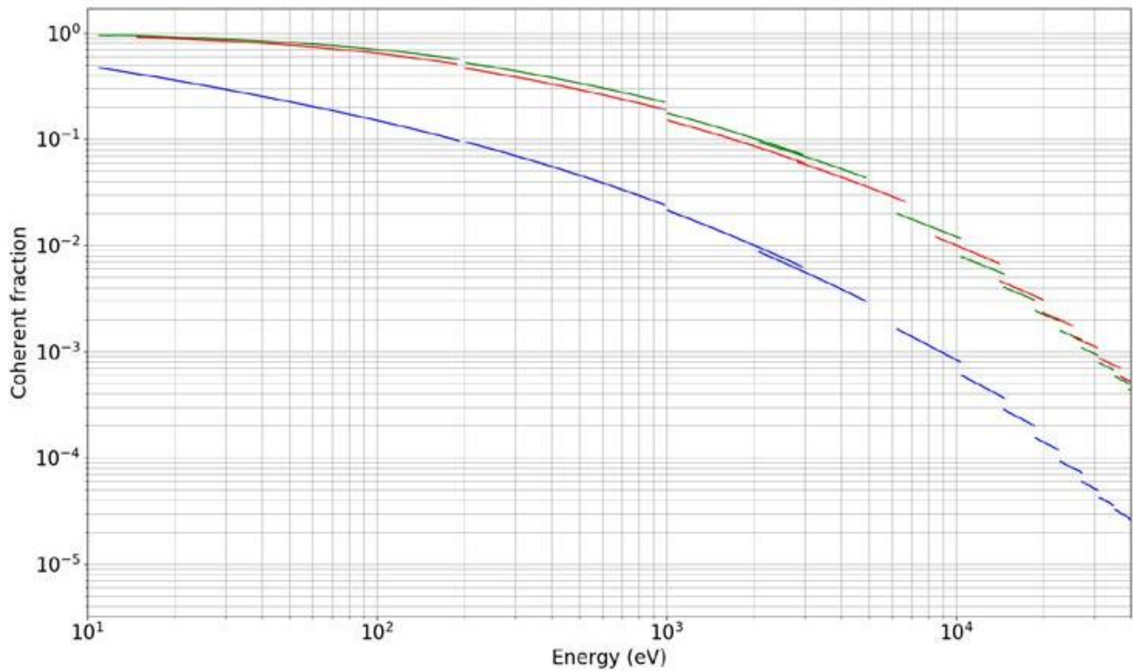


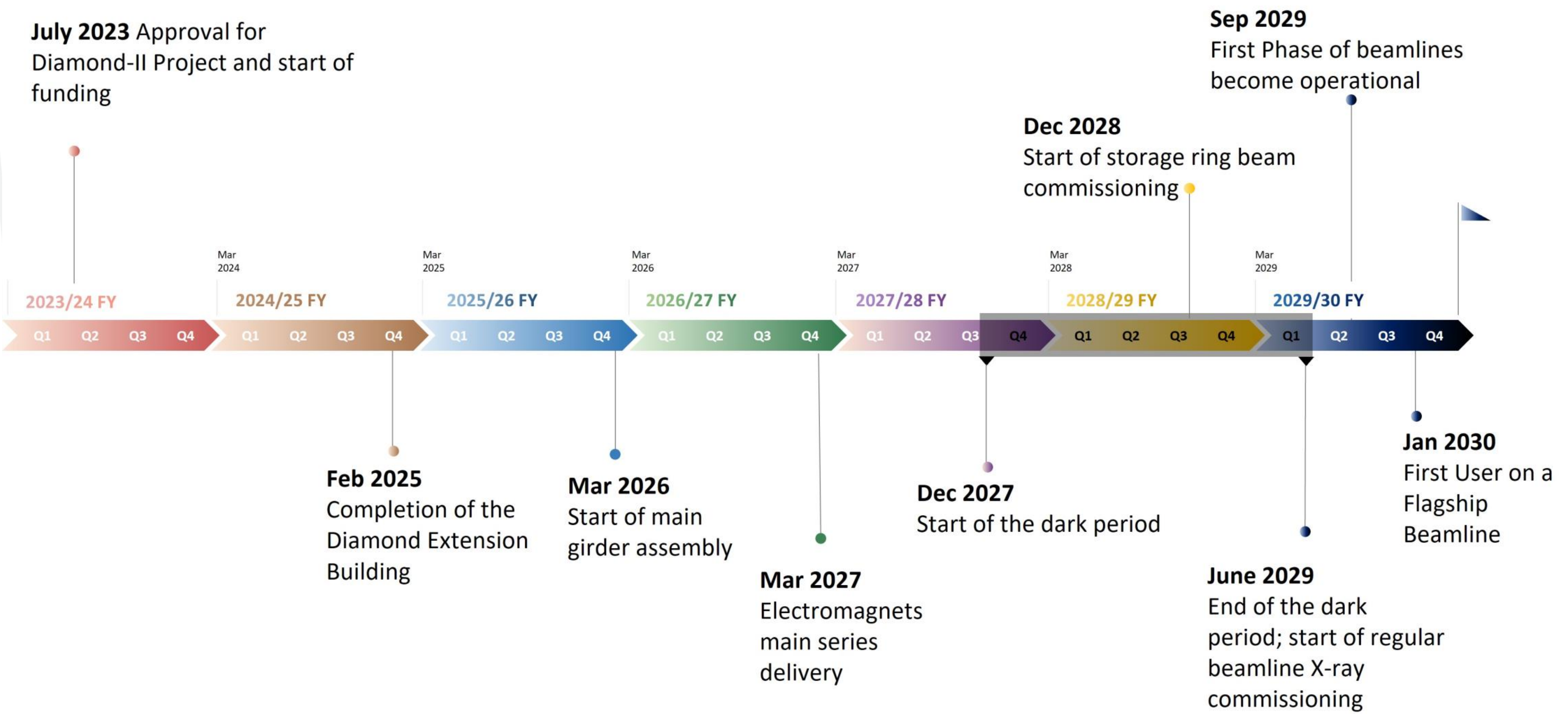
Figure 1-3 : Coherent fraction in the horizontal direction as a function of Energy for Diamond (blue), Diamond-II at 3 GeV (green) and Diamond-II at 3.5 GeV (red). All curves have been produced with Spectra using the Wigner function and approximating the coherent fraction as the ratio between the Brightness and the Brightness calculated in the limit of zero emittance and zero energy spread.

Diamond-II Project Structure

1. Diamond-II Project

- **WBS 1.1 Machine** — A major upgrade of the machine, replacing the Booster Synchrotron and Storage Ring.
- **WBS 1.2 Beamlines** — 3 new ‘flagship’ beamlines + significant upgrades to many existing beamlines.
- **WBS 1.3 Core Software, Controls & Computing** — A boost in data handing and analysis hardware & software, to manage the increased data rates.
- **WBS 1.4 Buildings & Infrastructure** — A new Diamond Extension Building for Diamond-II assembly work, as well as other infrastructure upgrades
- **WBS 1.5 Project Management** — Enhanced Project Management processes.

Timelines


July 2023 Approval for Diamond-II Project and start of funding
Sep 2029 First Phase of beamlines become operational
Dec 2028 Start of storage ring beam commissioning
Mar 2024
Mar 2025
Mar 2026
Mar 2027
Mar 2028
Mar 2029
2023/24 FY
2024/25 FY
2025/26 FY
2026/27 FY
2027/28 FY
2028/29 FY
2029/30 FY
Q1 Q2 Q3 Q4
Q1 Q2 Q3 Q4
Q1 Q2 Q3 Q4
Q1 Q2 Q3 Q4
Q1 Q2 Q3 Q4
Q1 Q2 Q3 Q4
Q1 Q2 Q3 Q4
Feb 2025 Completion of the Diamond Extension Building
Mar 2026 Start of main girder assembly
Mar 2027 Electromagnets main series delivery
Dec 2027 Start of the dark period
June 2029 End of the dark period; start of regular beamline X-ray commissioning
Jan 2030 First User on a Flagship Beamline

Diamond-II Beamlines

- **3 new Flagship Beamlines**
  - SWIFT: Fast Operando Spectroscopy
  - K04: Ultra-high throughput for MX and Xchem
  - CSXID: Coherent Soft X-Ray Imaging and Diffraction

- **4 Bending Magnet Beamlines converting to ID Beamlines**
  - B07: Versatile Soft X-ray (VerSoX) Beamline
  - B16: Test Beamline
  - B18: Core XAS
  - B21: High-throughput small-angle X-ray scattering

- **3 Bending Magnet Beamlines with extensive front-end changes**
  - B22: Multimode InfraRed Imaging and Microspectroscopy
  - B23: Circular Dichroism
  - B24: 3D Correlative Cryo-Imaging

- **Critical Beamline Upgrades**
  - Upgrades required to optics, shielding, slits, diagnostics, collimators, windows etc., to enable the beamlines to operate in Diamond-II.

diamond

Two New Flagship Beamlines

SWiFT and CSXID

Spectroscopy WIthin Fast Timescales: beamline SWIFT

Giannantonio Cibin,

Beamline project development lead

diamond

Diamond-II | Advancing Science

SWIFT: Science drivers

Nanoparticle chemistry
Time resolution

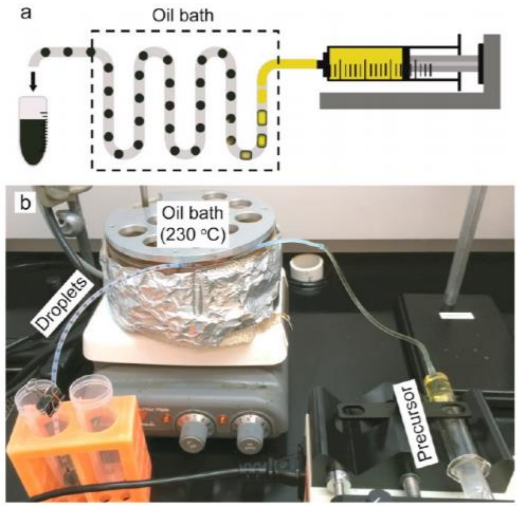
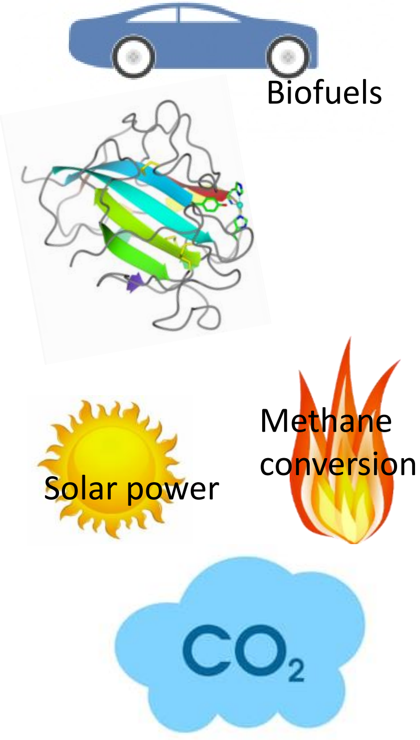
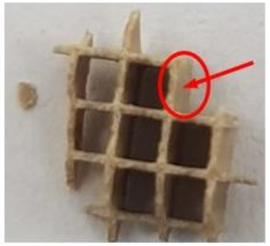


Figure 1. (a) Schematic illustration of the fluidic device used for generating droplets in situ, followed by the formation of Pt–Ni octahedral nanocrystals within each droplet. (b) Photograph showing the formation of droplets in a PTFE tube during the continuous pumping of a precursor solution containing $W(CO)_6$ at a concentration of 2.0 mg mL^{-1}.

Metalloenzymes
Flux And time resolution
Radiation damage



Catalysis:
Mapping, Spectroscopies
Time resolution



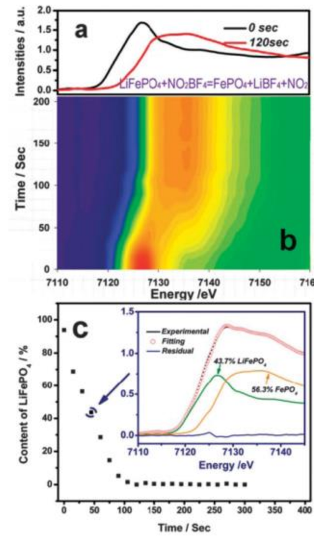
Energy:
spatial and time resolution in batteries

www.rsc.org/chemcomm COMMUNICATION

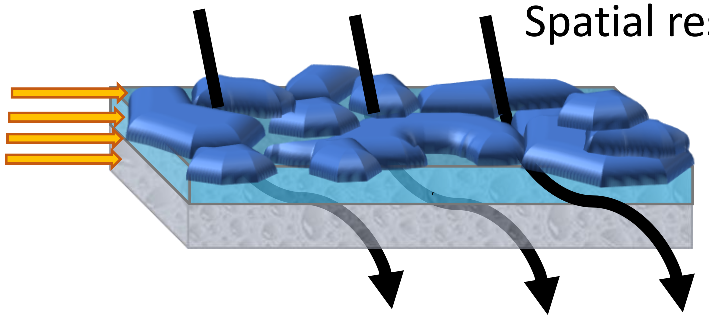
High rate delithiation behaviour of $LiFePO_4$ studied by quick X-ray absorption spectroscopy†

Xiqian Yu,[a] Qi Wang,[a] Yongning Zhou,[a] Hong Li,[b] Xiao-Qing Yang,*[a] Kyung-Wan Nam,*[a] Steven N. Ehrlich,[a] Syed Khalid[a] and Ying Shirley Meng[c]

Received 1st September 2012, Accepted 8th October 2012
DOI: 10.1039/c2cc36382h



Environment and Earth sciences
Spatial resolution, radiation damage control



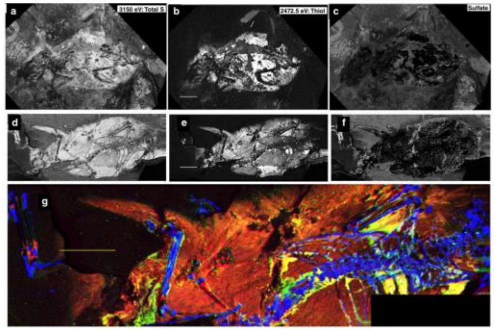


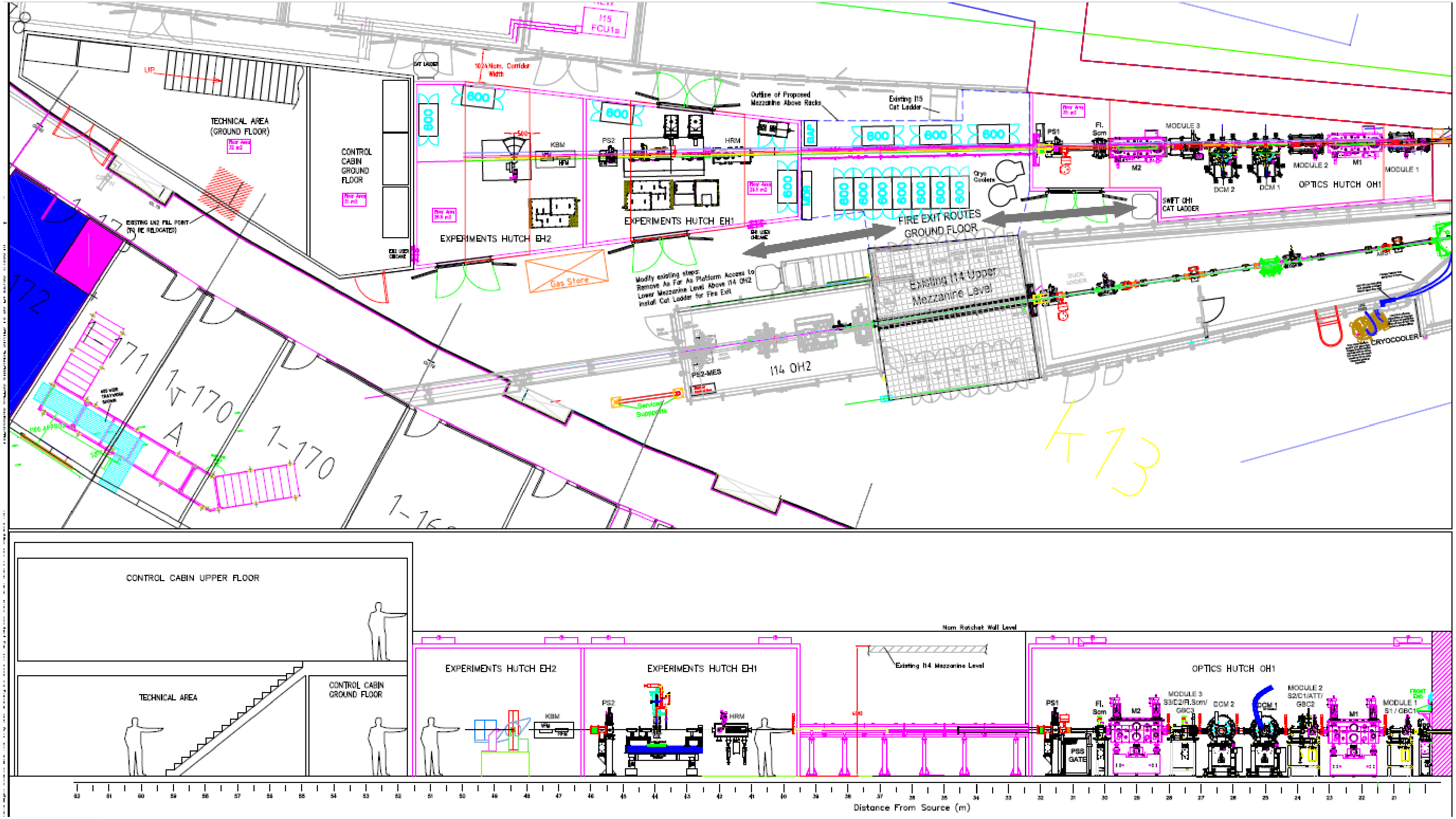
Fig. 2 X-ray image comparison of "lateral" and "dorsal" fossils. SRS-XRF map comparisons for the *A. atavus* lateral fossil (GZG.W.20027b: **a**–**c**) with the "dorsal" fossil (GZG.W.17393a: **d**–**g**). Maps **a** and **d** are total sulfur (incident beam energy 3150 eV). **b** and **e** show reduced organic species of sulfur (incident beam energy 2472.5 eV). **c** and **f** subtract the organic image from the total sulfur map, thus showing only inorganic sulfate. **g** is a false-color map (blue = P, green = Zn, and red = organic S) for the dorsal fossil comparable to that shown in Fig. 1b for the lateral fossil (scale bars = 1 cm). Bright yellow areas indicate a correlation between Zn and organic sulfur

diamond

Diamond-II

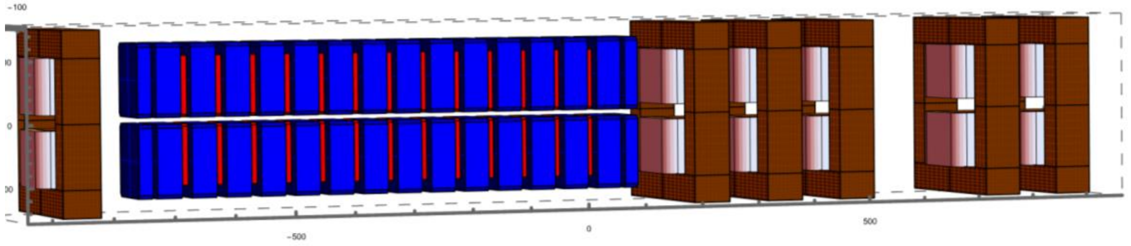
Courtesy of Giannantonio Cibin

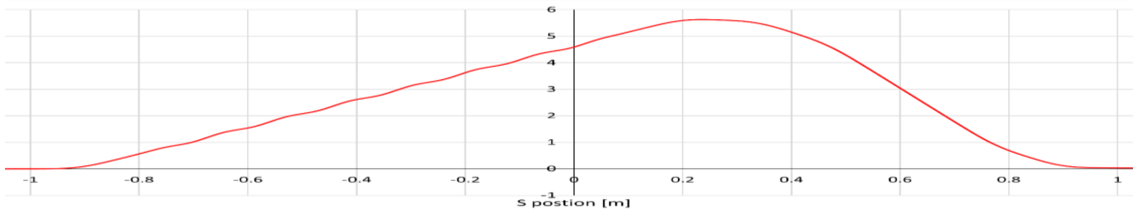
SWIFT beamline layout

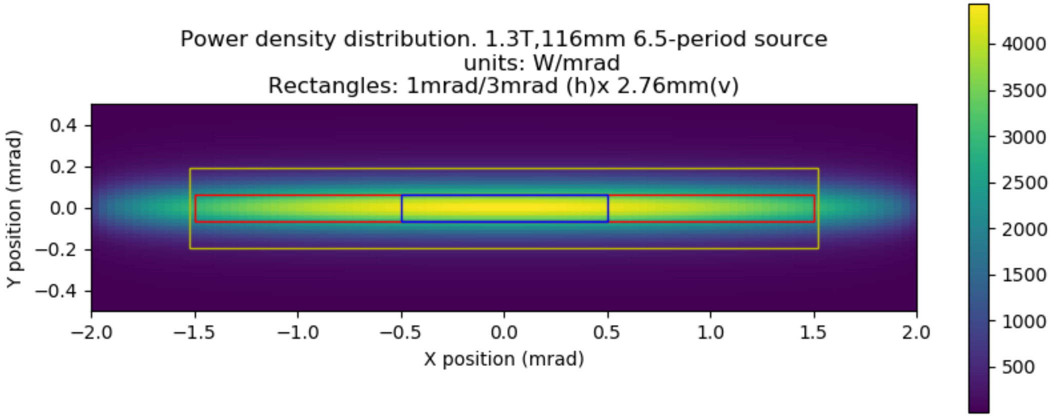


Courtesy of Giannantonio Cibin

Source: 13-pole wiggler in a mid-straight section

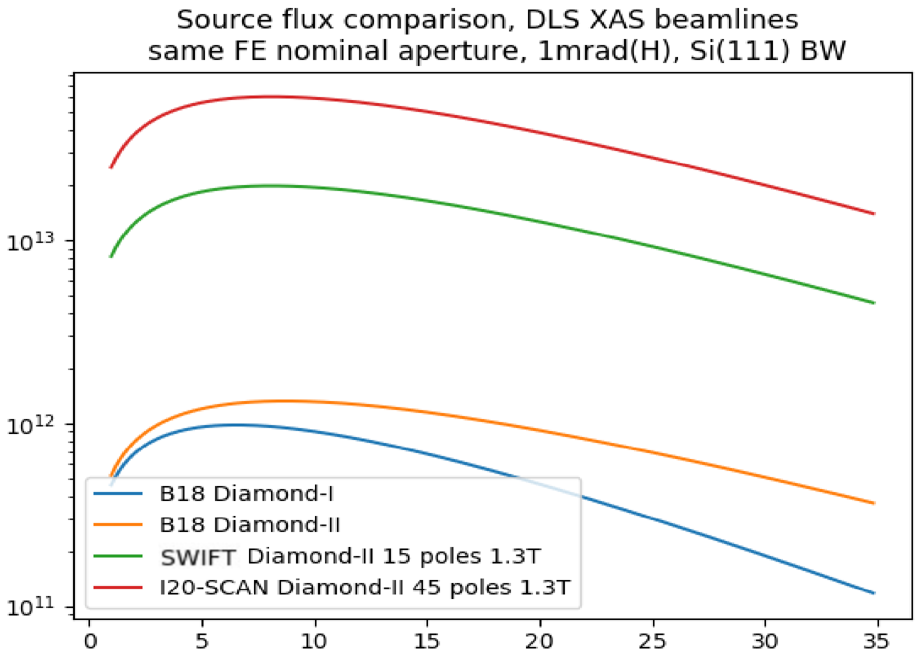






Multi-pole wiggler - 3.2 kW total power
Source is off-axis to the nominal trajectory

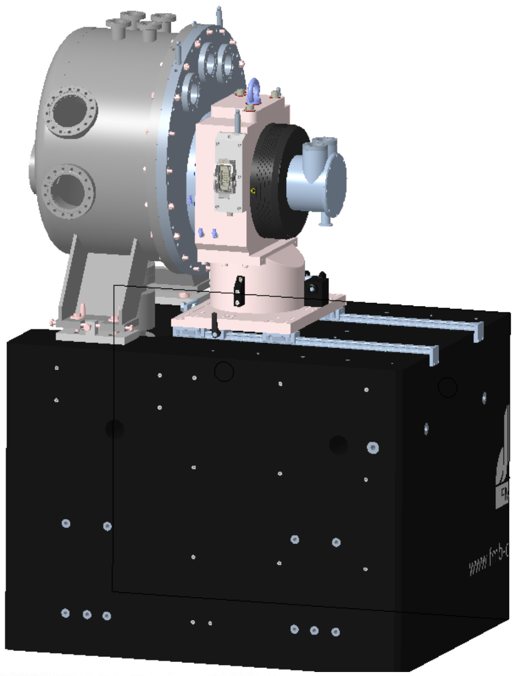
Will give 10-15 times more photons than B18

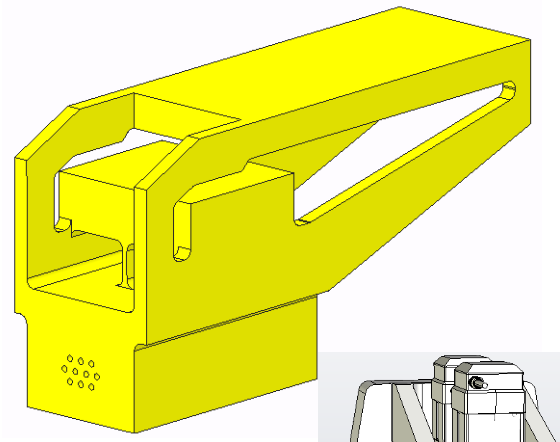


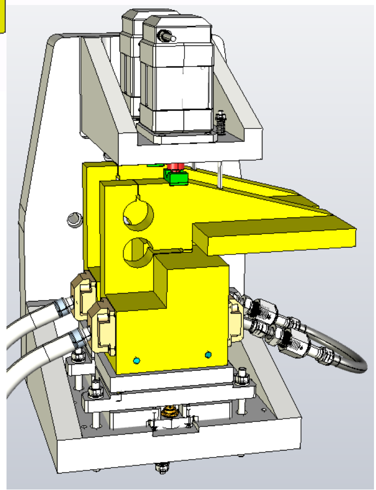
QUICK-EXAFS Monochromator

Monochromators: High power load, LN2 cooled

- **Quick-EXAFS**, fast-scanning DCM (50Hz, 4-35 keV)
  - Channel-cut, direct-drive, direct cooling
- **Continuous-scanning**, fixed exit ('conventional')





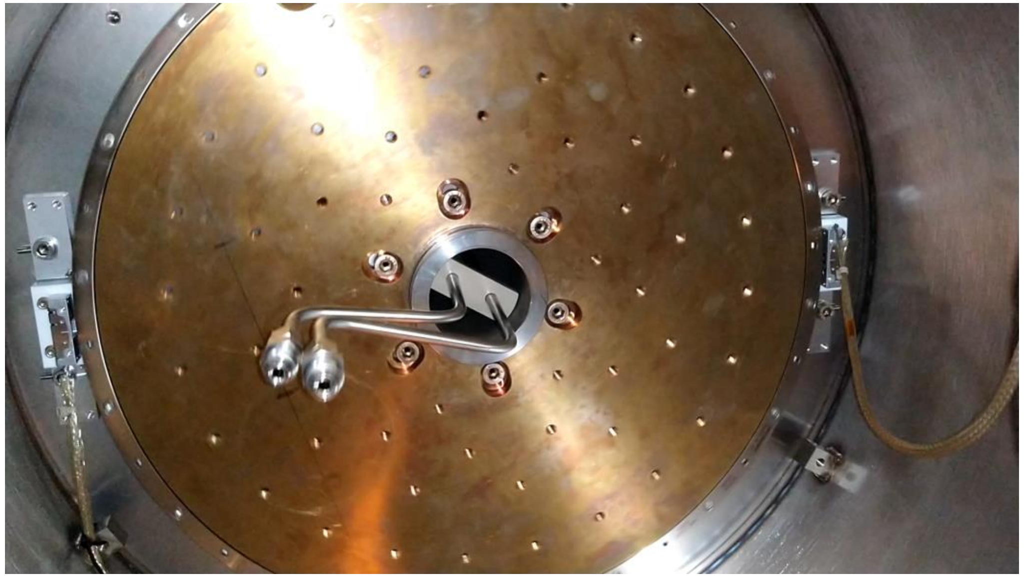


Courtesy of Giannantonio Cibin

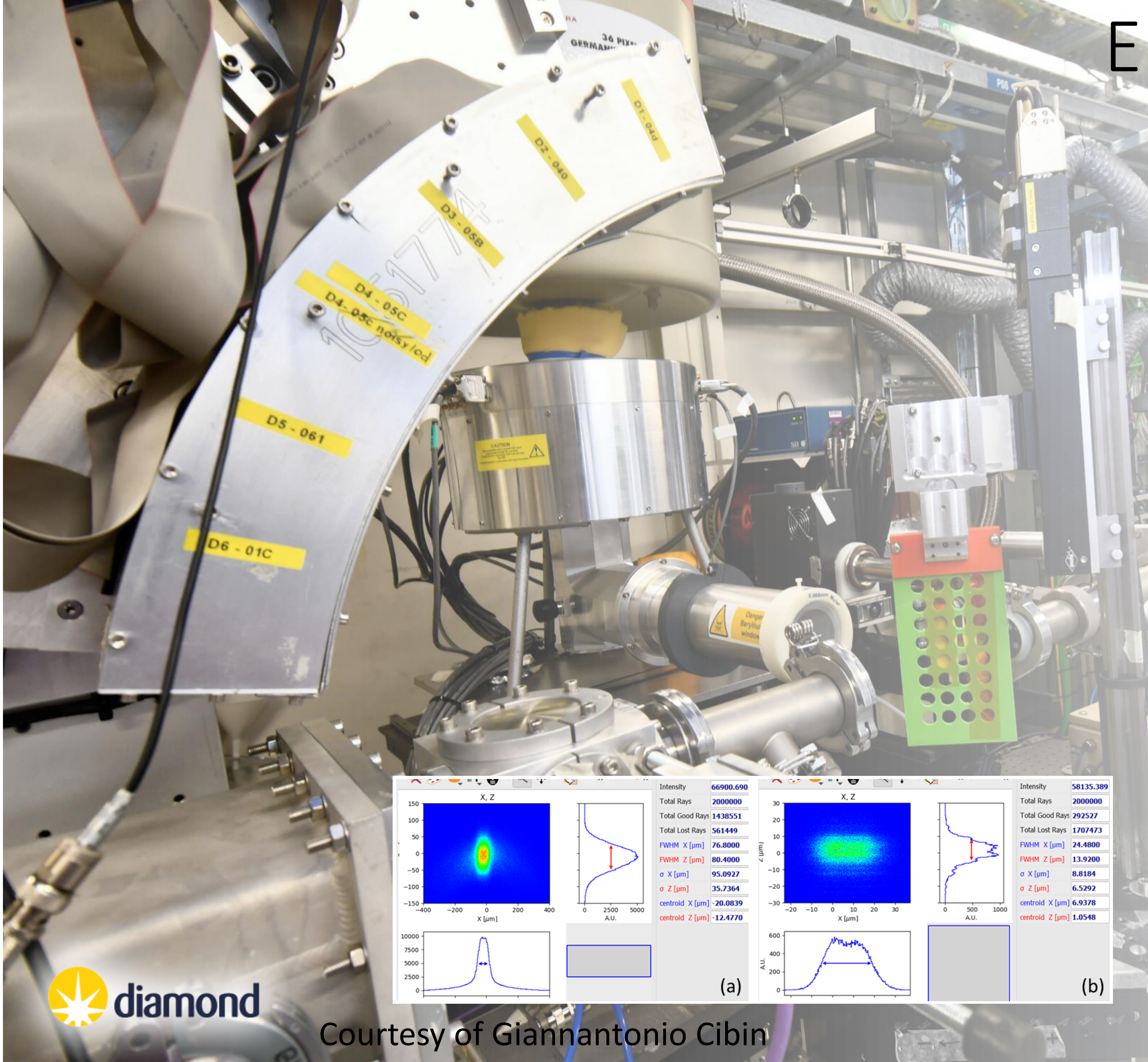
Preliminary studies quite advanced:

Challenges are thermal load and alignment accuracy under high dynamical conditions

Complex crystal design, direct LN2 cooling
LN2 joints under vibrations



Endstations



Experimental Hutch 1: bulk
- High flux
- Operando studies, dilute systems
- Beam size: 100 x 100 um

Experimental Hutch 2: microfocus
- Beam size: 20 x 20 um
- Sample chemical mapping, tomography

Operando sample environments
- High temperature
- Gas flow reaction cells
- Liquid flow reaction cells
- Electrochemistry

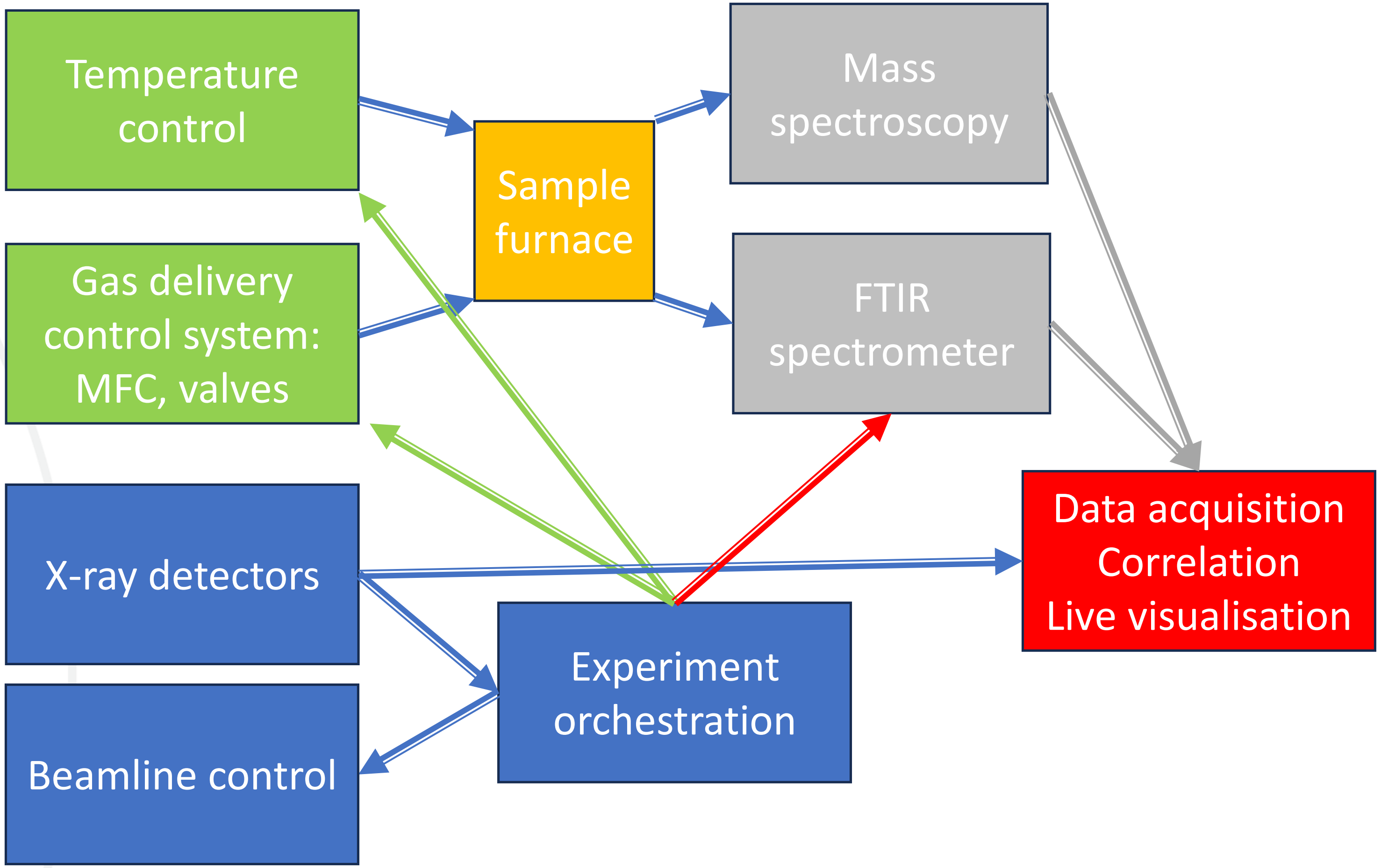
Courtesy of Giannantonio Cibin

Endstations: Ancillary instrumentation

Will expand on the experience from the present Spectroscopy beamlines

To characterise the sample conditions during operando experiments

- **Mass Spectrometers**
- **Potentiostats**
- **UV-VIS spectrometers**
- **FTIR, Raman**



- **Essential is development of software interfaces - EPICS, BlueSky**
  - Need: correlate time-resolved conventional instrumentation and beamline data
  - Control integrated with data acquisition system
  - Intake of time-resolved data for live processing

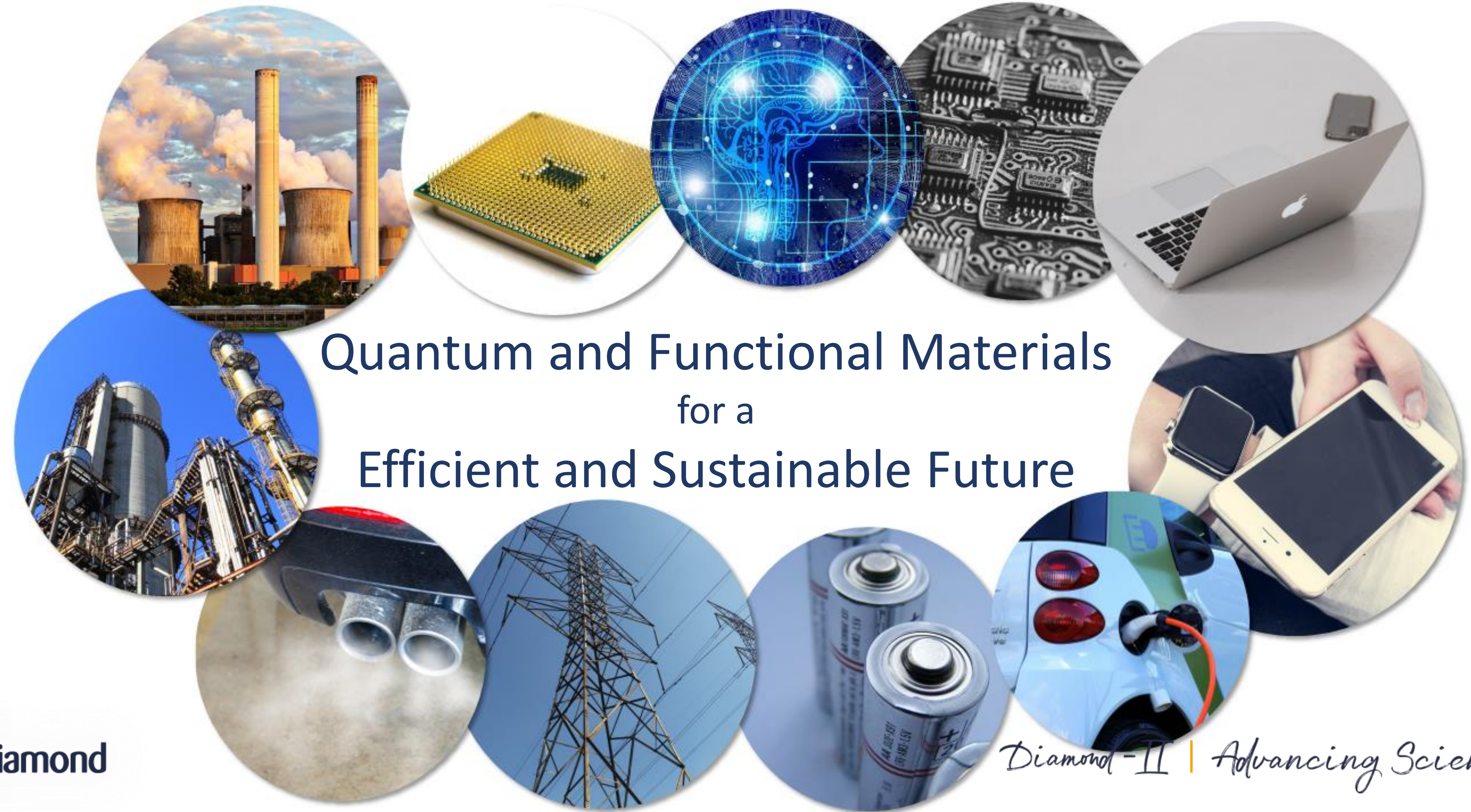
Courtesy of Giannantonio Cibin

The Coherent Soft X-ray Imaging and Diffraction beamline CSXID

David Burn

Beamline project development lead

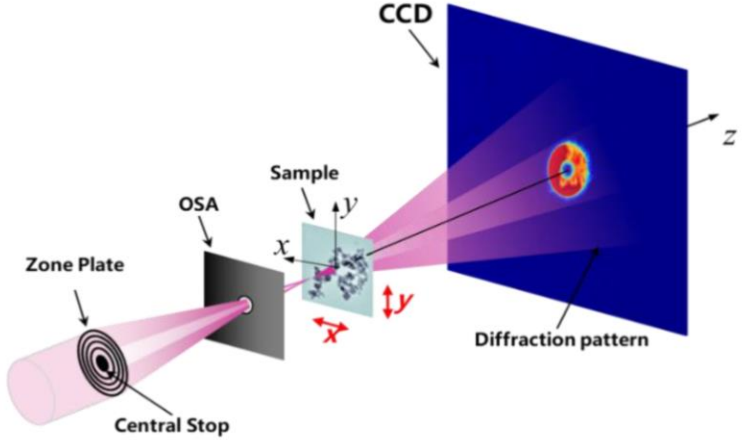
Science Drivers



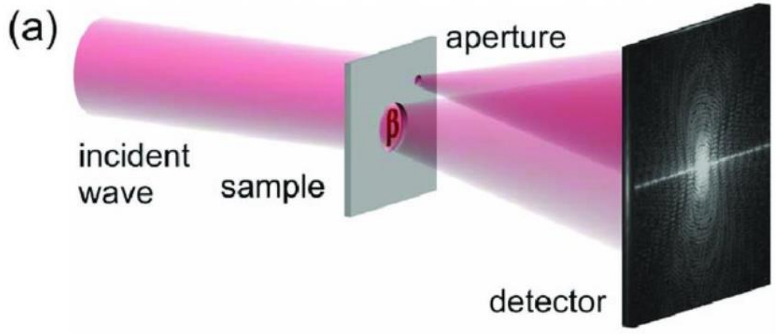
Quantum and Functional Materials
for a
Efficient and Sustainable Future

CSXID experimental techniques

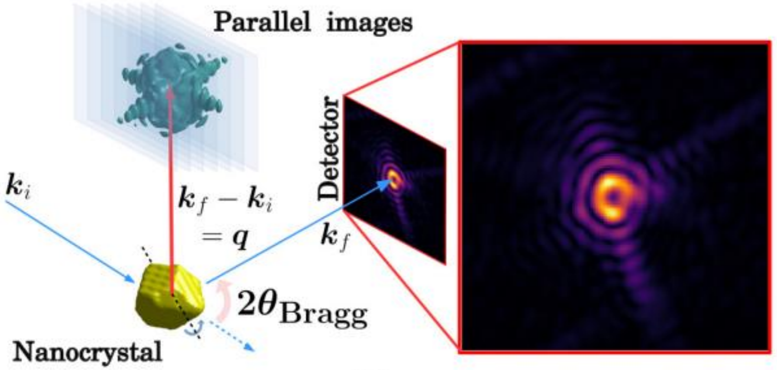
Ptychography



Holography

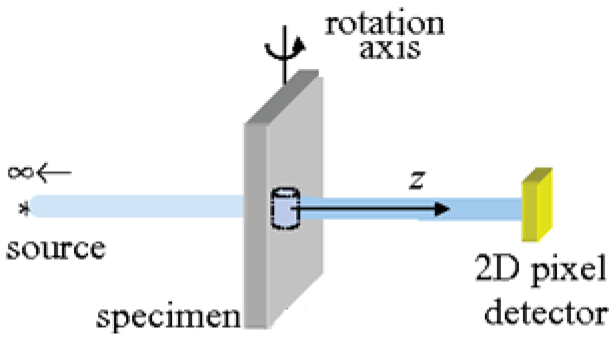


Bragg CDI

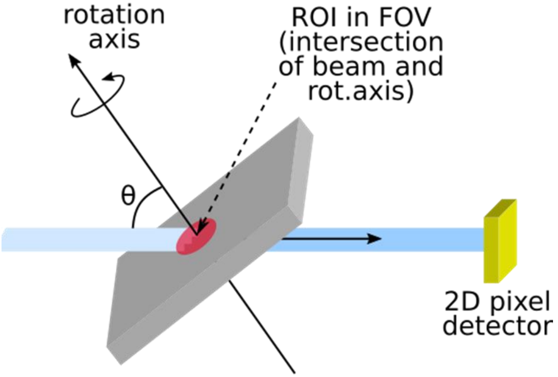


Phys. Rev. A 99, 053838 (2019)

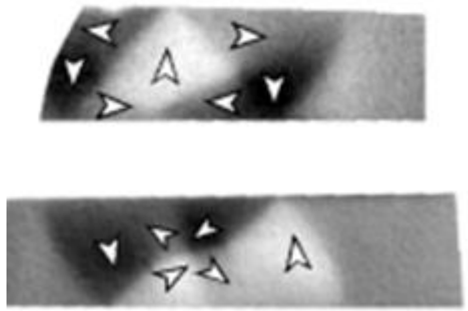
Tomography



Laminography

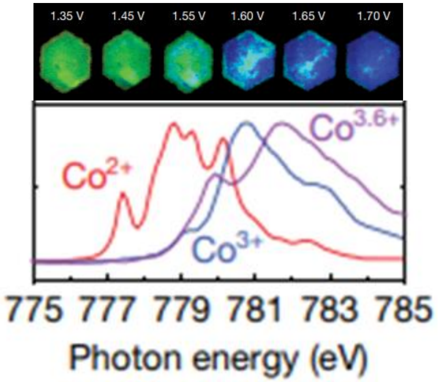


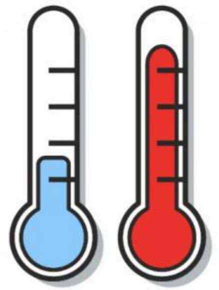
Magnetic contrast



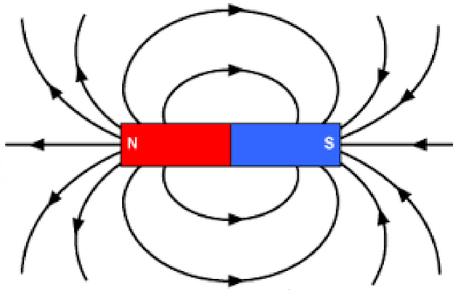
M. Klaui, et.al. Appl. Phys. Lett. 88 (2006) 232507.

Chemical contrast

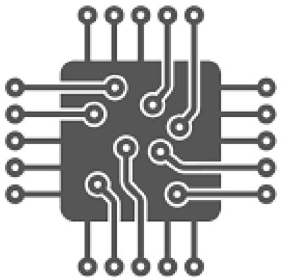




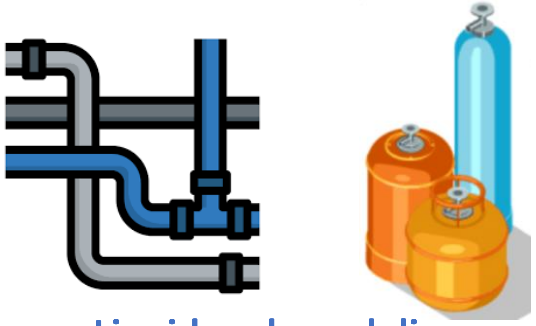
Temperature



Magnetic field



Electrical connections

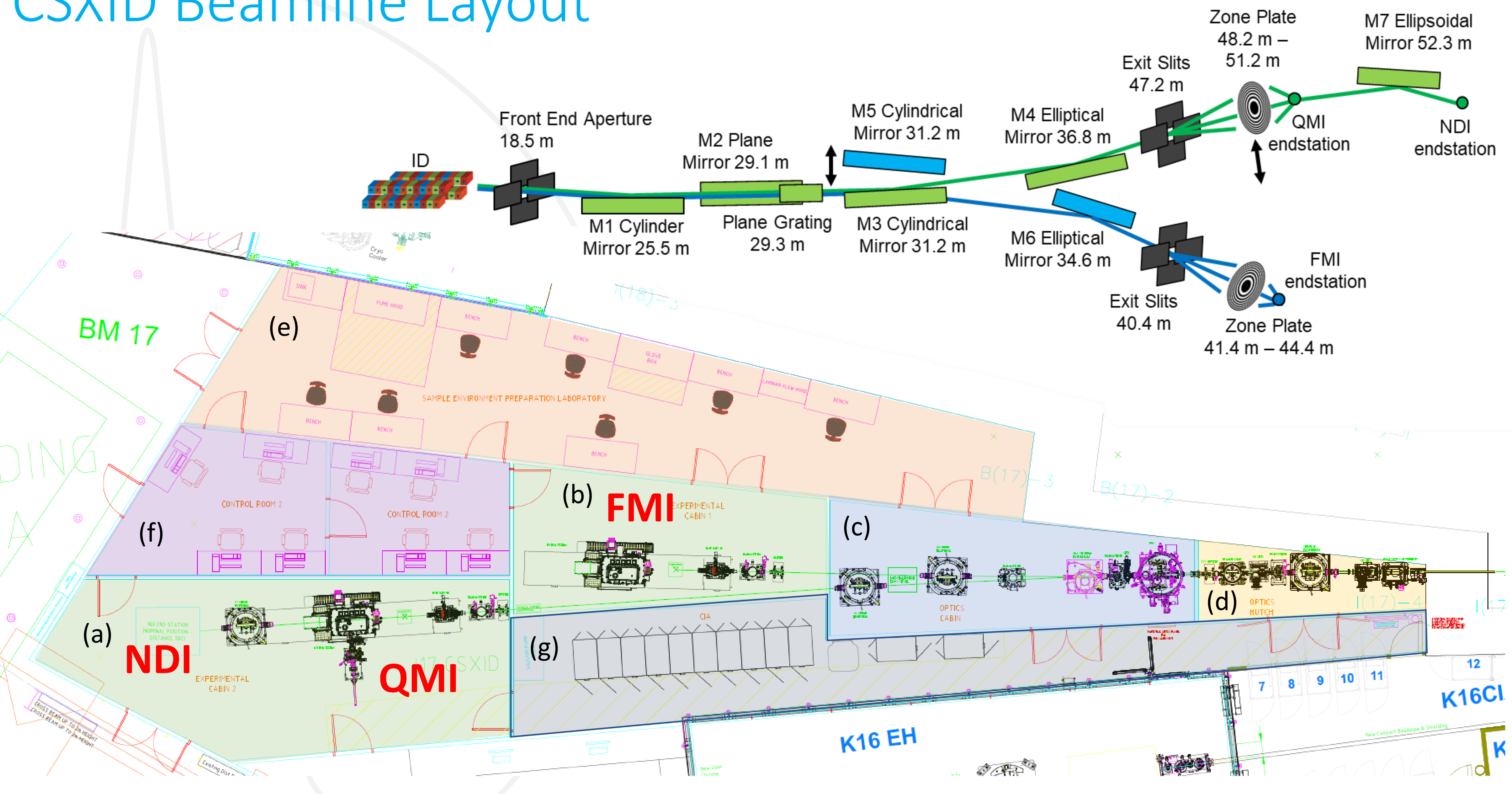


Liquid and gas delivery

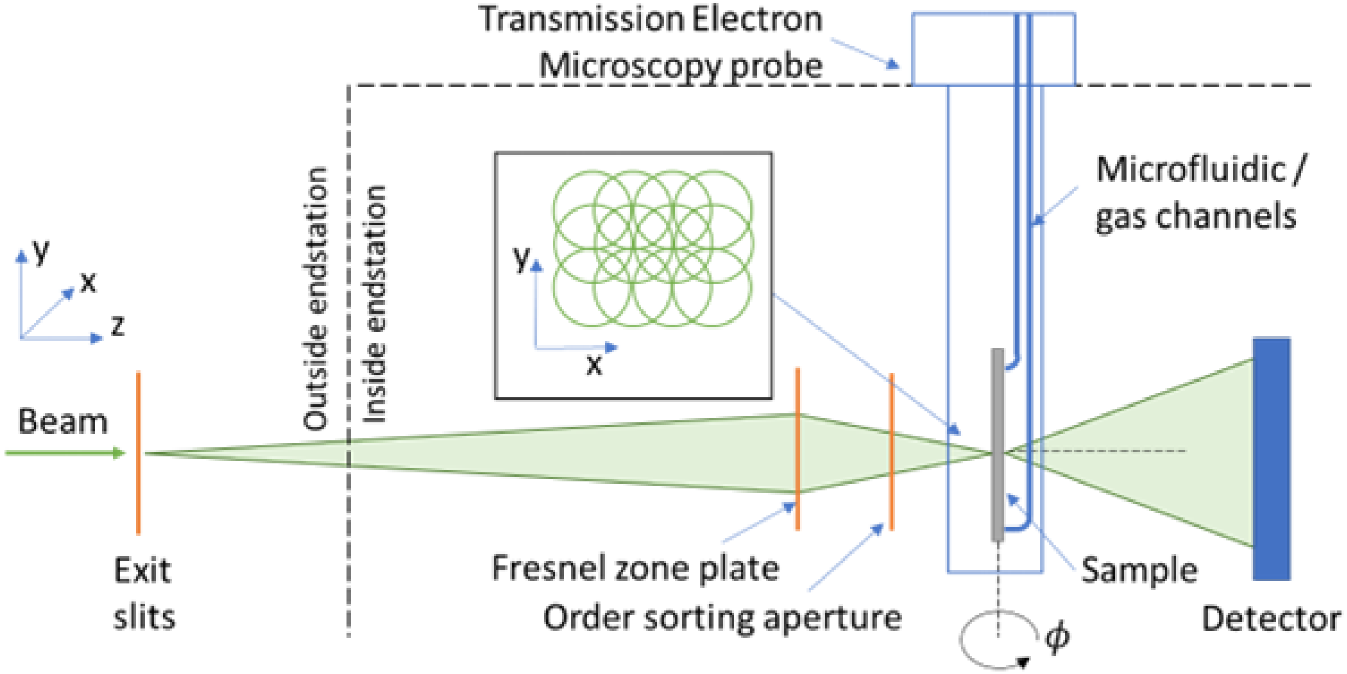
Time resolution

Environment development

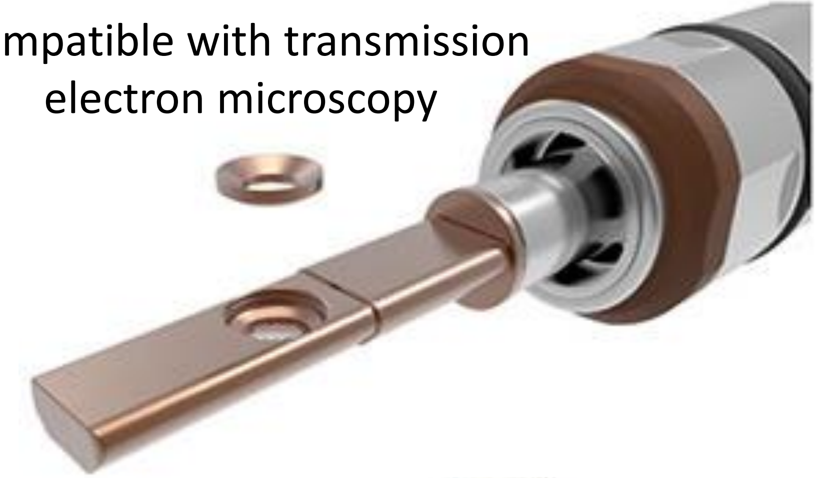
CSXID Beamline Layout



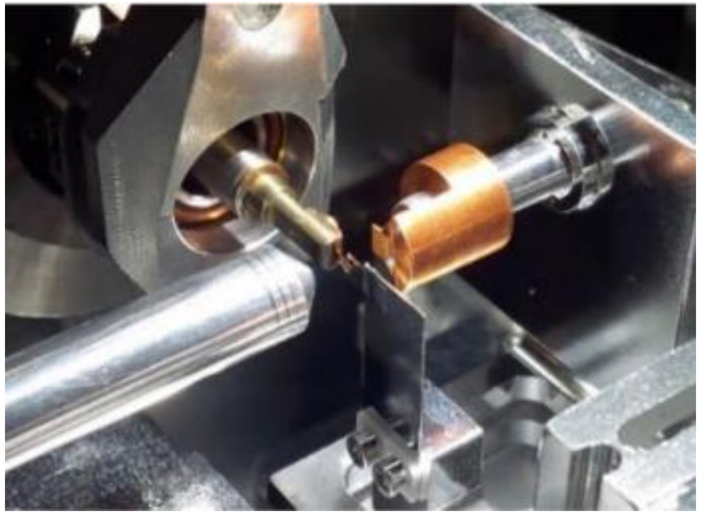
Functional Materials Imaging



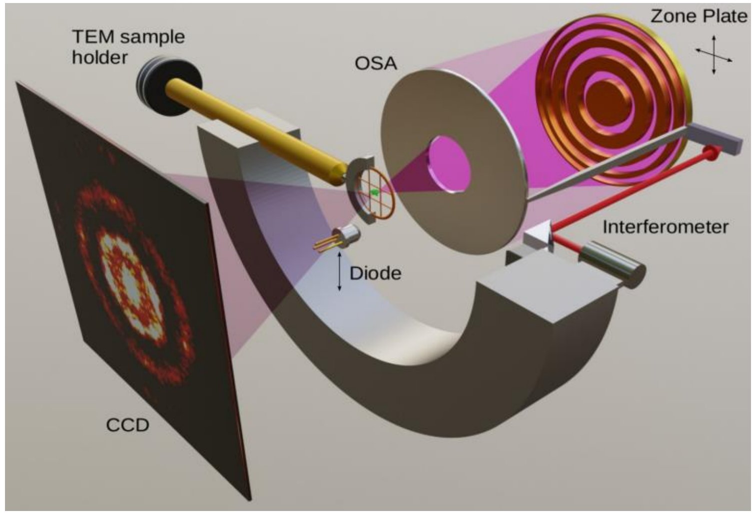
Compatible with transmission electron microscopy



Cryo STXM @ CLS



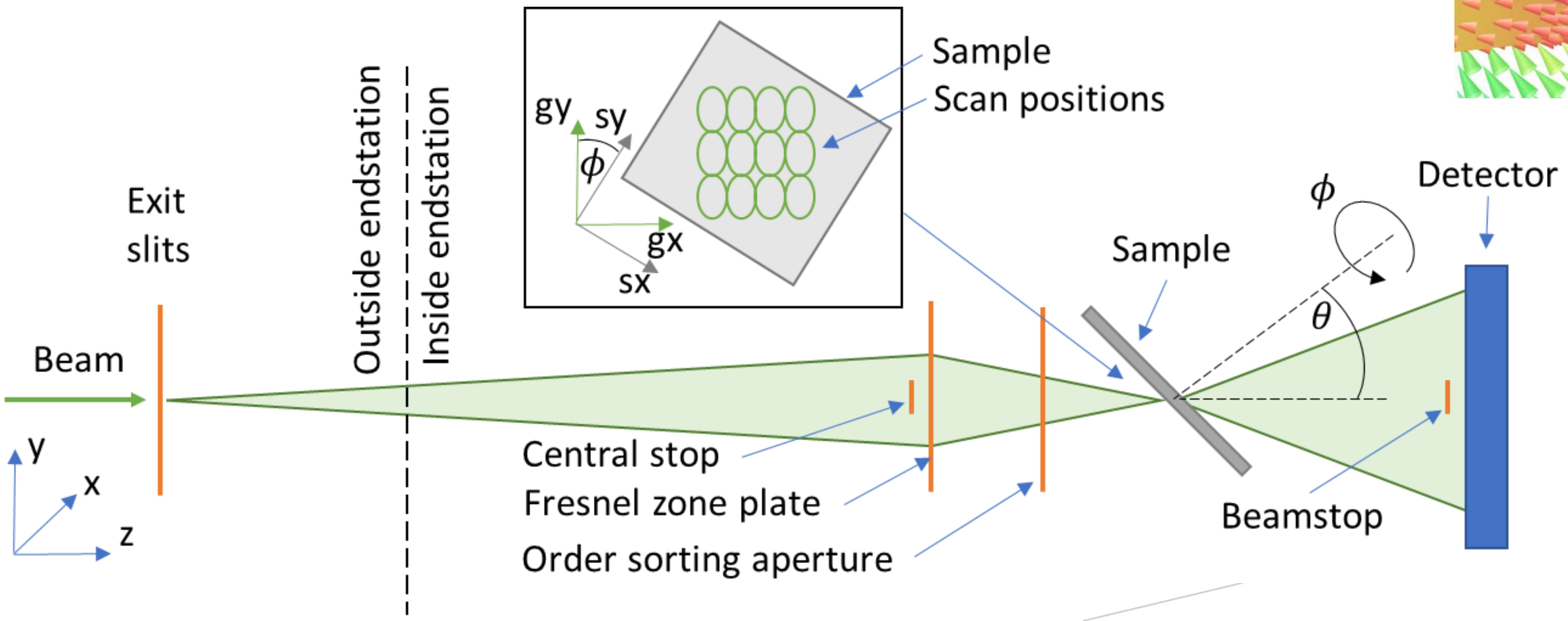
COSMIC @ ALS

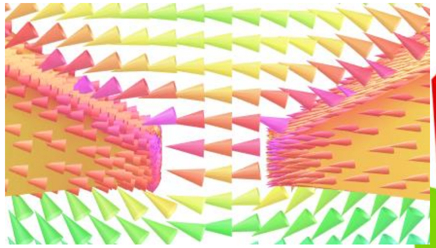


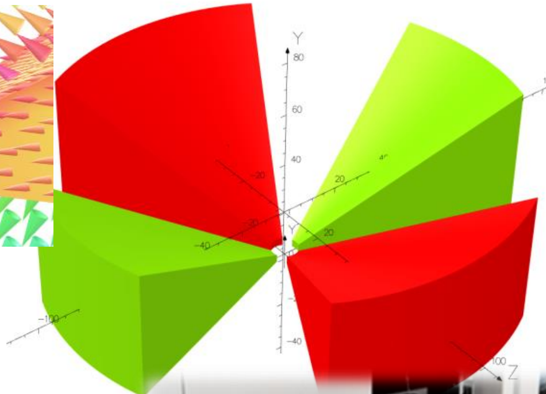
Gas/liquid cells
Electrical connections
cooling / heating

Diamond-II | Advancing Science

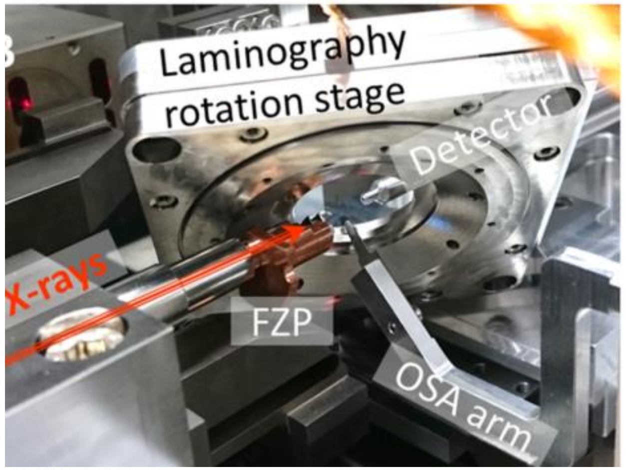
Quantum Materials Imaging



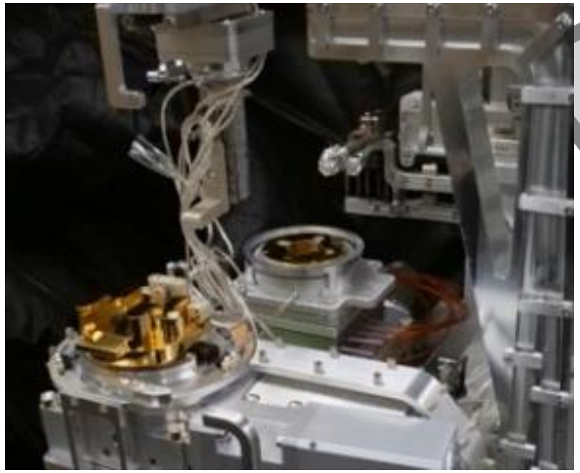


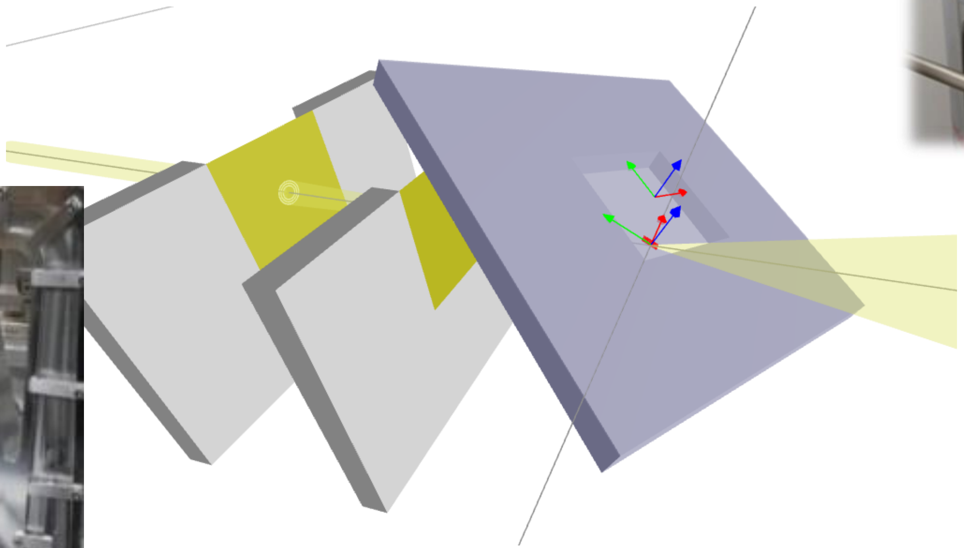


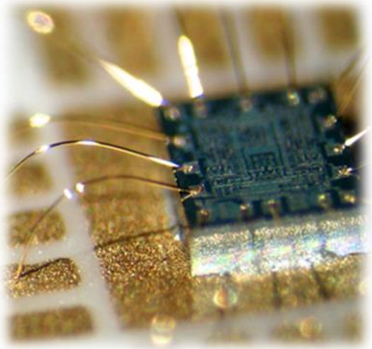
PolLux @ SLS



J08 @ DLS

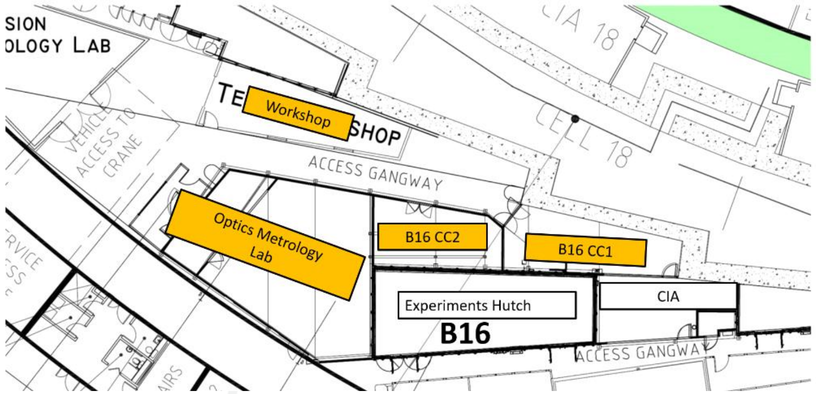




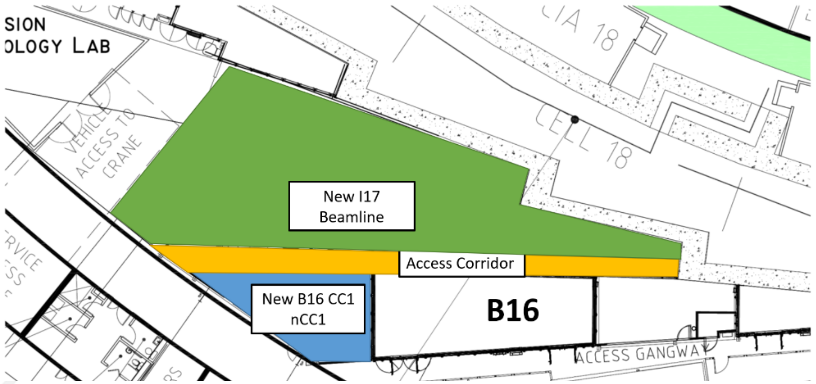


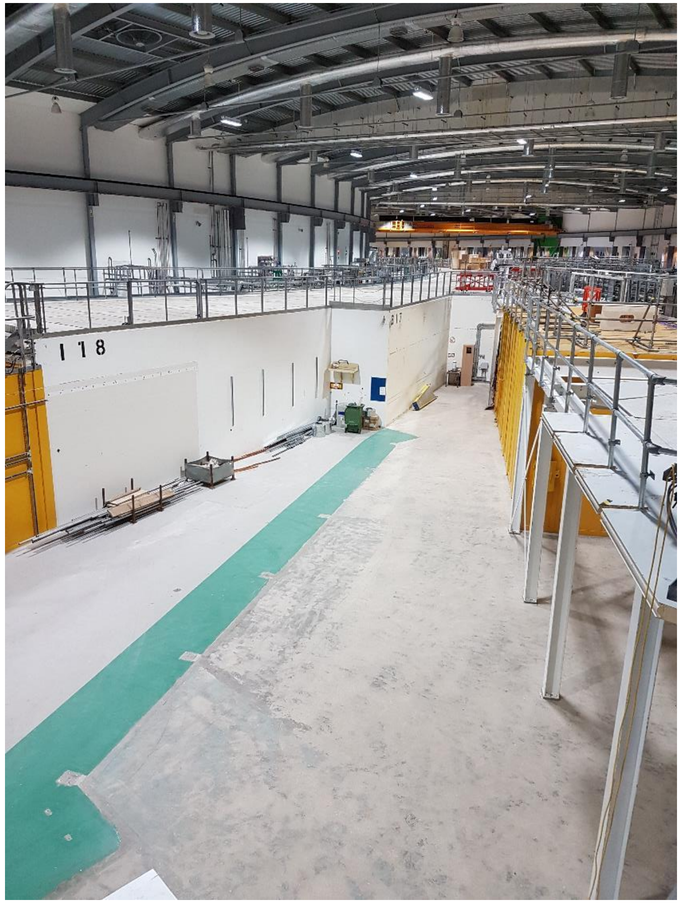
CSXID: space ready to install hutches

How it was:
All 'amber; areas now removed for installation of the Diamond-II flagship beamline CSXID (I17).



How it will be:

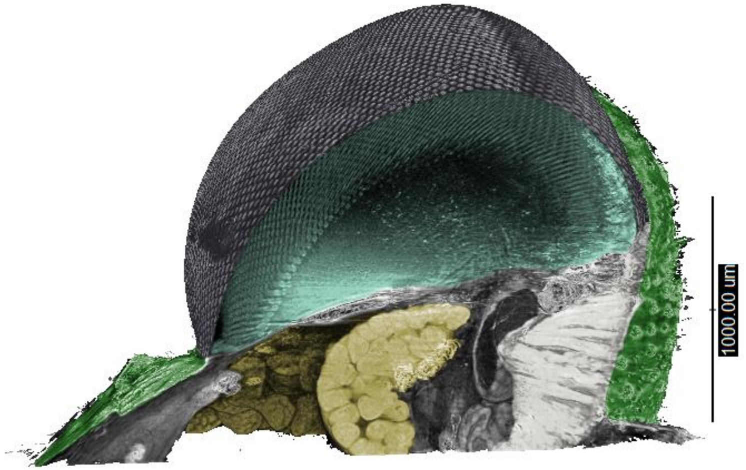




Other activities beyond the machine and beamlines

Software, Computing and Controls Drivers

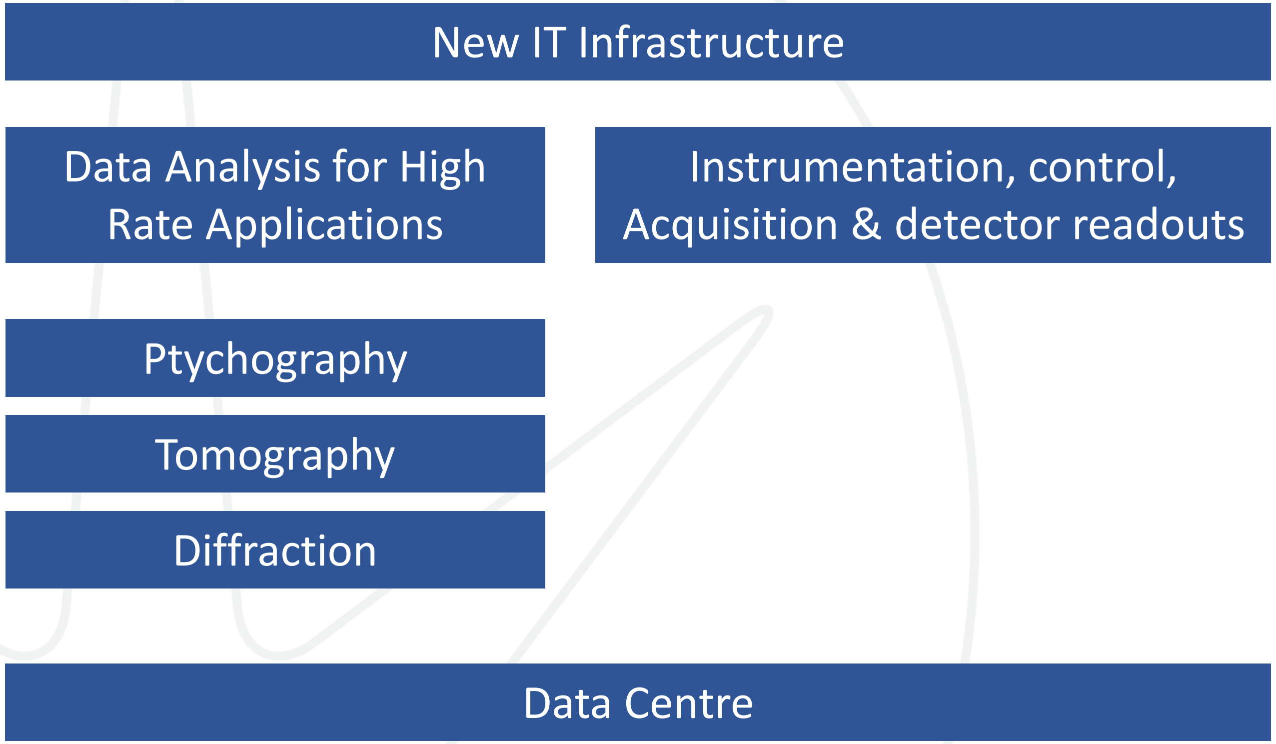
- Increased photon brightness will drive
  - New science
  - More complex experiments
  - Higher spatial and temporal resolution
  - Enable faster detectors
  - Greater automation of experiment
  - Faster data processing and reduction
  - New data processing techniques such as AI/ML ….
- Science benefits will also come from
  - More open software environment
  - Greater software-scientist collaboration
  - Lowering threshold of use
- Result in a **data tsunami**



The dataset that brought us past the 3PB mark: a coloured reconstruction of a bee's compound eye, produced from studies on I13. Courtesy of Gavin Taylor, Emily Baird, Andrew J Bodey & Andreas Enstrom (University of Lund)

diamond

Software and Controls Developments



- More holistic approach to software design and development
  - Greater functional integration
  - Richer metadata
  - Service orientated architecture
- Substantial software developments in:
  - Data to Knowledge
  - Realtime Data Management
  - Experiment Management
  - Information Management
- Facilitate greater use of
  - ML/AI technologies
  - Post visit data analysis services
  - Open data management

diamond

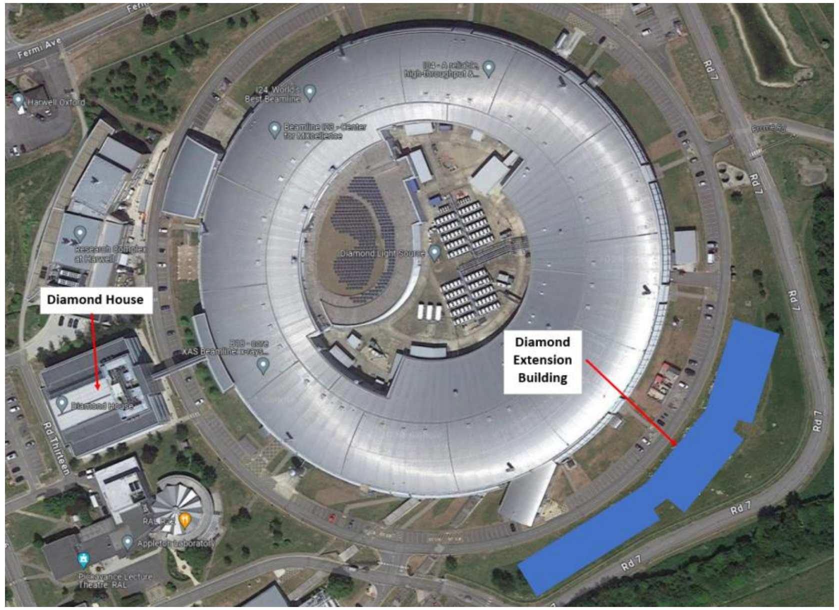
Diamond Extension Building (DEB)

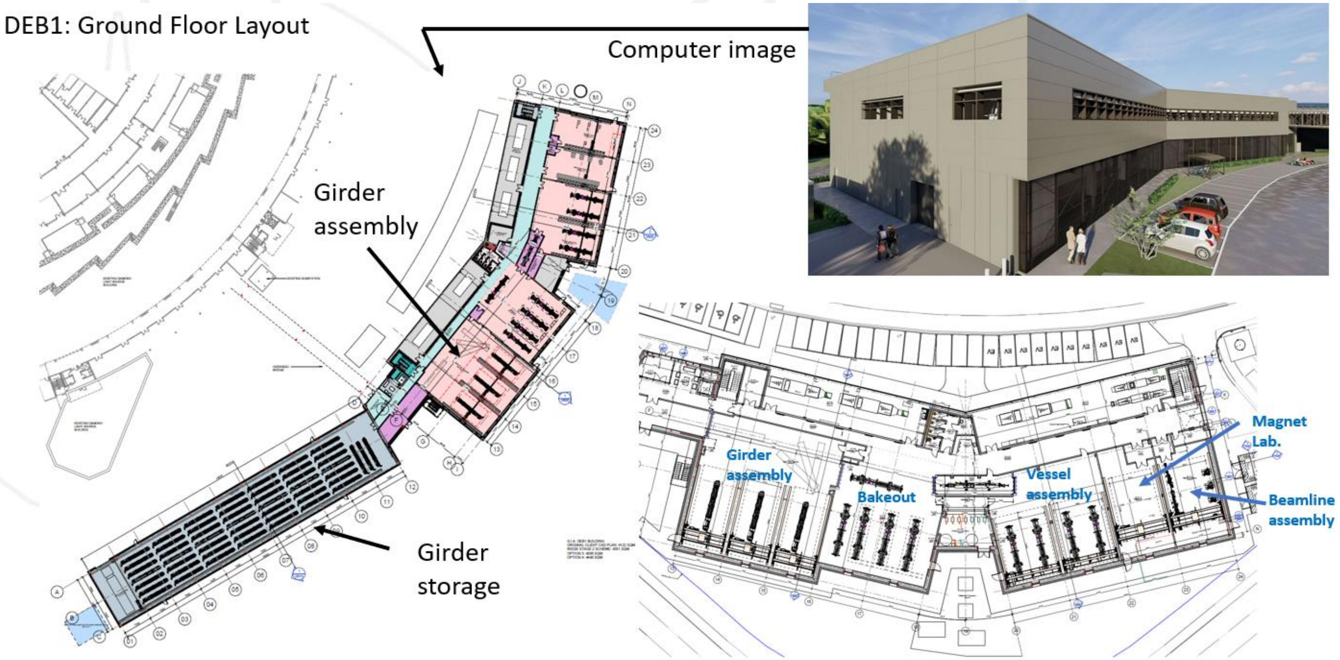
Purpose of the DEB prior to ‘dark period’

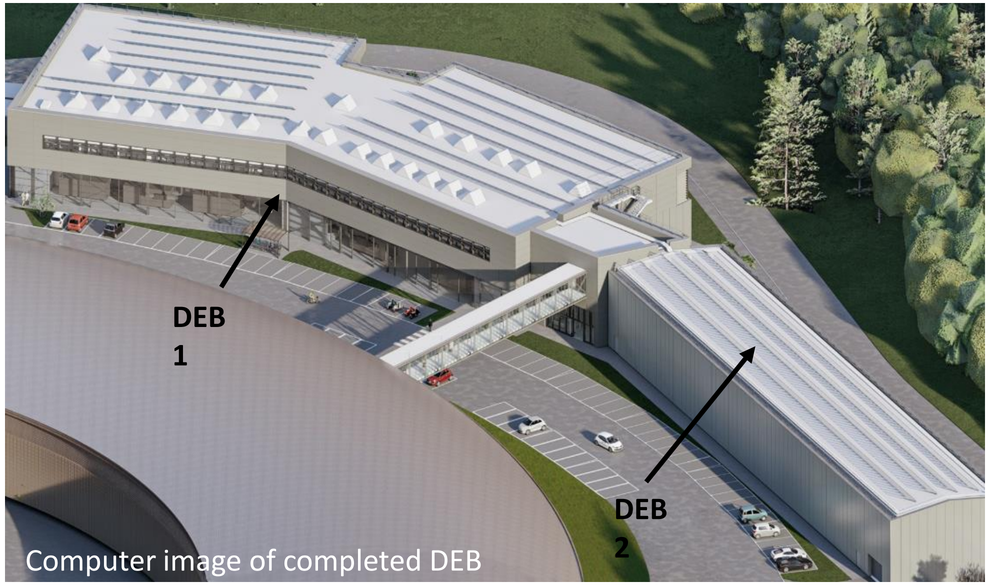
- **Critical to minimising the dark period**
- **DEB1**: magnet measurement, vacuum assembly and bakeout, girder assembly
- **DEB2**: girder storage and girder mock-up

Repurposed after the ‘dark period’

- Legacy of critical office and laboratory space
- possibility of creating a central stores/’goods-in’
- possibility of relocating Insertion Device area from R79 into DEB2







diamond

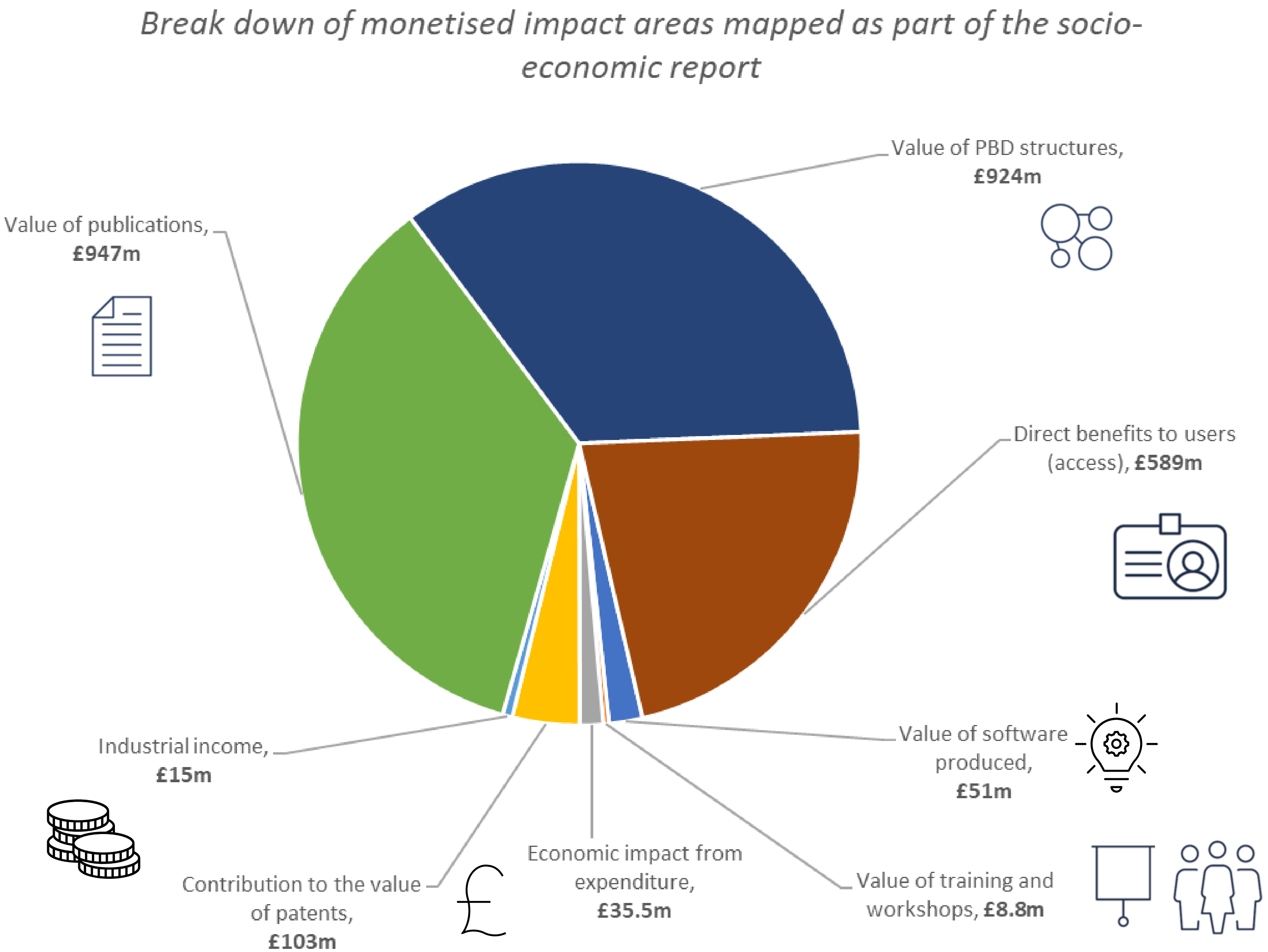
Key element to Diamond-II funding: Socioeconomic impact study

- The study estimates a cumulative monetised impact for Diamond of ***at least* £2.6 billion**
- This reflects very favourably with the **£1.4 billion investment** made in the facility to date
- **Covers 13 of the 17 UN-Sustainable Development Goals**

Lead of the study: Isabelle Boscaro-Clarke

diamond

Summary of Impact



Using published impact research - PatVal EU & PDB assessment carried out in 2017

...and societal

research that improves lives!

Summary

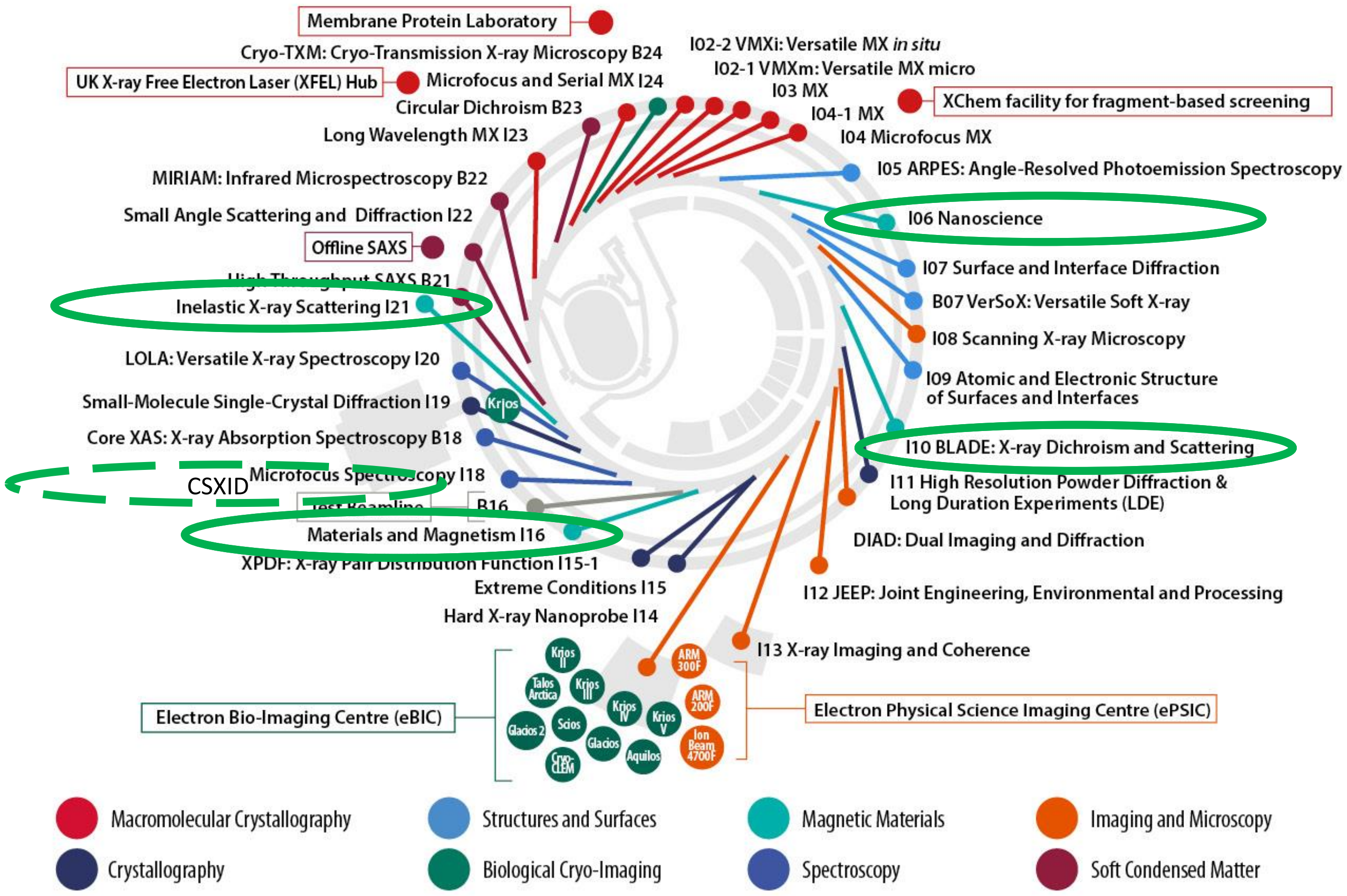
- Diamond: A facility continuing to provide new capabilities to support users doing outstanding research
- Diamond-II aims to maintain Diamond as a competitive facility
  - Strong engagement with the user base, provide key support,
  - Needed to show impact of Diamond
  - Not an easy time given financial challenges

Thank you!

Thank you.

Magnetic Materials

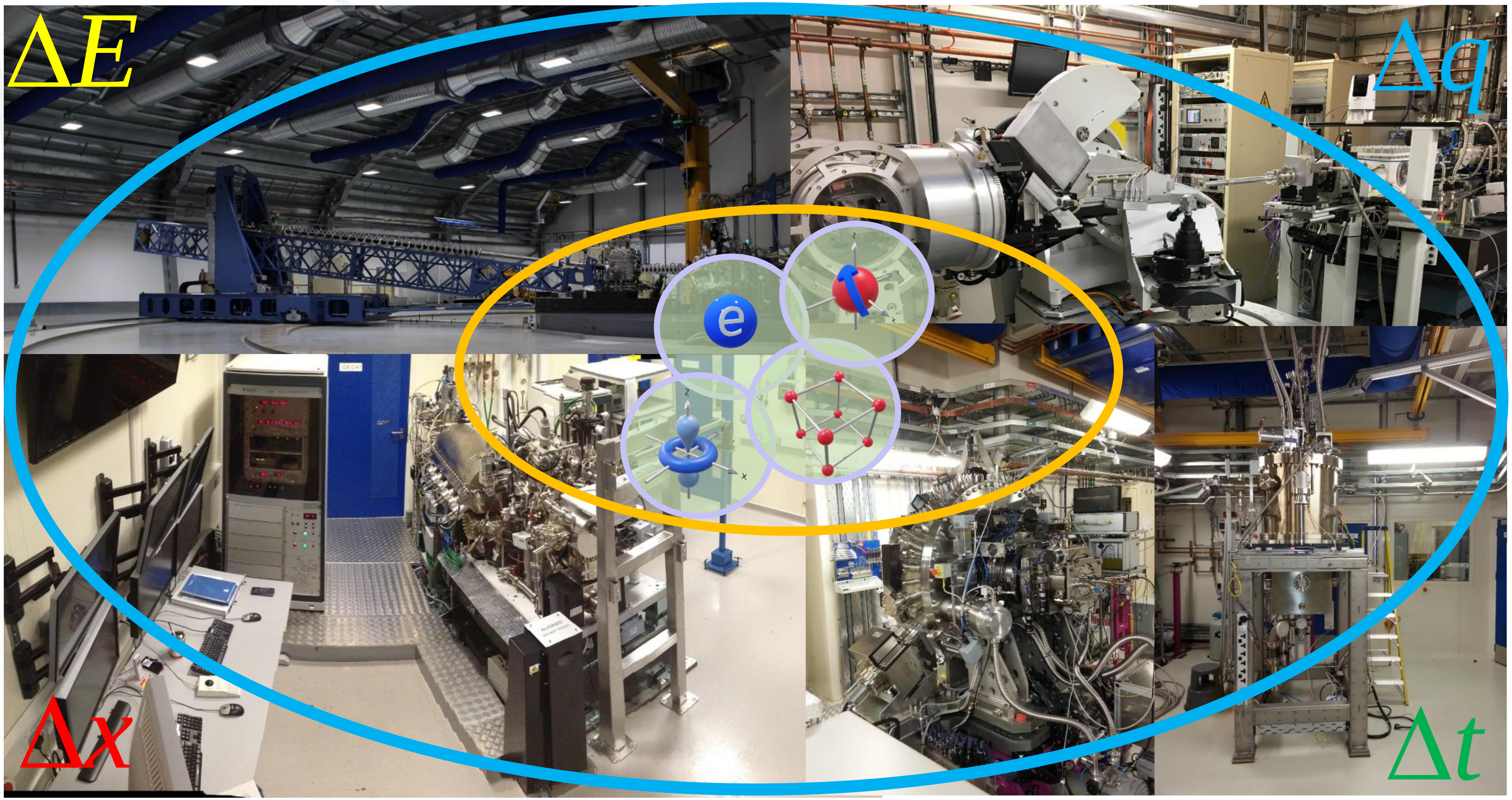
Infrastructure and capabilities



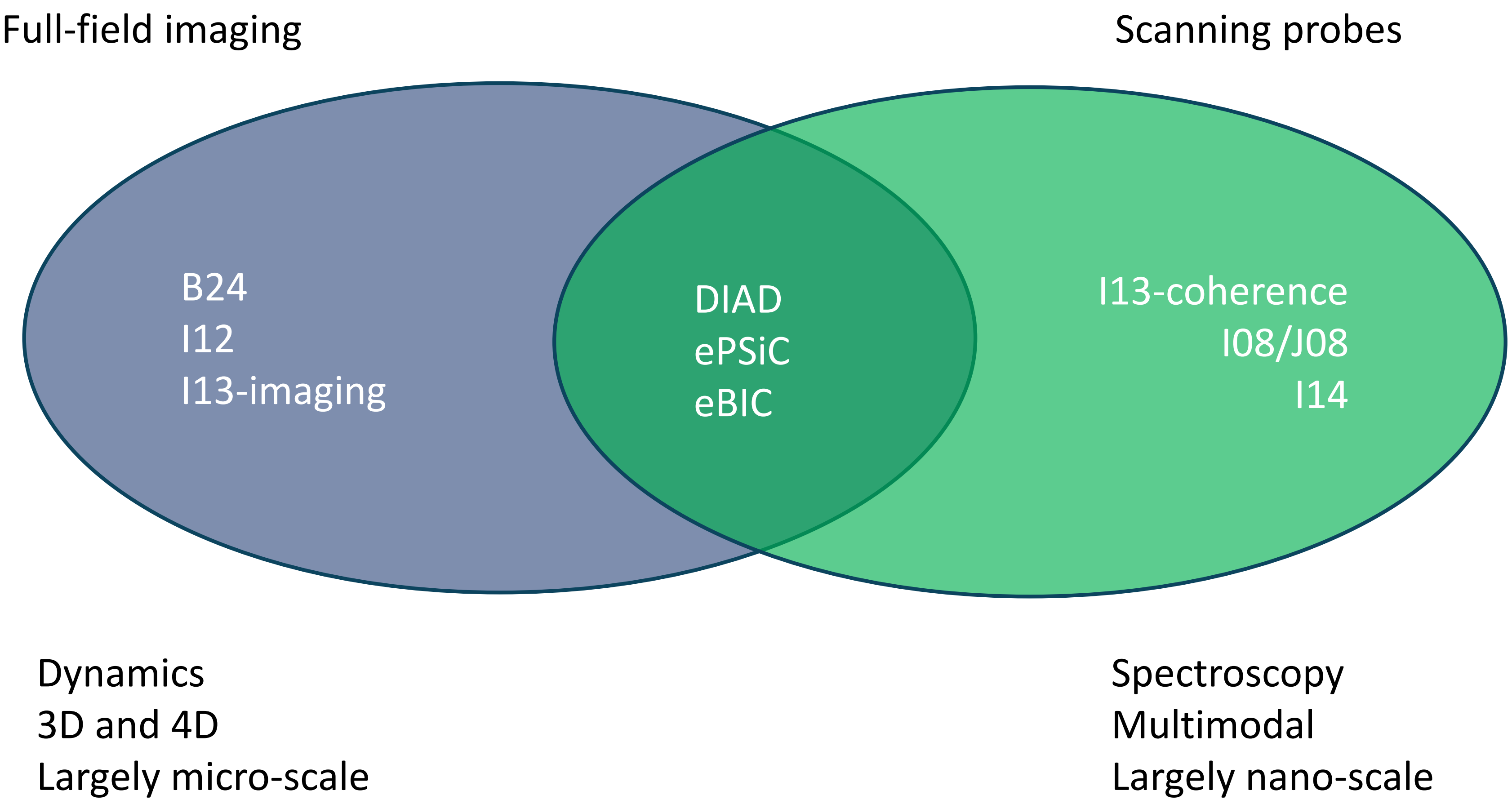
Magnetic Materials Group

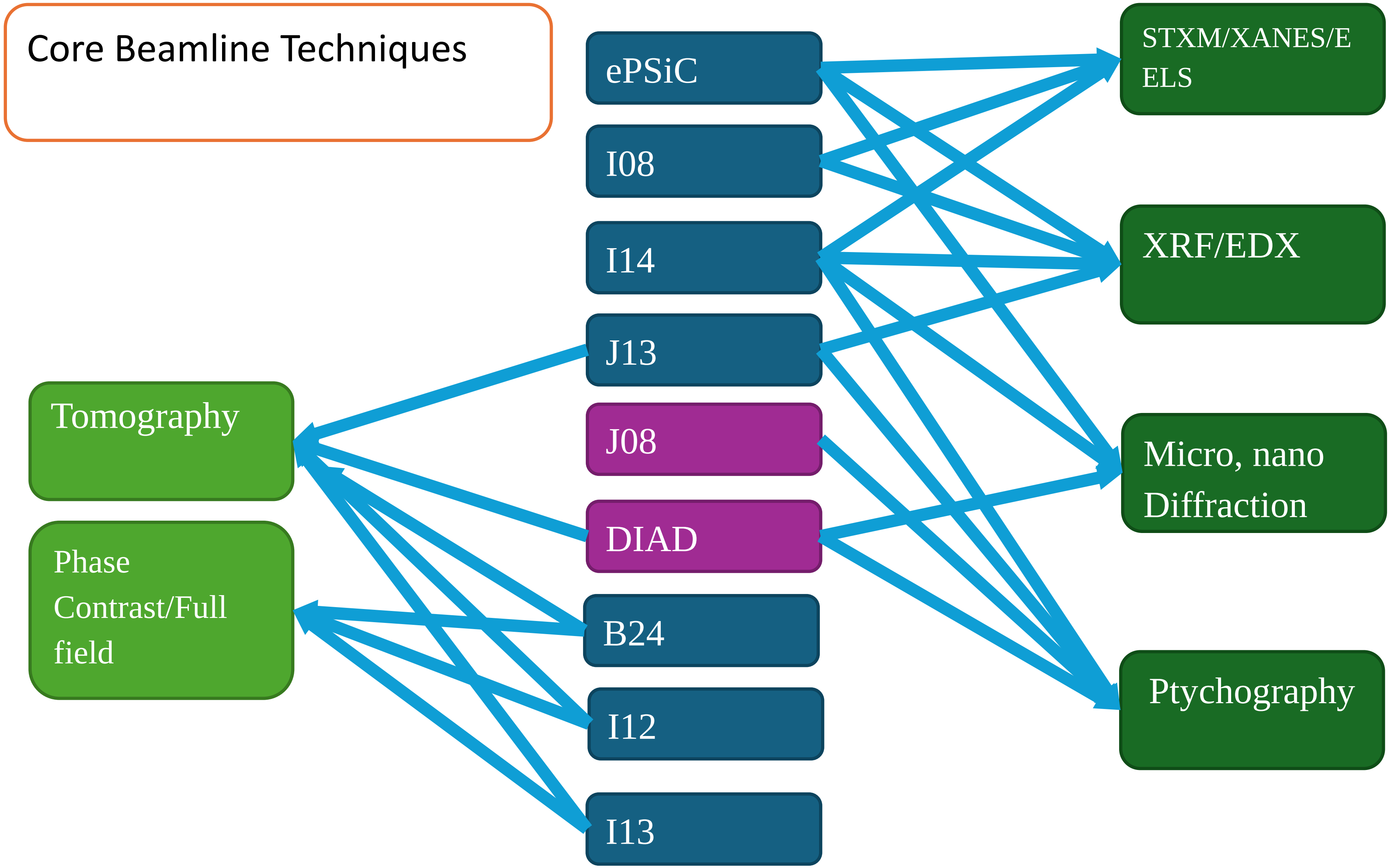
- I16 – Alessandro Bombardi
- I06 – Larissa Ishibe-Veiga
- I10 – Paul Steadman
- I21 – Kejin Zhou
- I17 – David Burn

Spectroscopy Scattering Imaging Dynamics



Diamond Imaging




Core Beamline Techniques
ePSiC
I08
I14
J13
J08
DIAD
B24
I12
I13
STXM/XANES/EELS
XRF/EDX
Micro, nano Diffraction
Ptychography
Tomography
Phase Contrast/Full field

RIXS - Superconducting nickelates

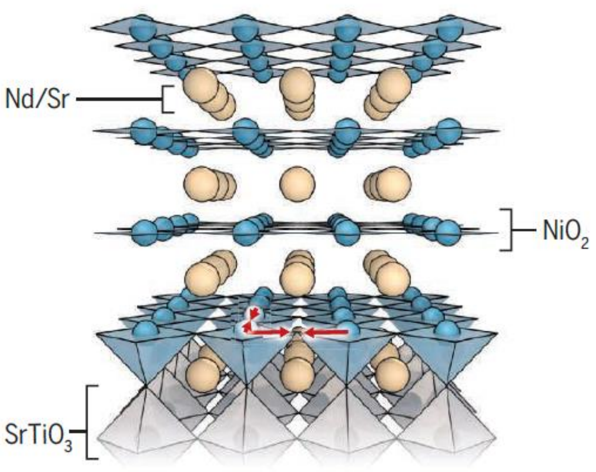
RESEARCH

SUPERCONDUCTIVITY

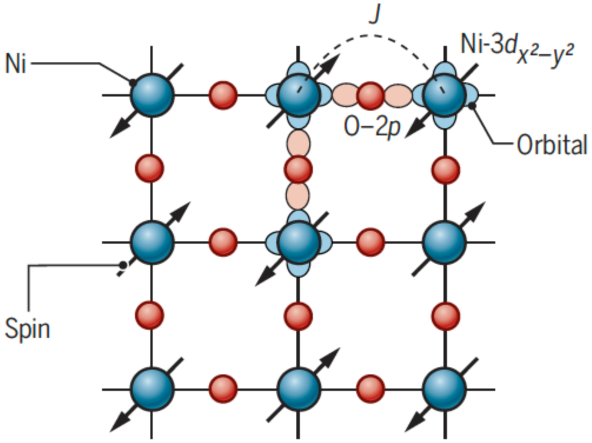
Magnetic excitations in infinite-layer nickelates

H. Lu[1,3], M. Rossi[1], A. Nag[2], M. Osada[3], D. F. Li[1]†, K. Lee[3], B. Y. Wang[3], M. Garcia-Fernandez[2], S. Agrestini[2], Z. X. Shen[1,3], E. M. Been[1], B. Moritz[1], T. P. Devereaux[1,3,4], J. Zaanen[5], H. Y. Hwang[1,3], Ke-Jin Zhou[2]*, W. S. Lee[1]*

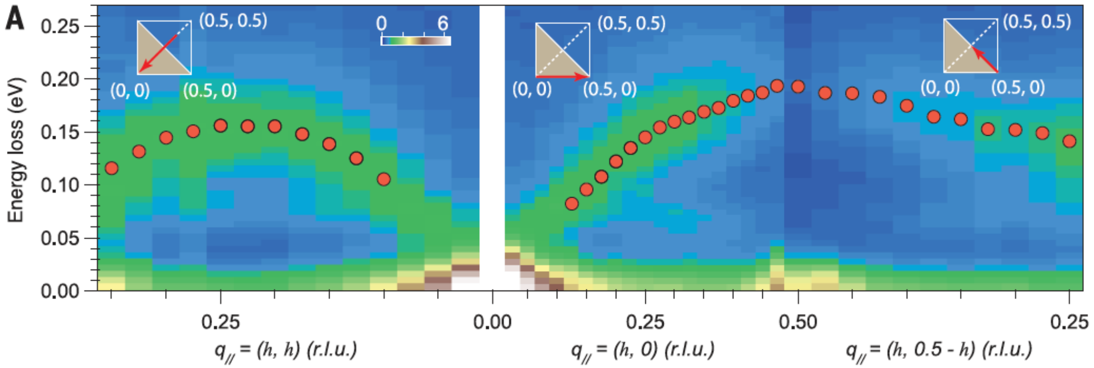
Superconducting nickelates

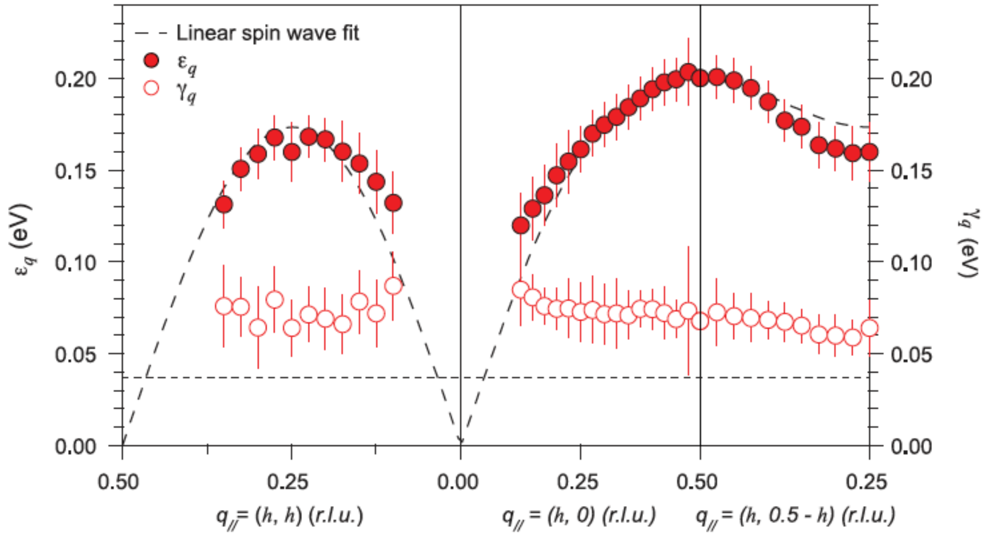


A structure on a substrate
The lattice mismatch with the $SrTiO_3$ substrate may affect the antiferromagnetic superexchange coupling (J).



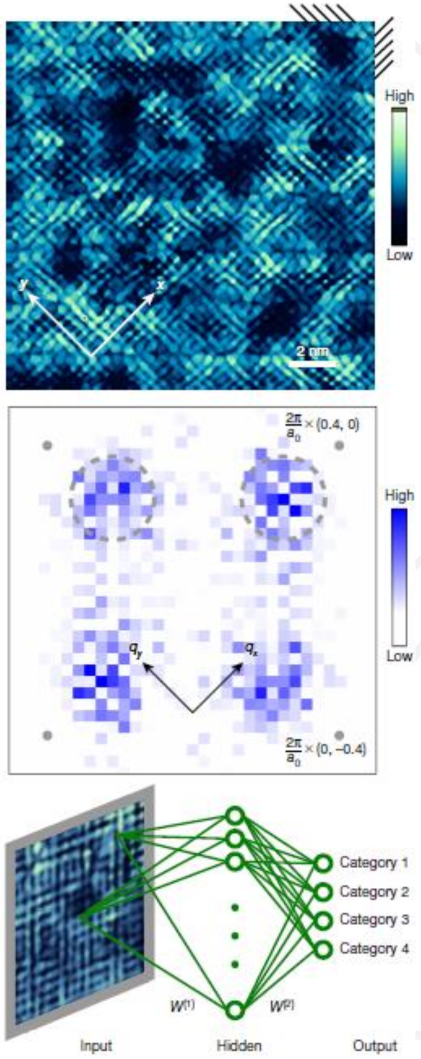
Magnetic interactions in the NiO_2 planes
Antiferromagnetic coupling of neighboring Ni spins arises from exchange interaction involving specific oxygen orbitals.





H. Lu *et al.*
Science **373**, 213-216 (2021)

Machine Learning and AI



Y. Zhang *et al.*, Nature **570**, 484 (2019)

Machine learning in electronic quantum matter imaging

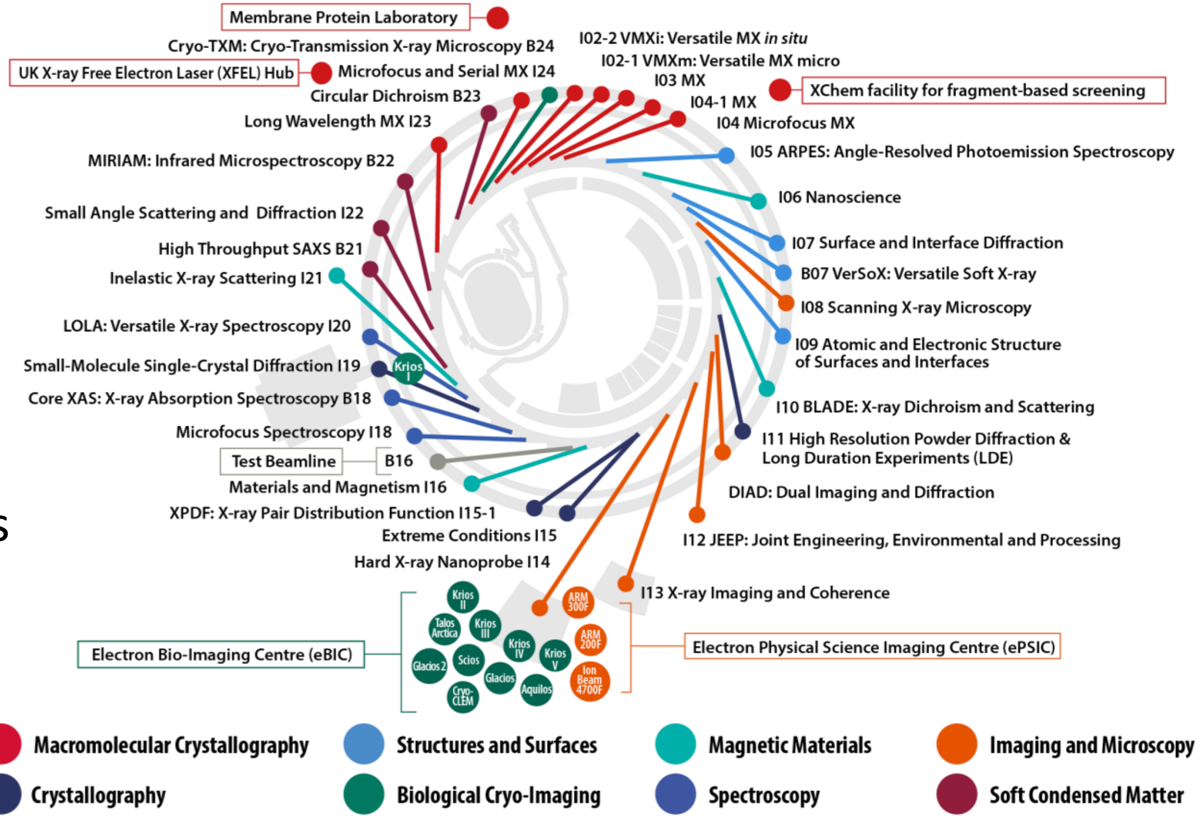
Strong Coulomb interactions produce charge localisation in an antiferromagnetic Mott insulator whilst hole doping leads to a pseudogap phase with rotational and translational symmetry breaking (perhaps).

Vast spectroscopic STM datasets from high-temperature superconductors exist, but often with considerable disorder and complexity in the mages.

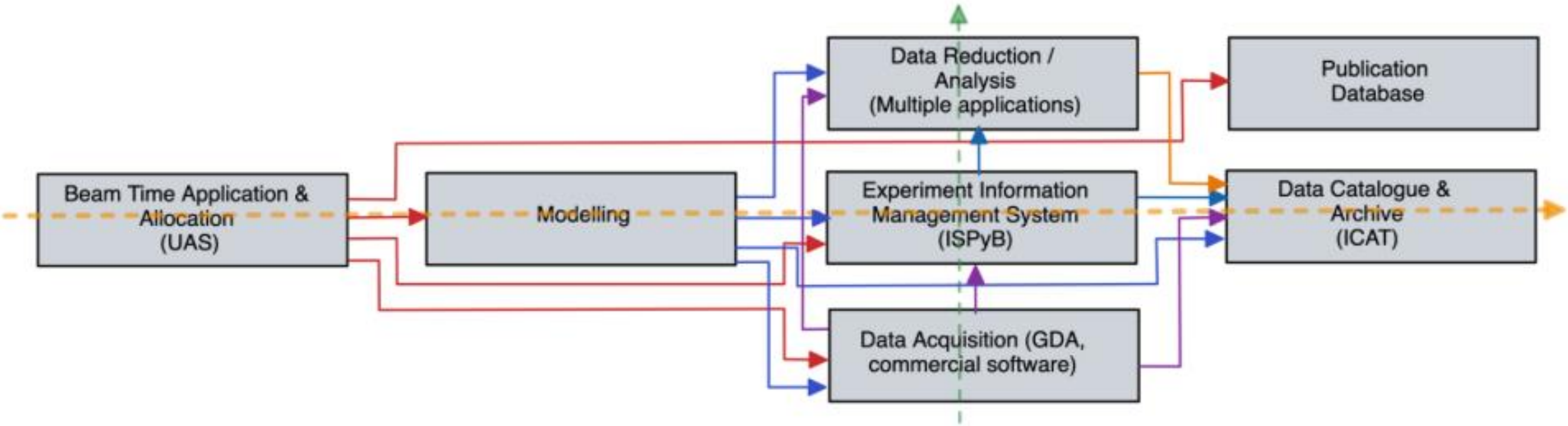
From the many noisy and complex datasets of spectroscopic STM images, ML has revealed the existence of a 4 unit-cell translational symmetry breaking phase within the pseudogap phase.

Diamond Light Source

- The UK's national synchrotron radiation facility, funded by Government (86%) and the Wellcome Trust (14%).
- Since starting operations in 2007 it has:
  - served over 14,000 scientists from academia and industry
  - hosted over 220 companies paying for commercial access, across multiple sectors
  - provided training for 8,000 PhD students
  - hosted over 6,000 visitors each year
- We have:
  - 33 beamlines
  - 36 independently operating instruments
  - 11 electron microscopes for Physical and Life sciences

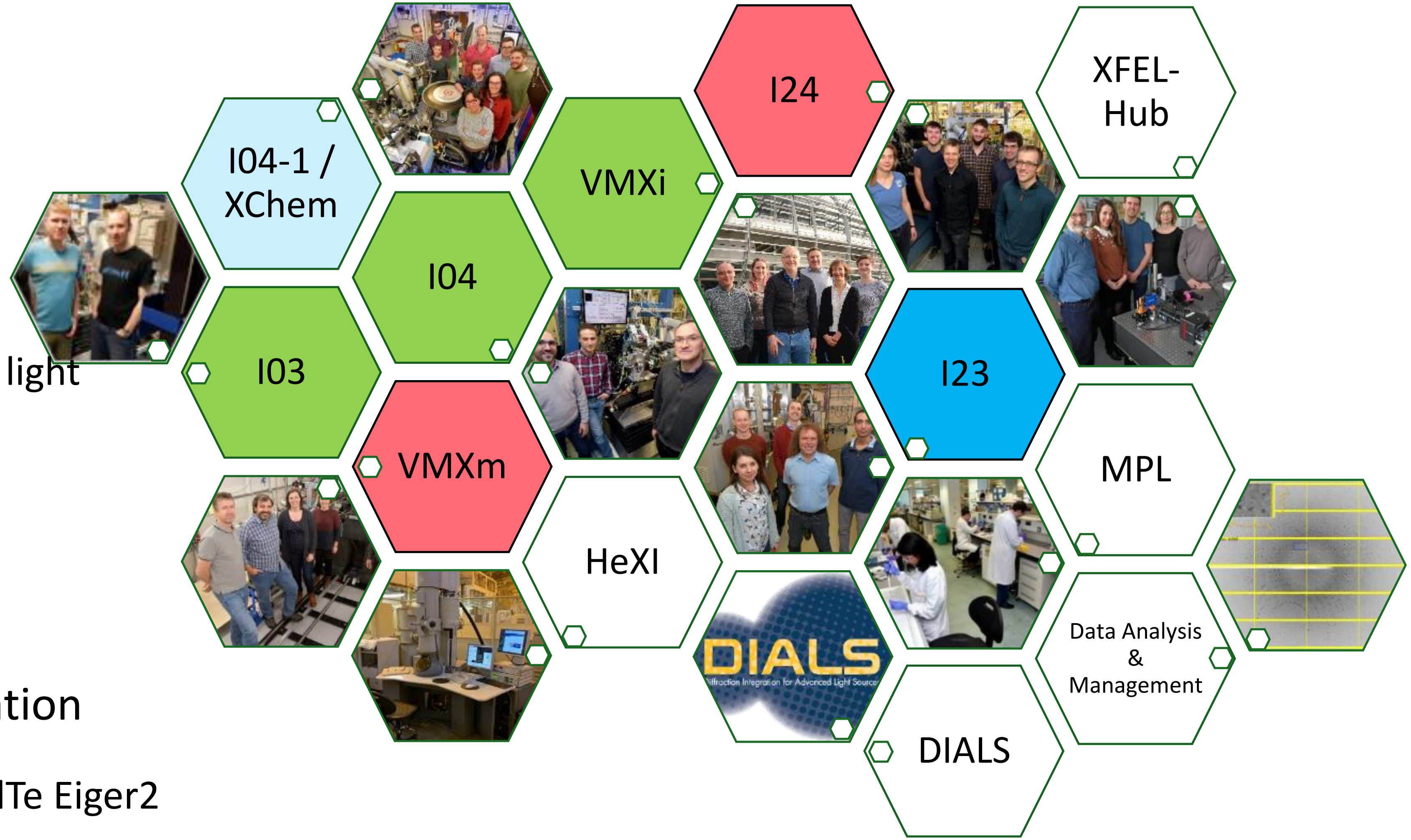


Not only the hardware but also a total redesign of software and controls

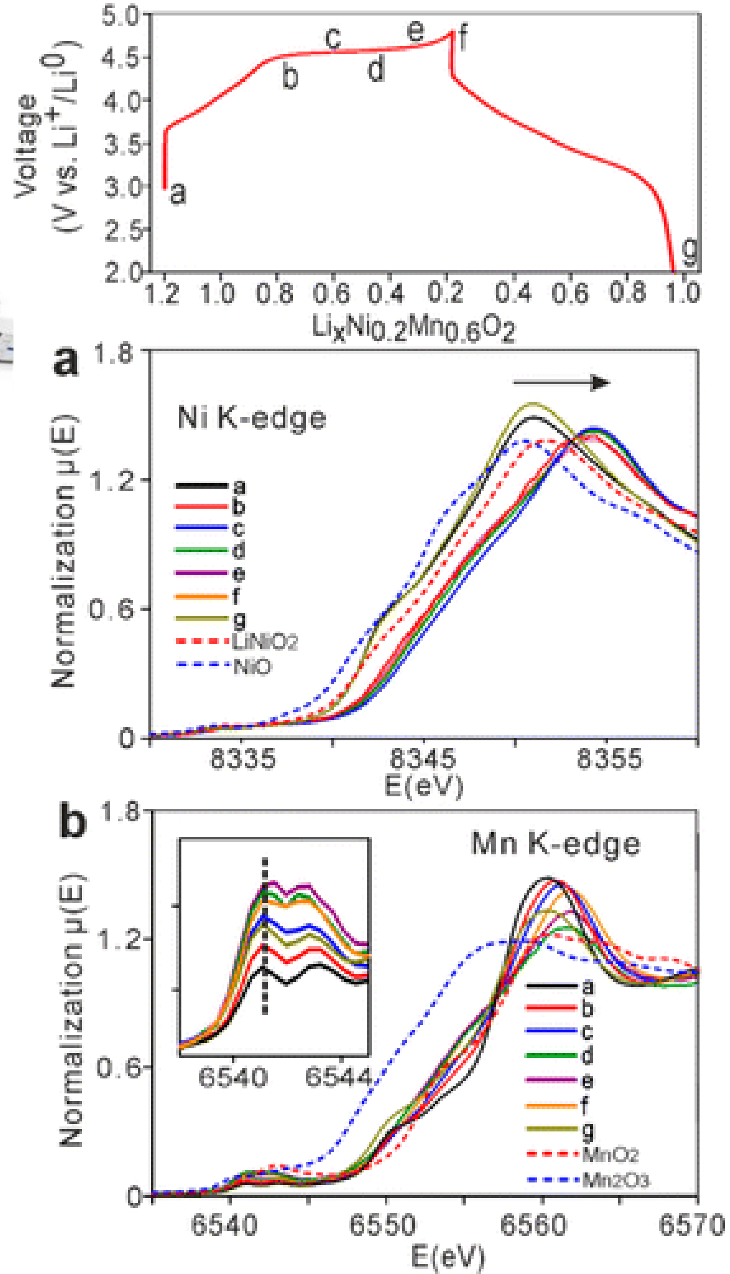


Energy Extremes – Low (2.1keV) to High (28 keV)

- All tuneable (except I04-1)
- High resolution data
- Metal identification
  - I23 uniquely equipped to look at light elements such as Na, K, Cl
  - Assist model building (S, P)
- Phasing
- High energies – minimising radiation damage
  - I24 and VMXm equipped with CdTe Eiger2 9M detectors



Li ion batteries charge/discharge mechanism

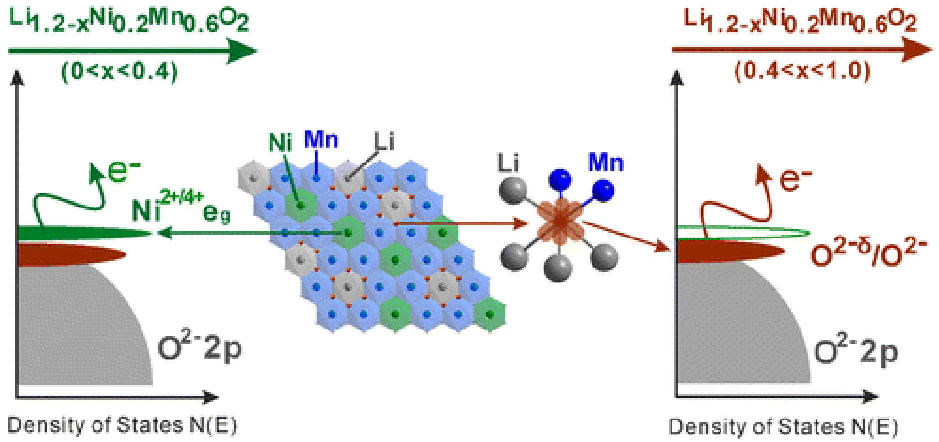


nature chemistry | ARTICLES

PUBLISHED ONLINE: 21 MARCH 2016 | DOI: 10.1038/NCHEM.2471

Charge-compensation in 3*d*-transition-metal-oxide intercalation cathodes through the generation of localized electron holes on oxygen

Kun Luo[1†], Matthew R. Roberts[1†], Rong Hao[1], Niccoló Guerrini[1], David M. Pickup[2], Yi-Sheng Liu[3], Kristina Edström[4], Jinghua Guo[3], Alan V. Chadwick[2], Laurent C. Duda[5] and Peter G. Bruce[1*]



Energy materials

Courtesy of Diego Gianolio

Diamond-II | Advancing Science

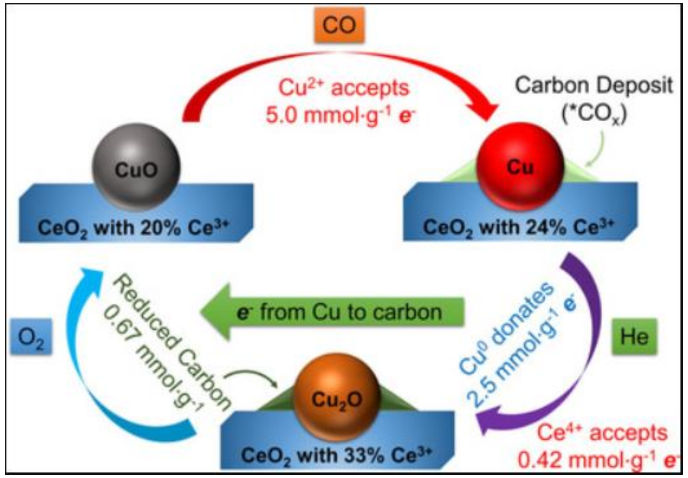
Angewandte Chemie International Edition
GDCh A Journal of the German Chemical Society

Research Article | Open Access

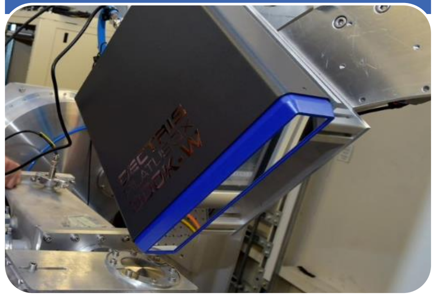
The Electrophilicity of Surface Carbon Species in the Redox Reactions of CuO-CeO_2 Catalysts

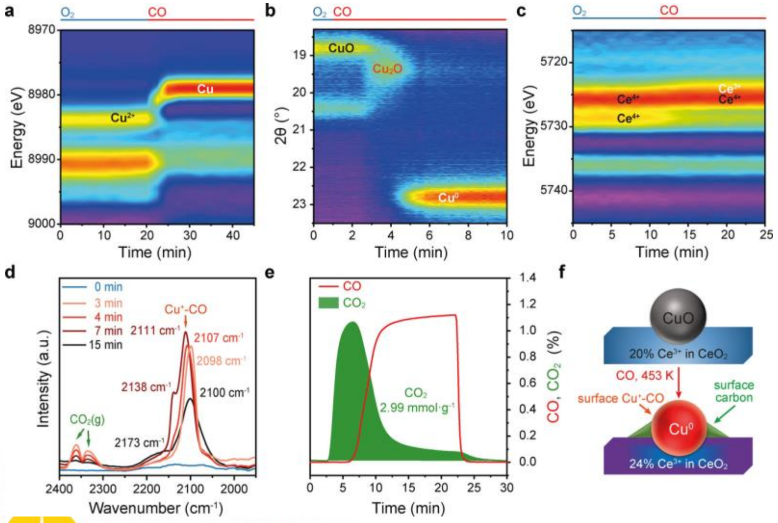
Liqun Kang, Dr. Bolun Wang, Dr. Andreas T. Güntner, Siyuan Xu, Xuhao Wan, Yiyun Liu, Sushila Marlow, Yifei Ren, Dr. Diego Gianolio, Dr. Chiu C. Tang, Dr. Vadim Murzin ... See all authors

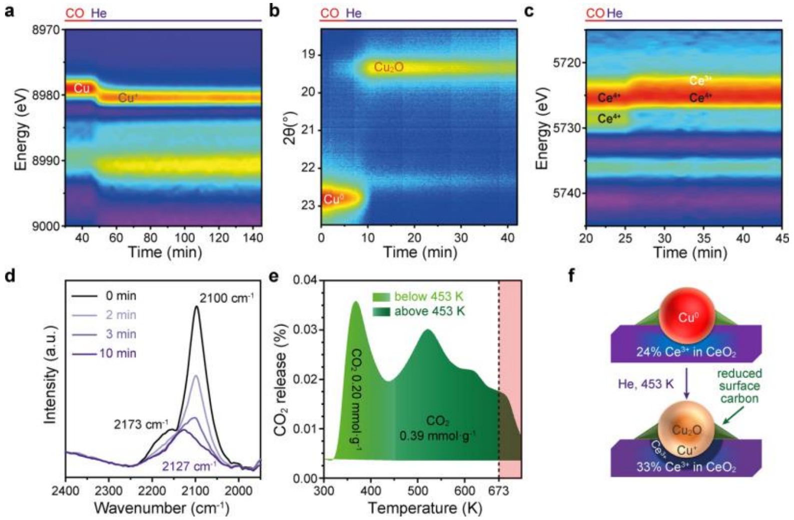
First published: 17 March 2021 | https://doi.org/10.1002/anie.202102570 | Citations: 4

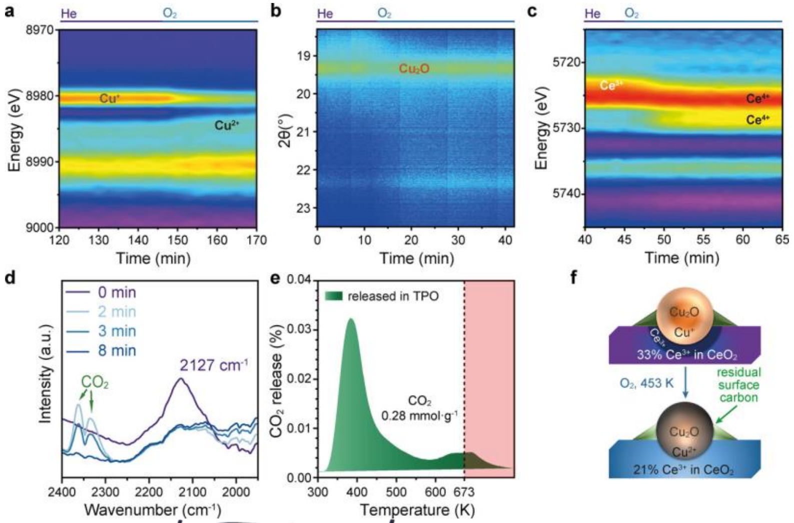


Prof. R. Wang UCL,
procurement and commissioning of Pilatus detector in B18









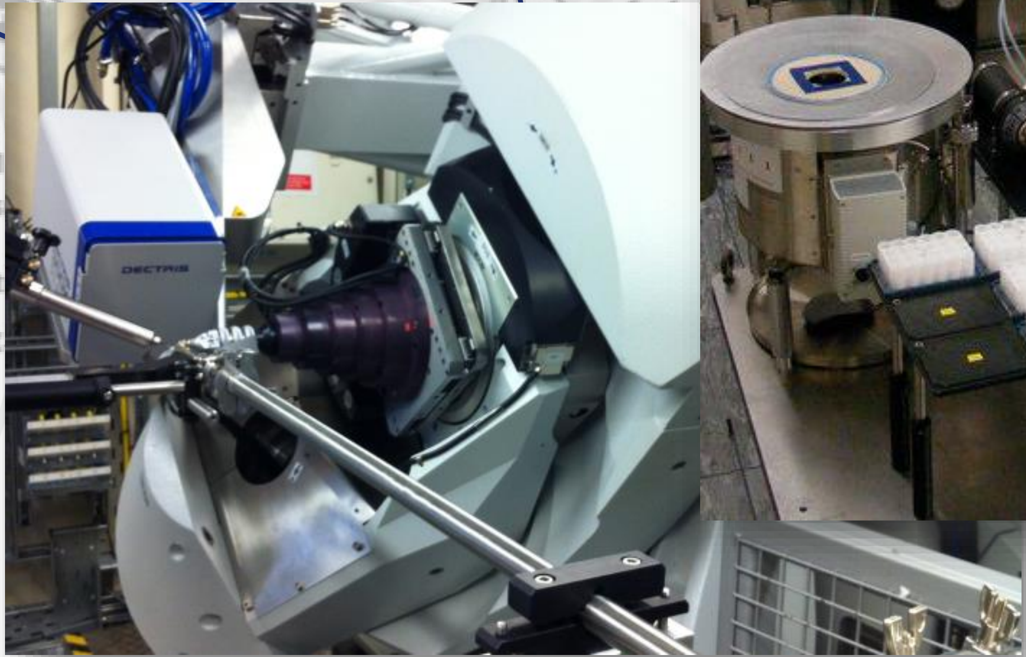
Courtesy of Diego Gianolio

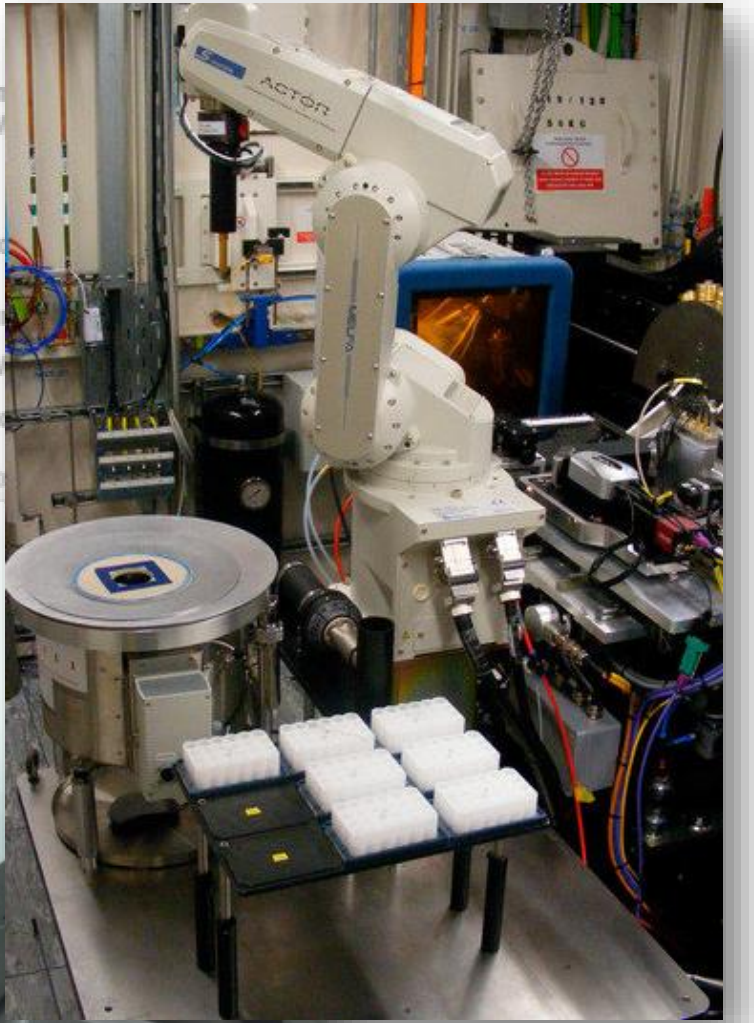
Diamond-II | Advancing Science

I19 Small-Molecule Single-Crystal Diffraction

- Undulator, 5 – 25 keV (2.5 – 0.5 Å)
- EH1 for standard chemical crystallography, 85 × 65 um beam with pin/col to 30 um
- EH2 for in situ, time resolved, DAC…
  100 × 120 um beam with pin/col to 50 um

Small-Molecule Single-Crystal Diffraction I19

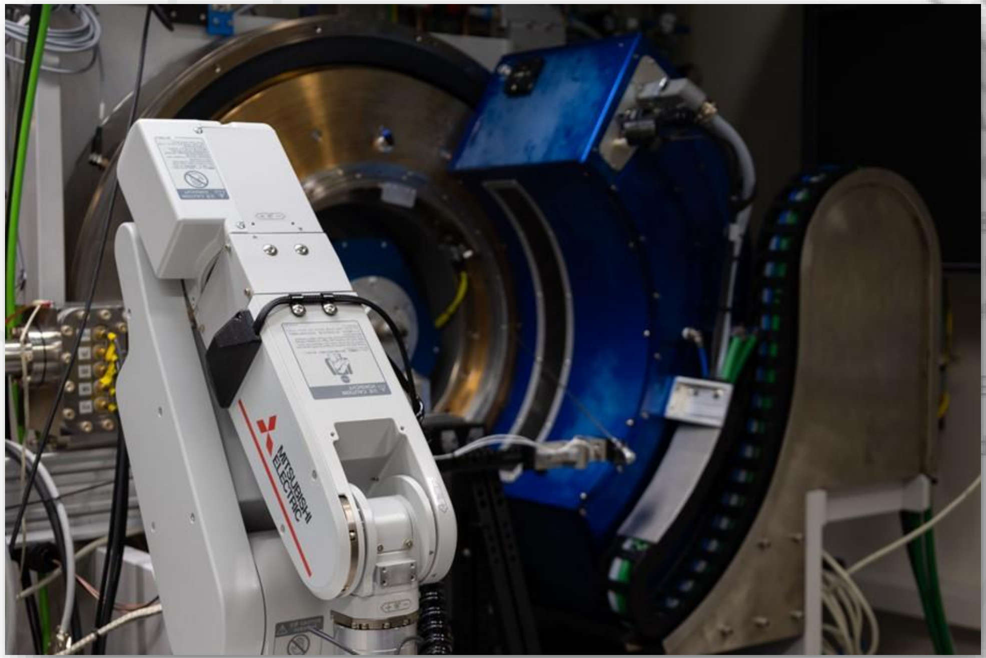


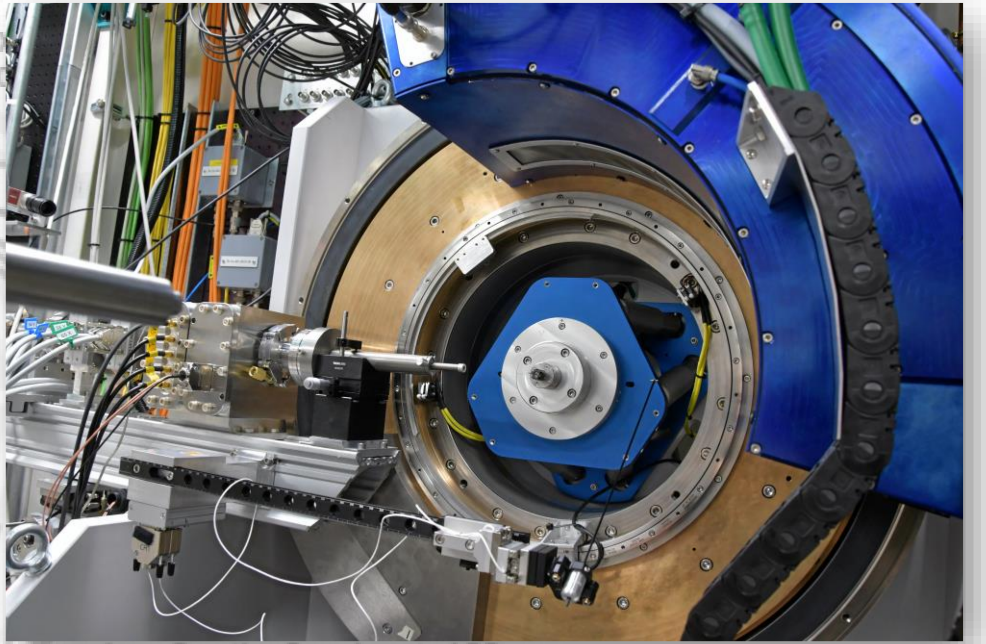


I15-1 X-ray Pair Distribution Function

- Wiggler, 40, 65 or 76 keV (0.31, 0.19 or 0.16 Å)
- 700 (H) × 10-150 (V) µm

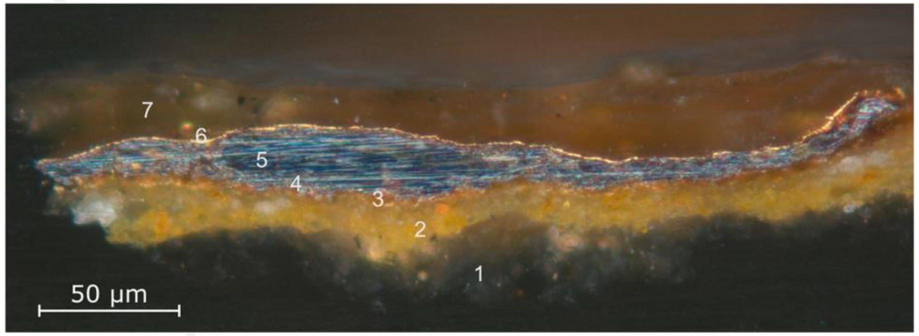
XPDF I15-1

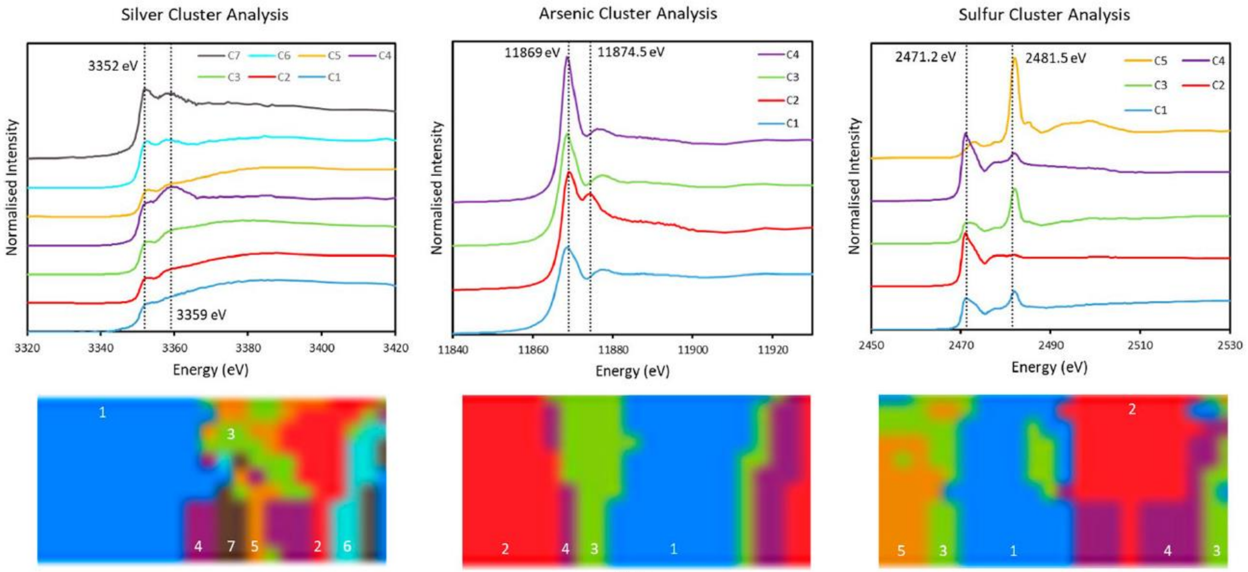




I18 Science Highlight

Degradation of Fourteenth-century Mordant Gilding Layers: Synchrotron based Microfocus XRF, XRD, and XANES Analyses of Two Paintings by Pietro Lorenzetti



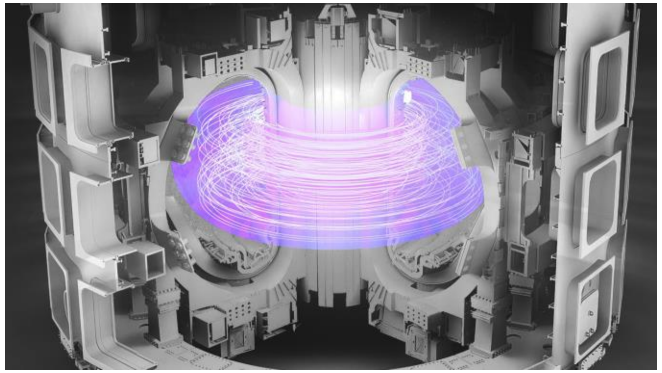


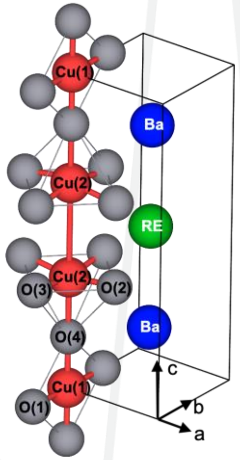
The thin layer of silver leaf has either reacted with surrounding sulfur-bearing compounds in the orpiment or atmospheric hydrogen sulfide. The darkening of the mordant was most likely caused by finely dispersed grey-coloured silver sulfide particles, although it also contains some silver oxide. There is evidence of arsenolite.

I20 Science Highlight

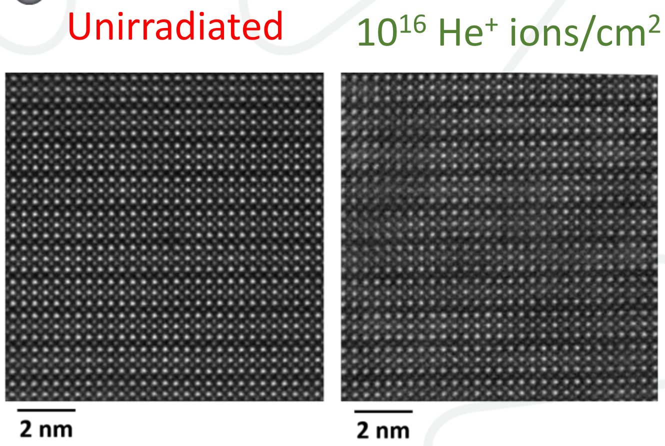
Understanding irradiation damage in high-temperature superconductors for fusion reactors using high resolution X-ray absorption spectroscopy

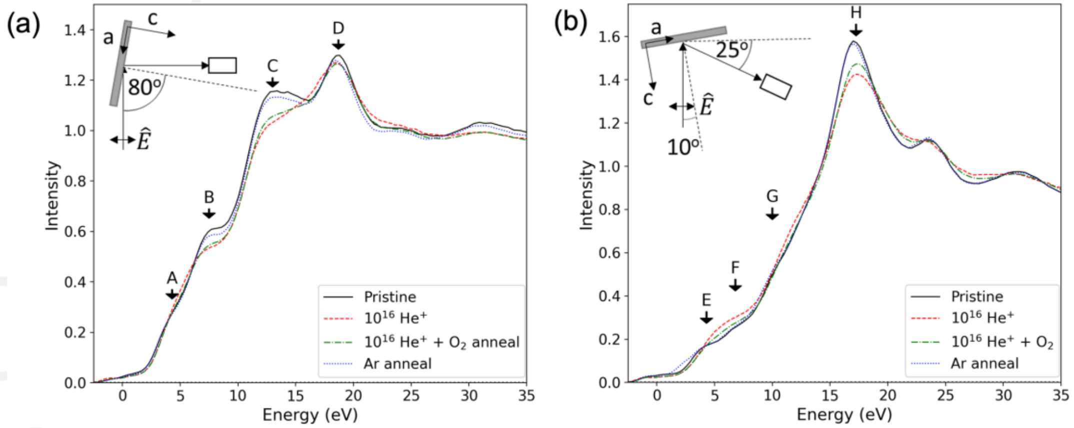
One of the most promising alternatives to clean energy is fusion, and tokamaks are considered the solution for commercial options. A tokamak uses high magnetic fields to confine the plasma in which the deuterium/tritium reaction takes place.

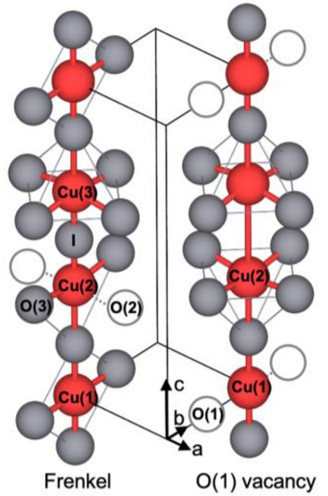




The most promising high-temperature superconducting materials for small fusion tokamaks are rare-earth barium copper oxides. However, tokamaks produce high energy neutrons that supress the superconducting properties of the oxide.

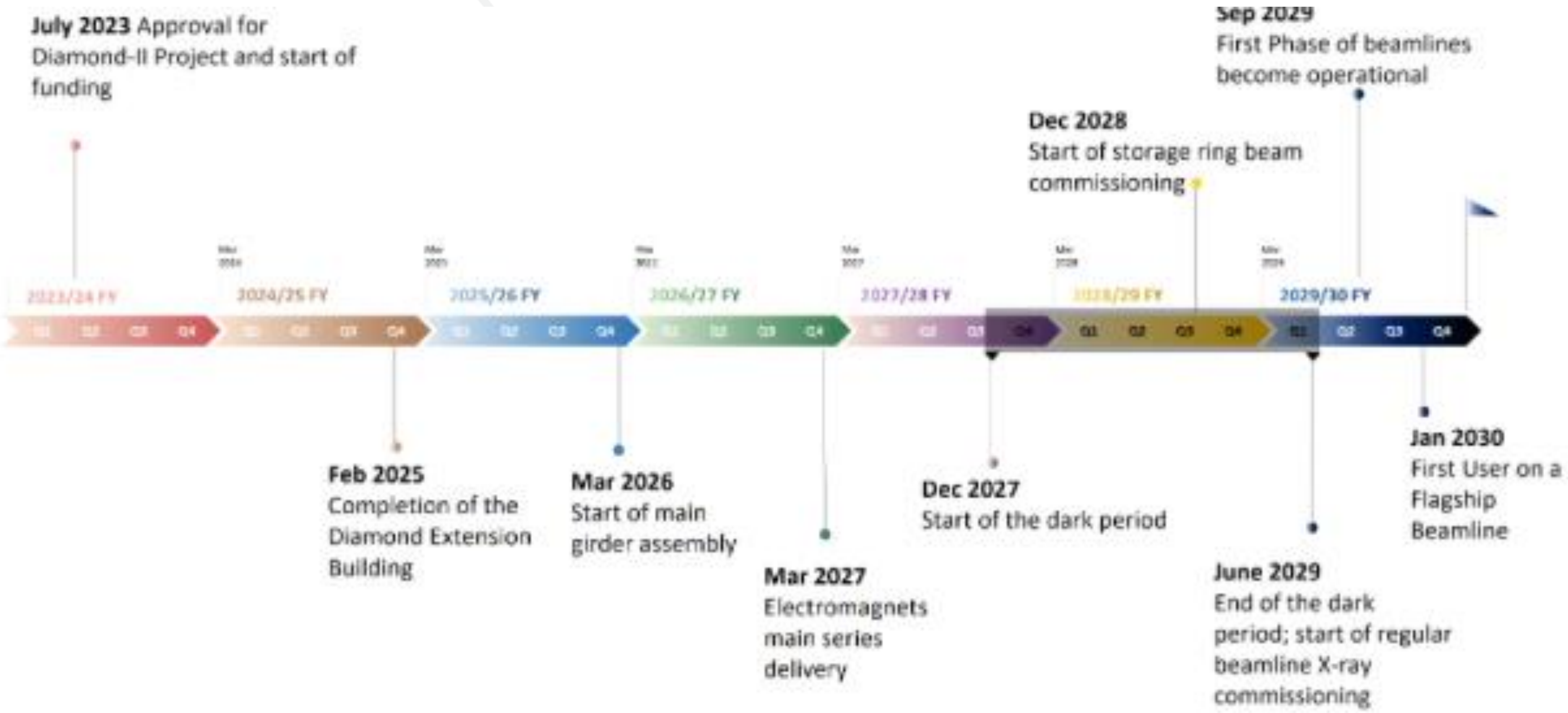






Thank you!

Timelines



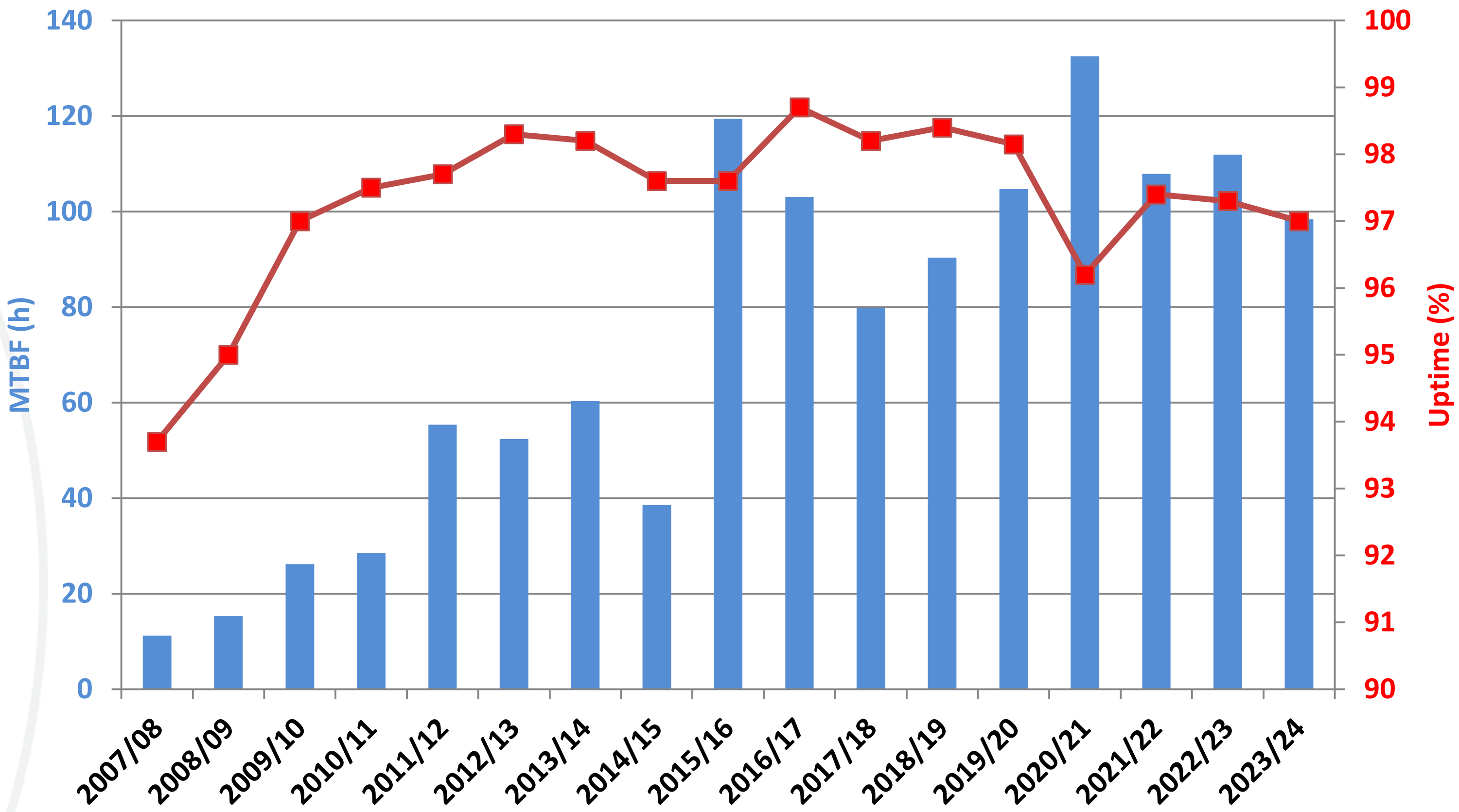
diamond

Diamond-II Design Goals and Main Features

- ❖ Increased brightness and coherence → low emittance MBA lattice
  → increase in energy from 3 GeV to 3.5 GeV
- ❖ Increased capacity for insertion devices → inclusion of 'mid straights' in a 6BA lattice
- ❖ Maintain ID source points where possible → adjustment of straight section lengths
- ❖ Minimise downtime → detailed planning
  → do what is possible before the dark period
  many activities already underway

Diamond Operations FY 23/24

- 4822 hours of User operation
- Mean Time Between Failures (MTBF) 98.4h
- All 5 operating Runs MTBF > 72 h target
- Up-time 97.0%



Thank you!

Diamond-II: Use of the 24 mid-straights

- 2 used to maintain two existing mid-straight ID beamlines which would be lost without mid-straights
- 2 for IDs for new Diamond-II flagship beamlines
- 4 will be used to convert existing bending magnet beamlines into ID beamlines
- **5 reserved for future ID beamlines**

- 5 will be used for RF cavities
- 1 will be used as part of the injection scheme
- 1 will be used for diagnostics
- 1 allocated for beam abort kickers
- 3 unallocated

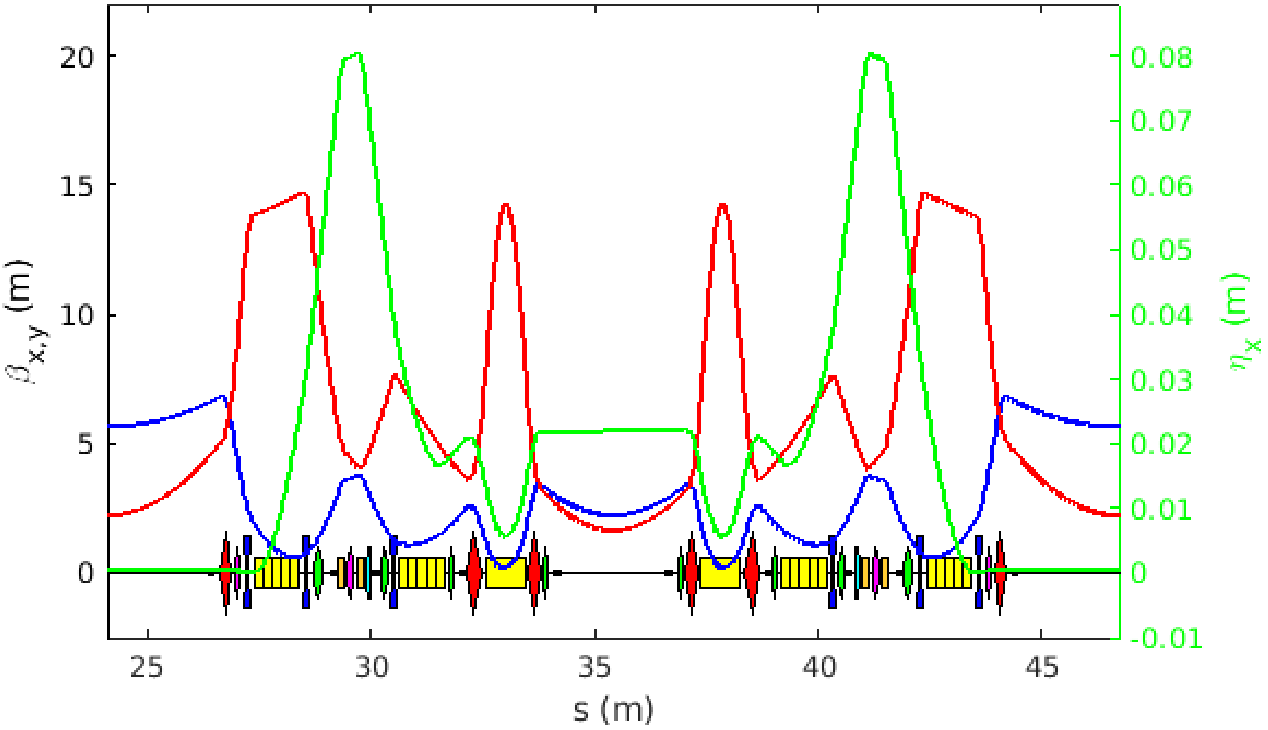
Note] none of these straights could be used for new IDs as there is no space on the experimental hall floor for a beamline.

diamond

Diamond-II Lattice Design

The Diamond-II lattice is a 'Modified Hybrid 6 Bend Achromat', which combines two concepts:

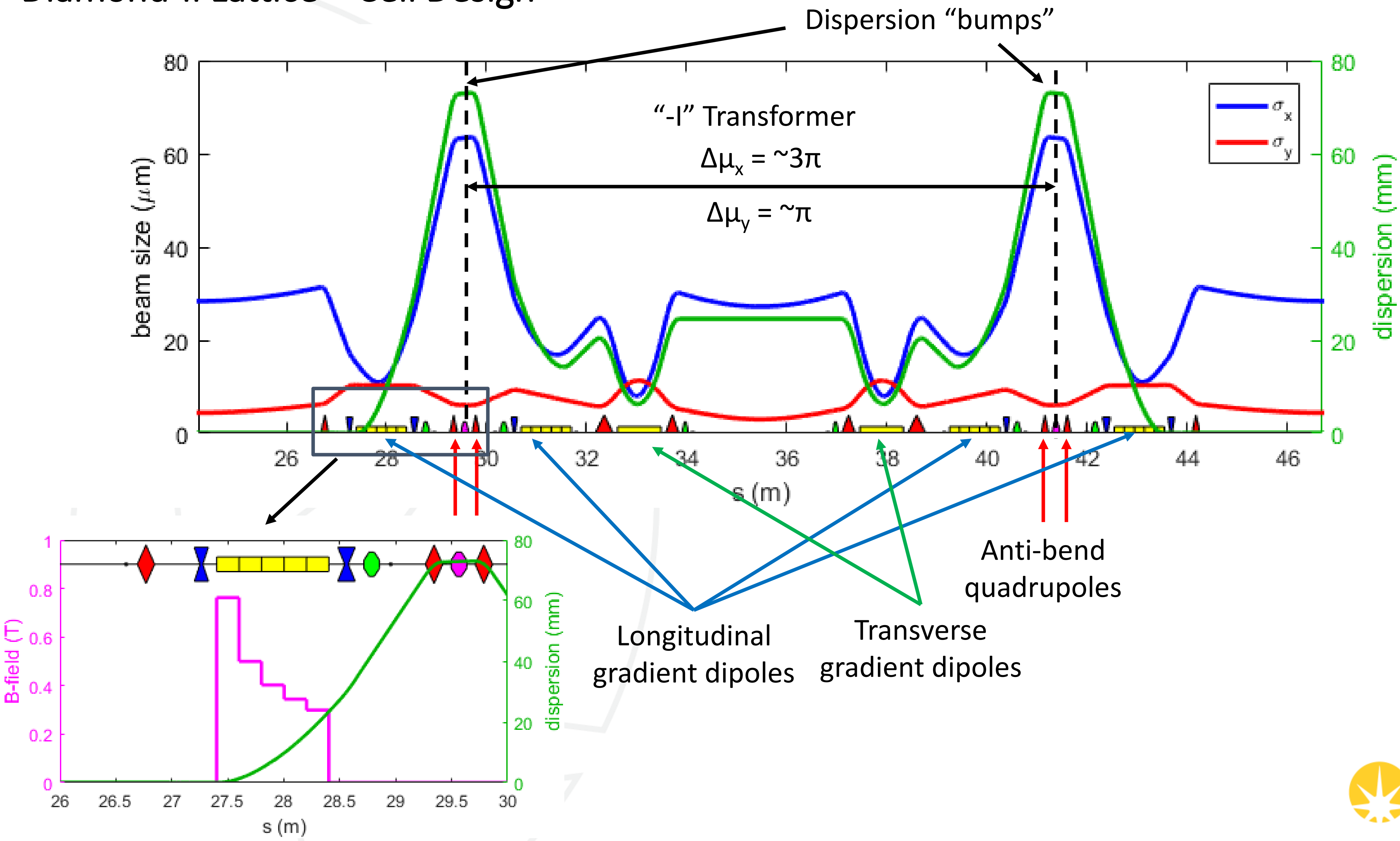
- The ESRF-EBS cell (Hybrid 7 Bend Achromat)
- The Diamond Double-Double Bend Achromat (DDBA) cell



	Diamond	Diamond-II
Lattice Type	DBA	M-H6BA
Circumference	561.6 m	560.561 m
Total Bend Angle	360º	388.8º
Straight Sections	24	48
Energy	3 GeV	3.5 GeV
Beam Current	300 mA	300 mA
Natural Emittance	2.7 nm.rad	161 pm.rad
Natural Energy Spread	0.096 %	0.094 %
Long Straight (x6) Length	11.3 m	7.545 m
Standard Straight (x18) Length	8.3 m	5.065 m
Mid-straight (x24) Length	-	2.872 m
Lattice magnets per cell	19	36(37)

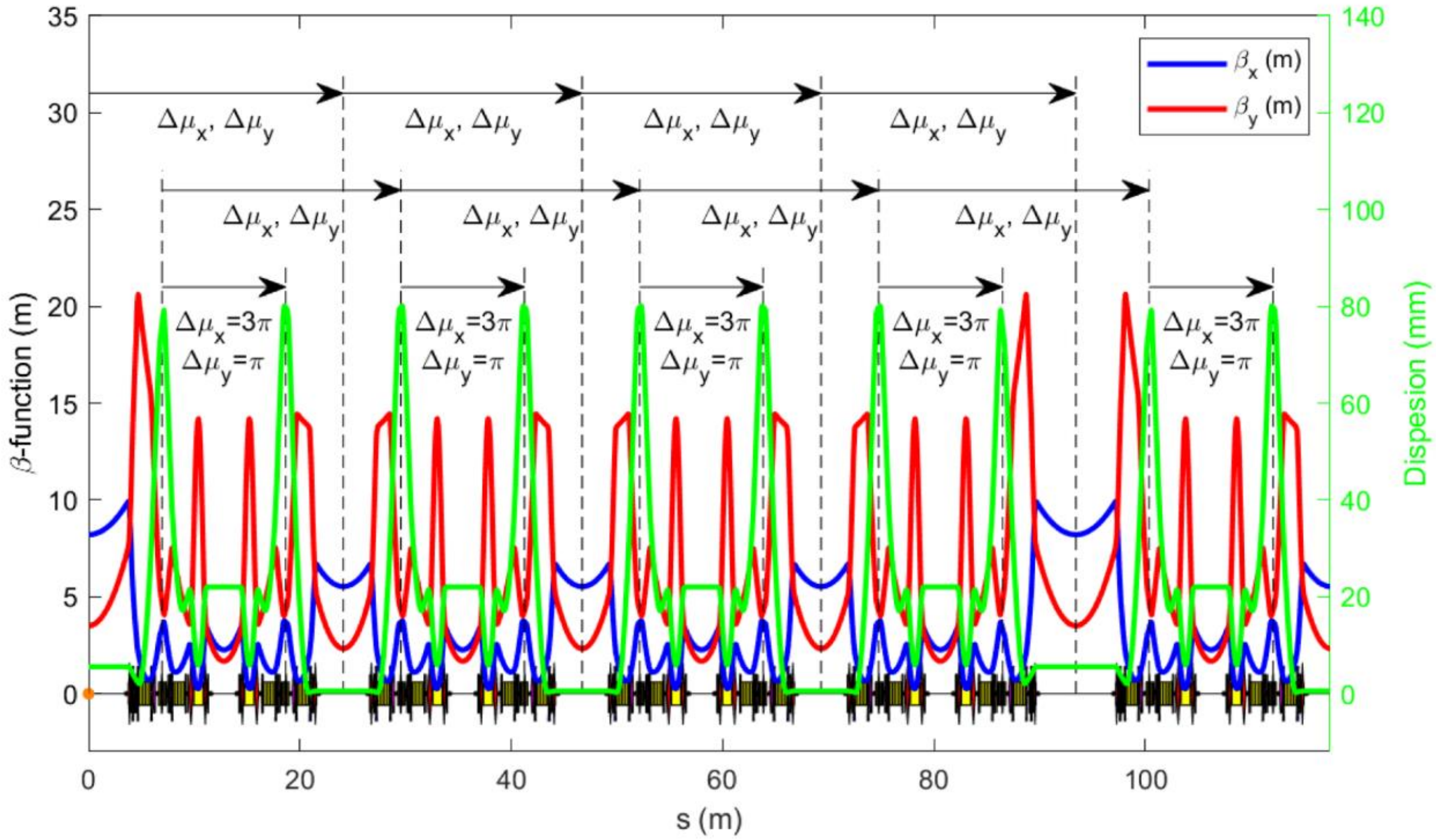
diamond

Diamond-II Lattice – Cell Design



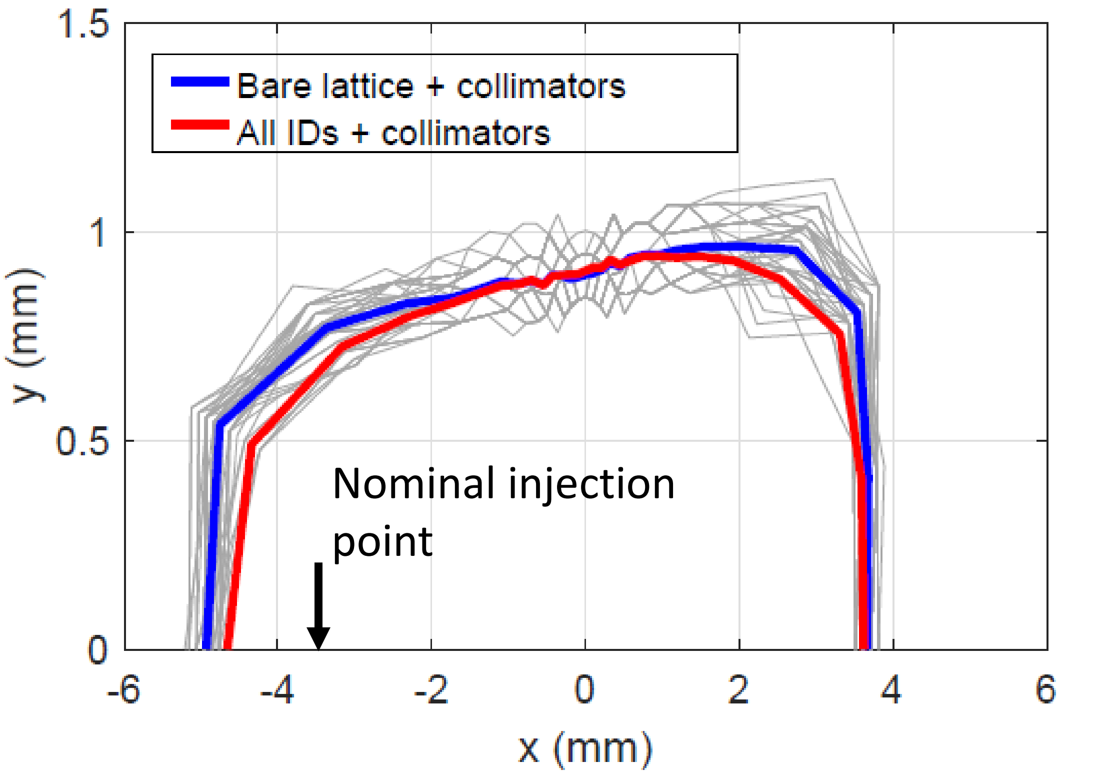
diamond

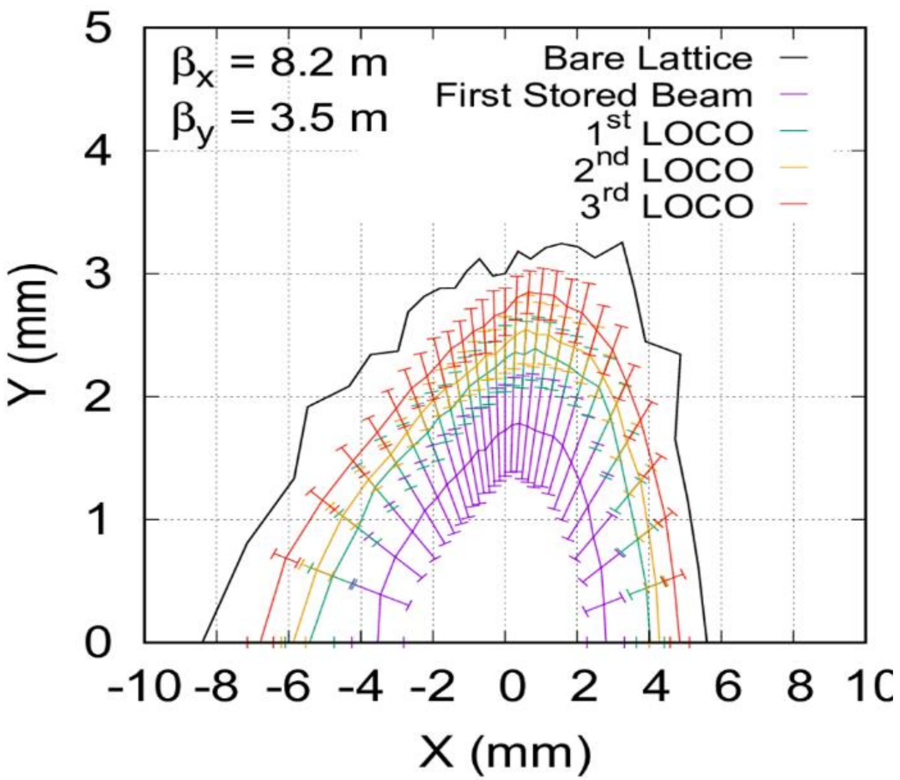
Diamond-II Lattice – Super-period Design



- Diamond (and Diamond-II) has 6-fold symmetry.
- “pseudo- symmetry” - fixing the cell tunes to be the same regardless of whether they contain long or standard straight sections has also been found to be beneficial for non-linear dynamics.

Diamond-II Lattice – Performance



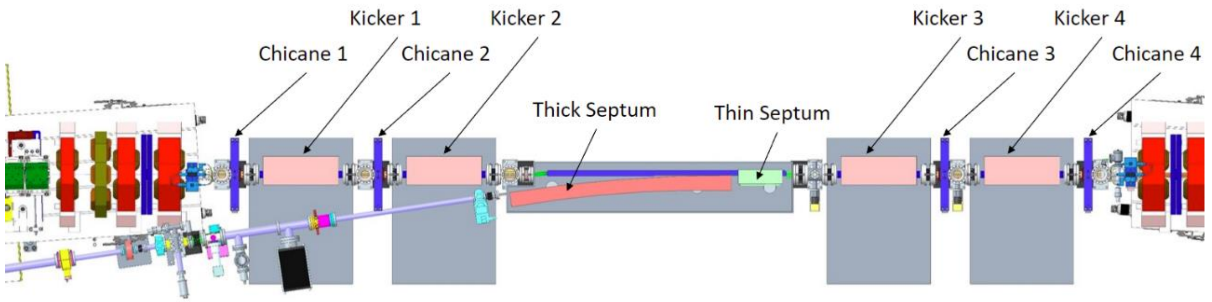


- Dynamic Aperture from 6D tracking including physical apertures (including collimators), magnet alignment and multipole errors after simulated commissioning.

- Detailed simulated commissioning calculations have been carried out to show sufficient dynamic aperture is available at each stage of commissioning. (This is with collimators open).

Injection – two different schemes

1) **Standard four-kicker bump** (single/multi-bunch)

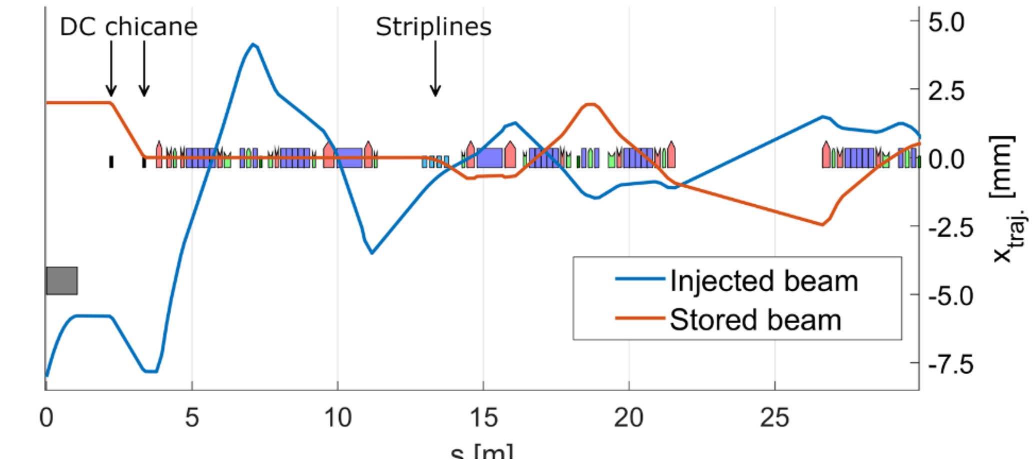


- Robust, proven technology
- Can be used for single shot on-axis injection (during commissioning), and off-axis accumulation.
- Baseline injection scheme for re-filling during operations

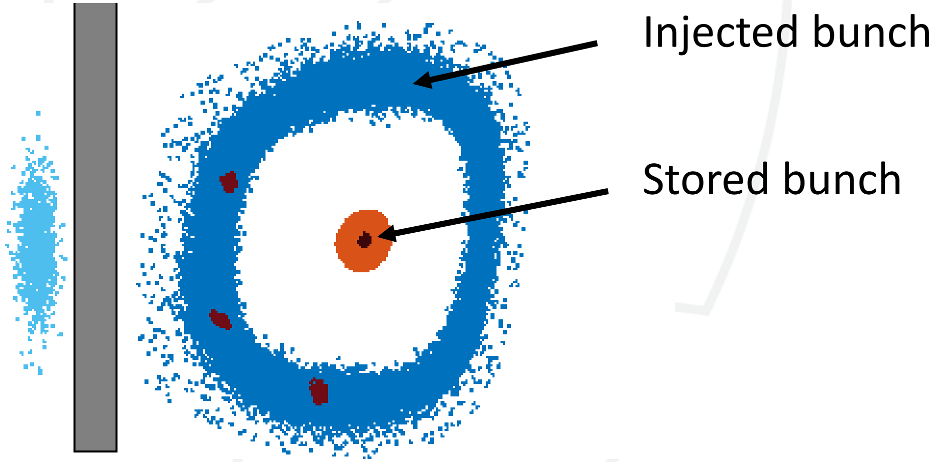
2) **Stripline kicker injection** (single bunch)

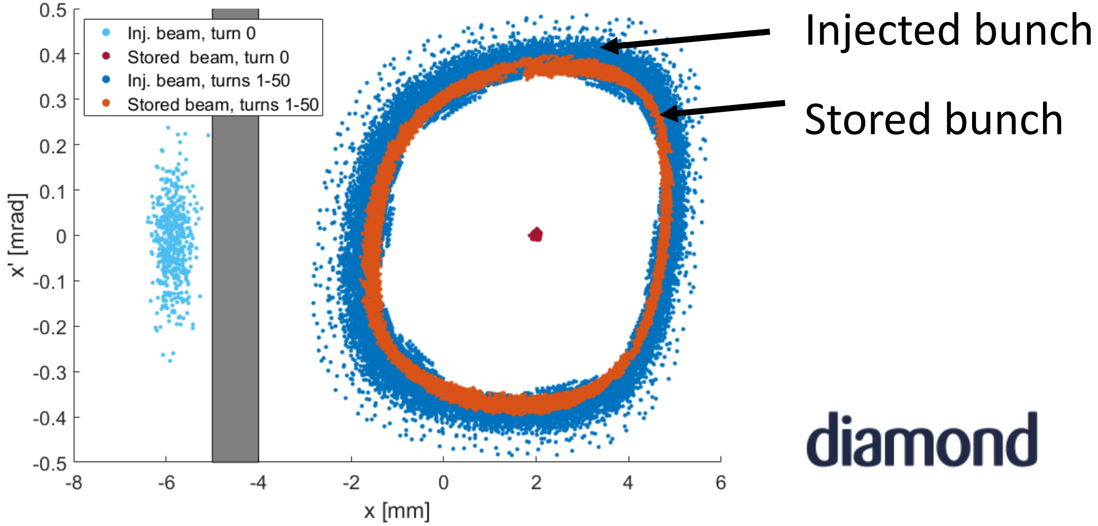
- For transparent injection during top-up in user-mode
- Two modes, “aperture sharing” and “kick-and-cancel”

Aperture sharing injection:



Kick-and-cancel injection:





diamond

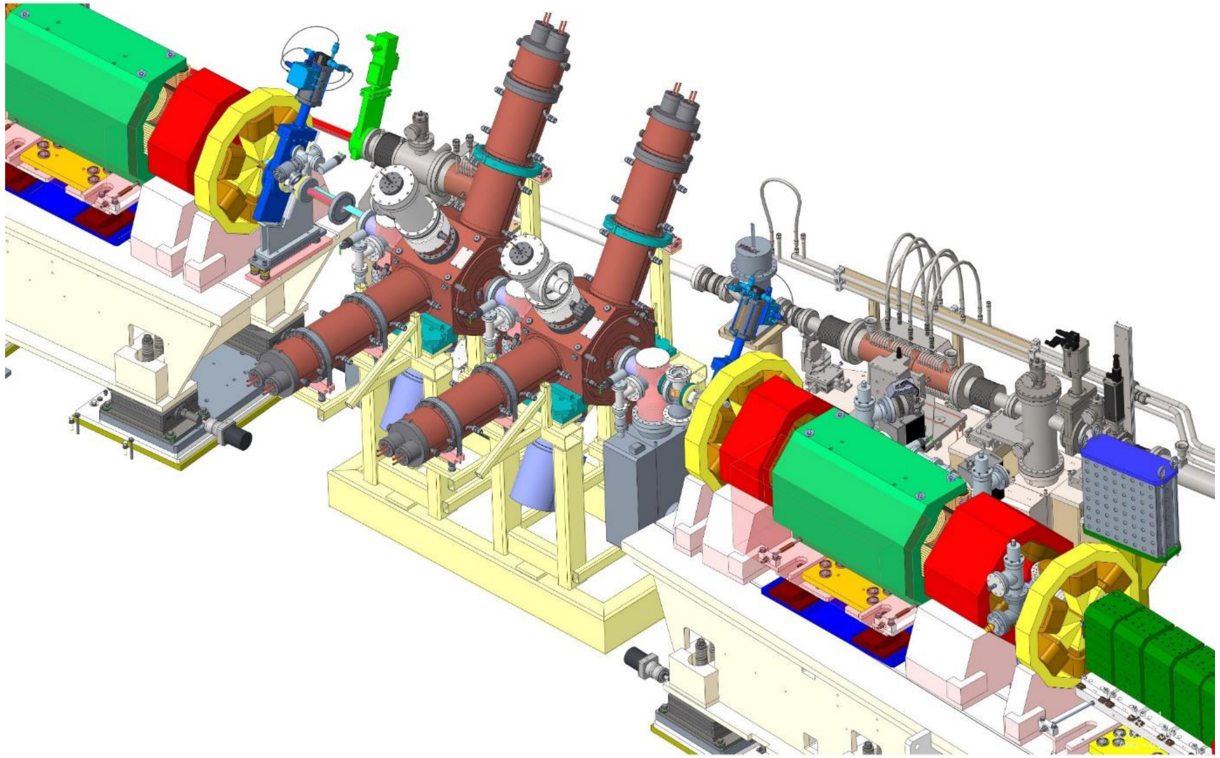
Radiofrequency

- **8 x 500 MHz EU normal conducting HOM damped cavitie**s, to replace the existing superconducting cavities which can't operate at the new storage ring RF frequency.

- The new cavities will be distributed around the ring, in pairs in the mid-straights. This frees the long RF straight for use for the ID for one of the new 'flagship' beamlines.

- Each cavity will be powered by an individual **120 kW solid-state amplifier**, replacing the unreliable and now obsolete IOT amplifiers.

- A passive superconducting **3rd harmonic cavity** will also be installed.



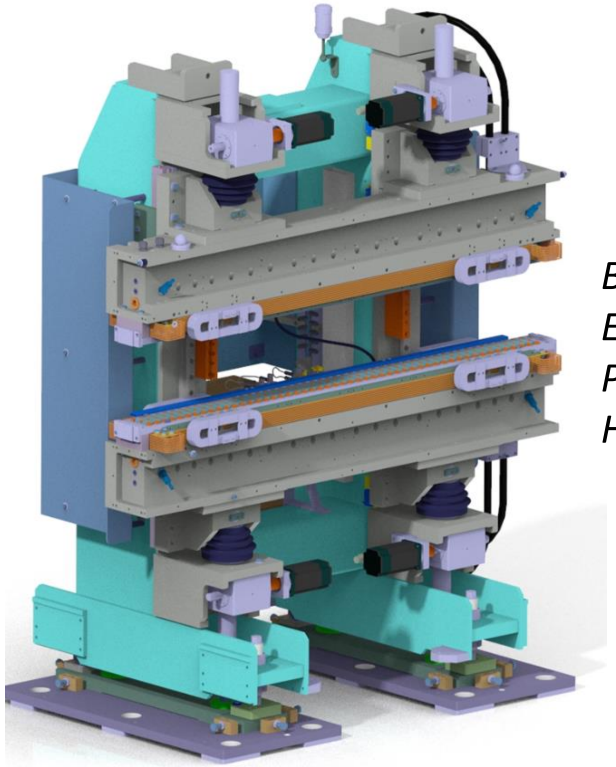
diamond

Insertion Devices

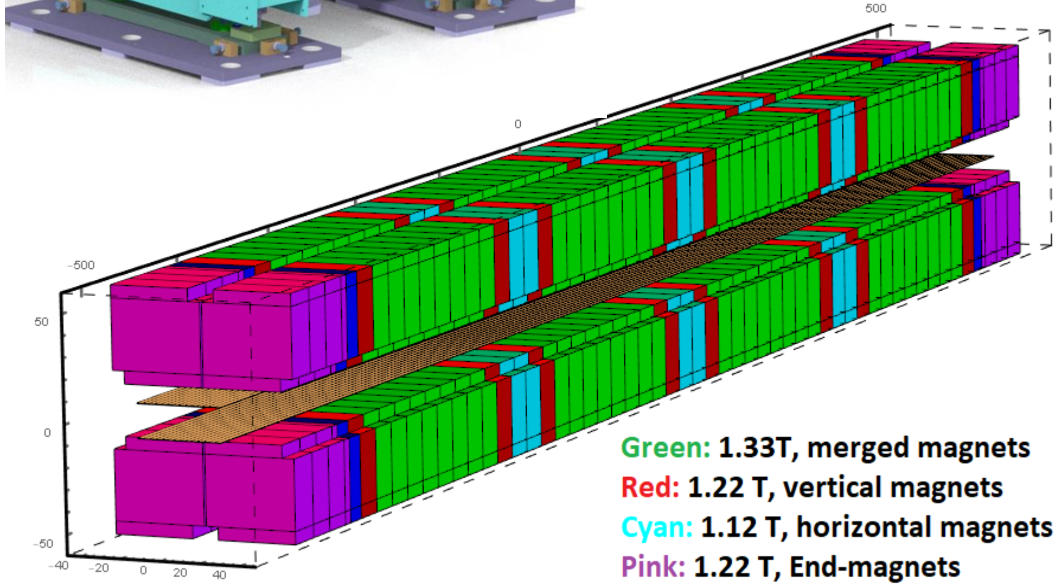
- **12 new Insertion Devices are needed for Diamond-II:**
  - 2 for new ‘flagship’ beamlines
  - 4 for beamlines switching from an existing bending magnet to an insertion device source
  - 3 to replace existing devices which are too long to fit in Diamond-II
  - 3 to replace existing devices with improved versions

- Comprising:
  - 1 x CPMU
  - 2 x HPMU
  - 5 x APPLE-II
  - 1 x MPW
  - 1 x 3PW
  - 1 x EMPHU for circular polarization switching
  - 1 x APPLE-Knot to reach 10 eV with low on-axis radiation power in all polarization modes

With a mixture of in-house and industry build.



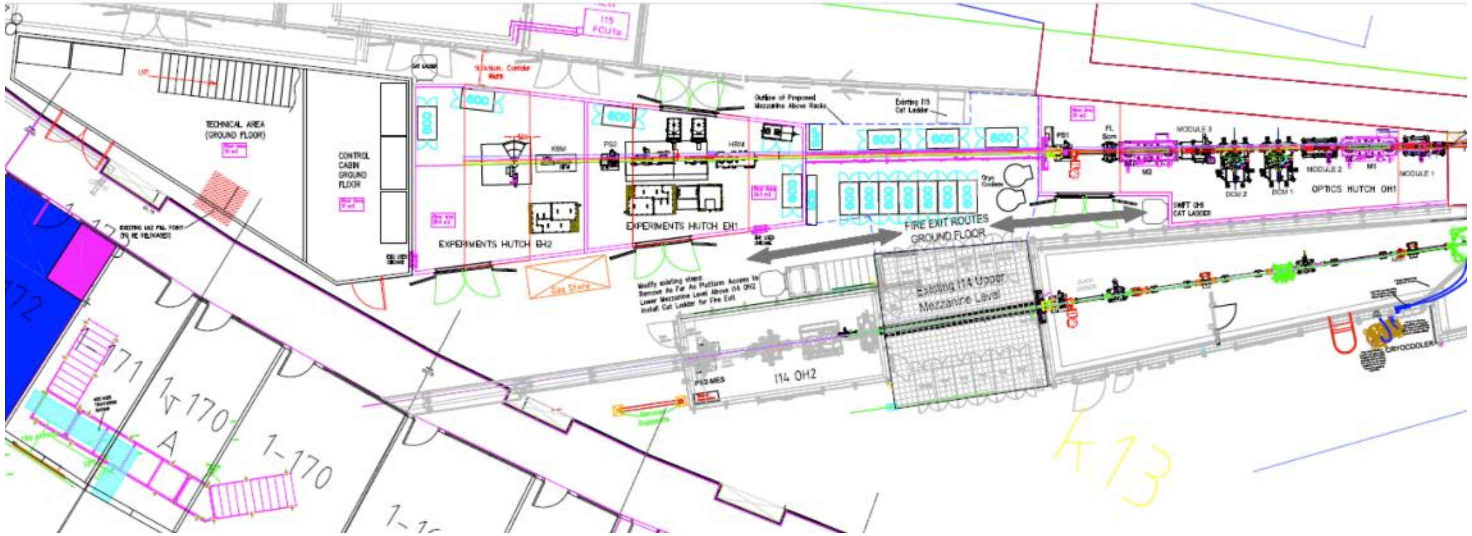
Based on the SOLEIL Electro-Magnetic Permanent magnet Helical Undulator

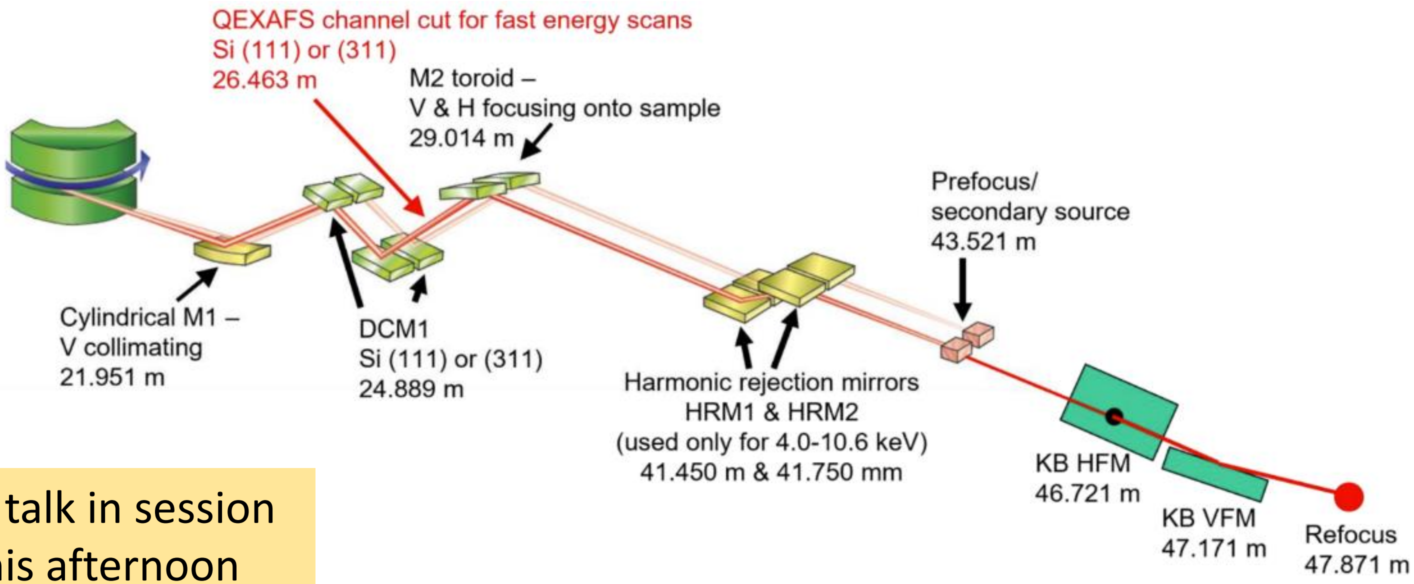


Green: 1.33T, merged magnets
Red: 1.22 T, vertical magnets
Cyan: 1.12 T, horizontal magnets
Pink: 1.22 T, End-magnets
Blue: 1.33T, merged End-magnet

SWIFT – Spectroscopy WIthin Fast Timescales

- Studies of dynamic phenomena with Quick-EXAFS in the Hard X-ray region
- Nanoparticle chemistry, metalloenzymes, catalysis, battery research, environmental and earth sciences
- Multipole wiggler source
- Fast-scanning DCM (50Hz, 4-35 keV), fast detectors and data acquisition
- End-station 1: high flux, operando studies, dilute systems, 100 μm x 100 μm
- End-station 2: microfocus 20 μm x 20 μm , chemical mapping, tomography
- Operando sample environments:
  - high temperature (1000 °C furnace)
  - gas flow reaction cells
  - liquid flow reaction cells
  - electrochemistry

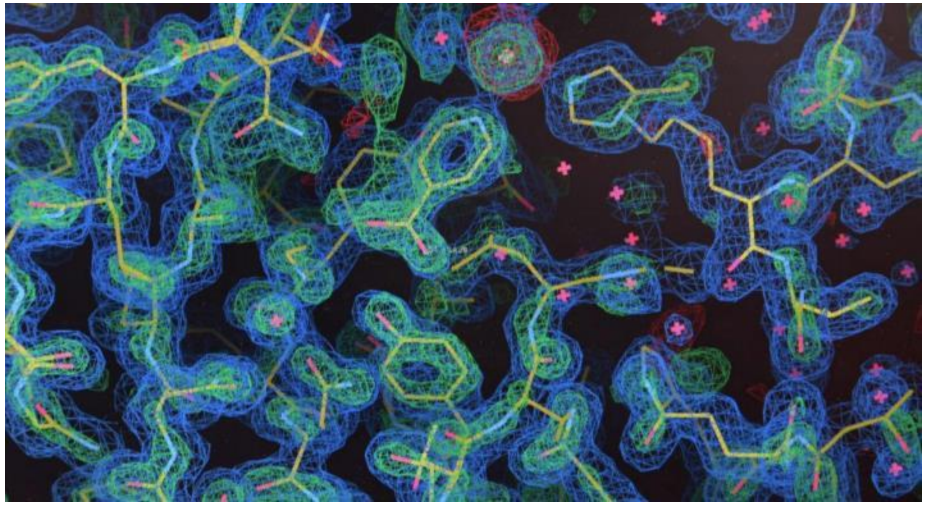


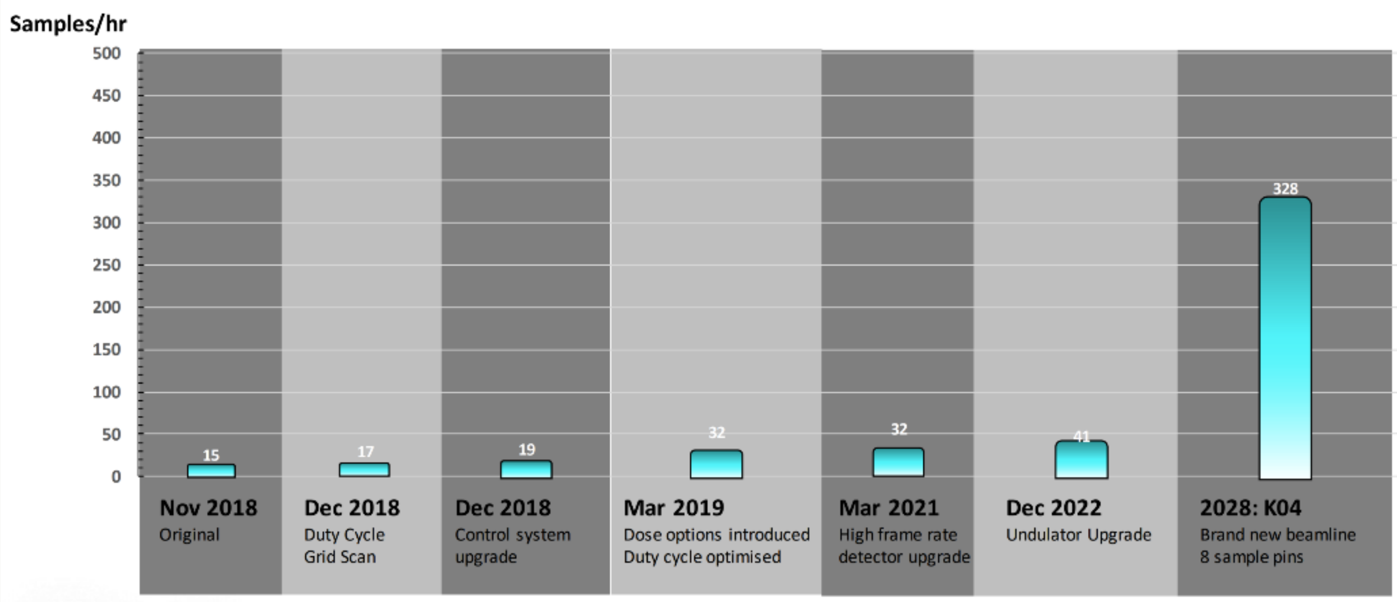


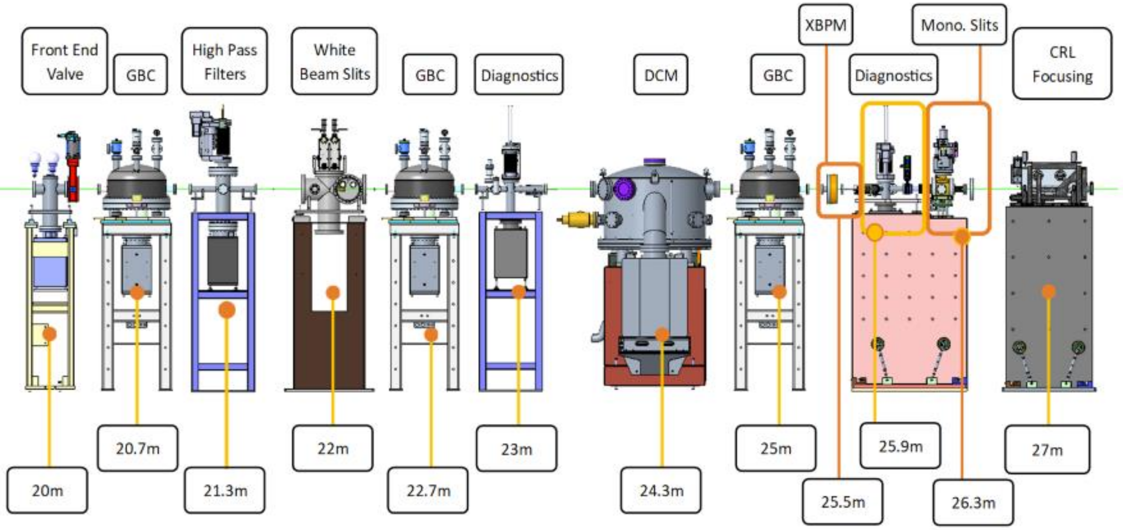
See Invited talk in session MS 2-2 this afternoon

K04 – Macromolecular Crystallography and Fragment Based Drug Discovery

- New beamline as part of a suite of 7 MX beamlines
- Replacement of the existing I04-1 Xchem fixed-energy side-station with a new variable energy beamline in a different location
- Massively increased throughput and automated data collection: 1,500 single crystal samples per day, or > 5,000 of multiple crystal samples per day
- Beam sizes 5-50 μm, crystals down to 10 μm in size.

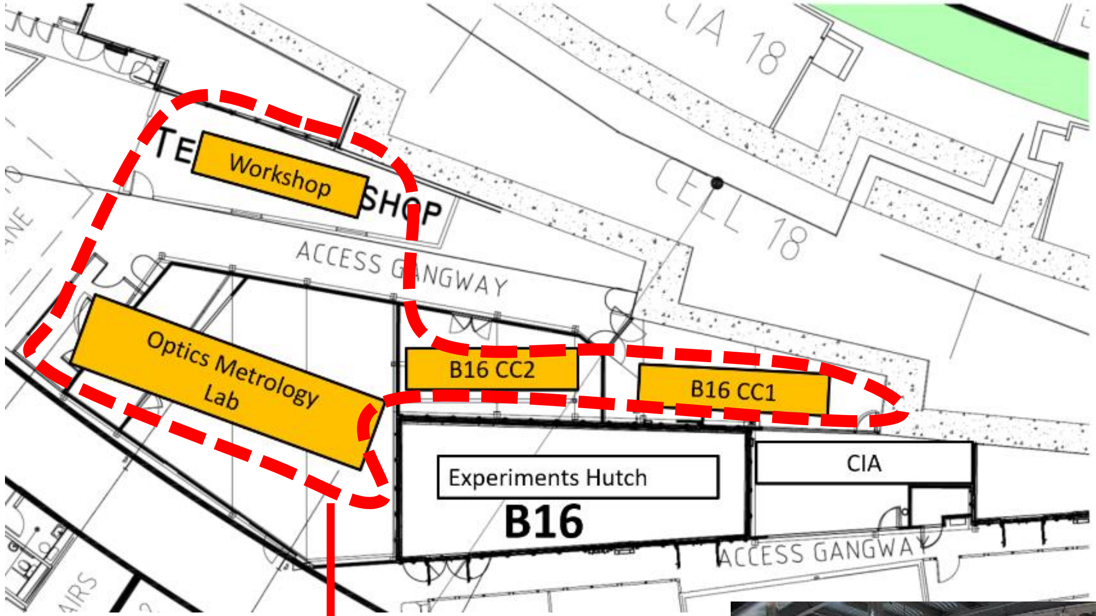


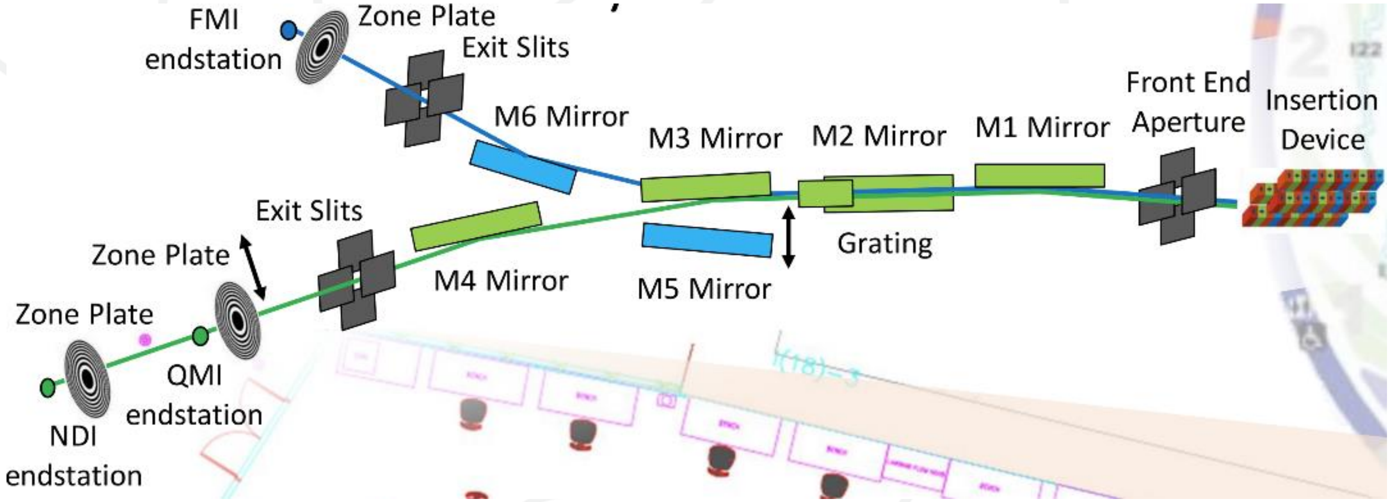




CSXID – Coherent Soft X-ray Imaging and Diffraction

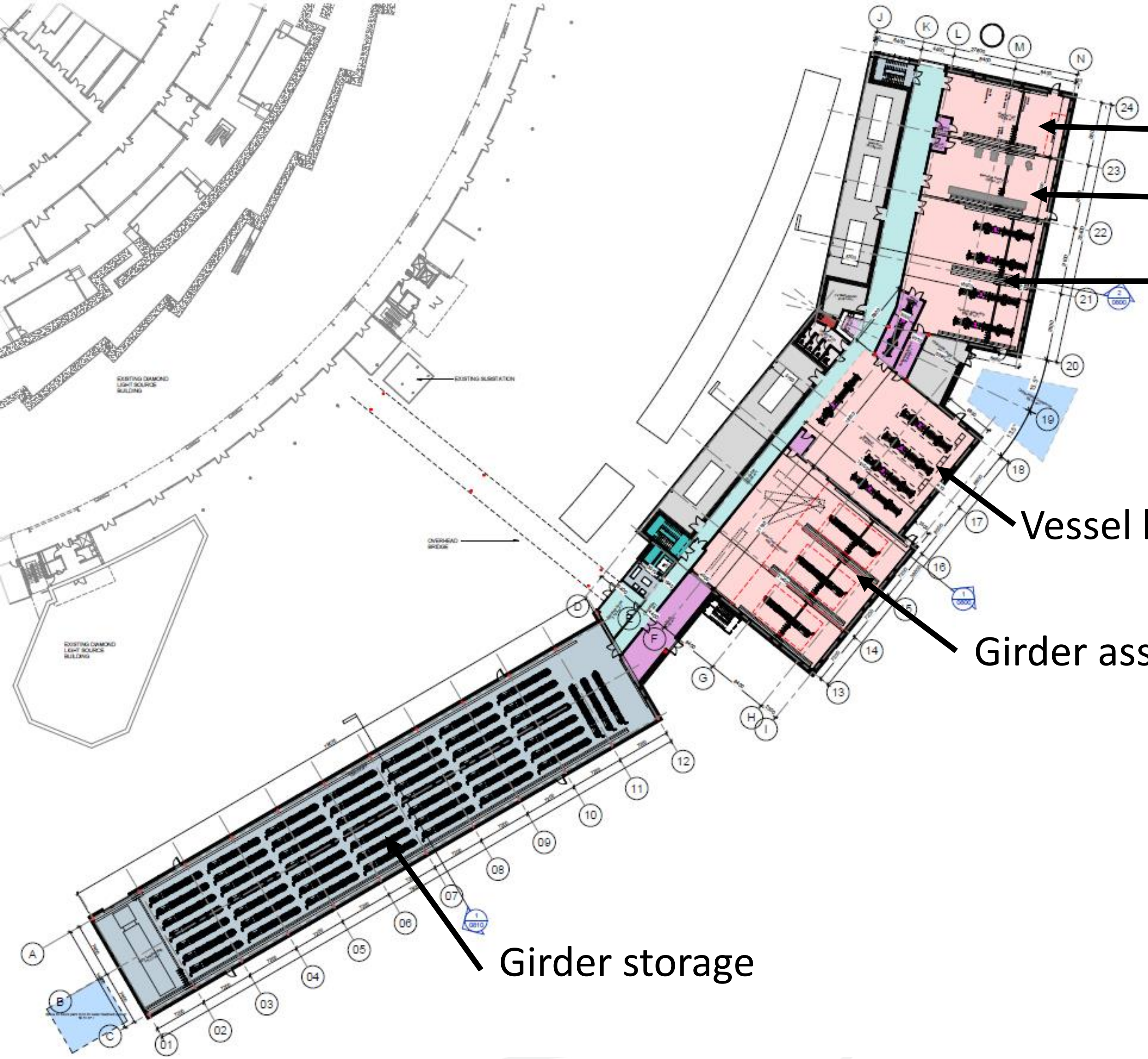
- 5m APPLE-II undulator source using the current long RF straight (I17)
- 0.25 – 3.5 keV
- End-station 1: quantum materials imaging
  - 0-250 mT, 20-300K, electrical excitation and biasing
- End-station 2: functional materials imaging
  - gas mixing cell for catalysis studies etc.
  - liquid flow cell for battery research etc.





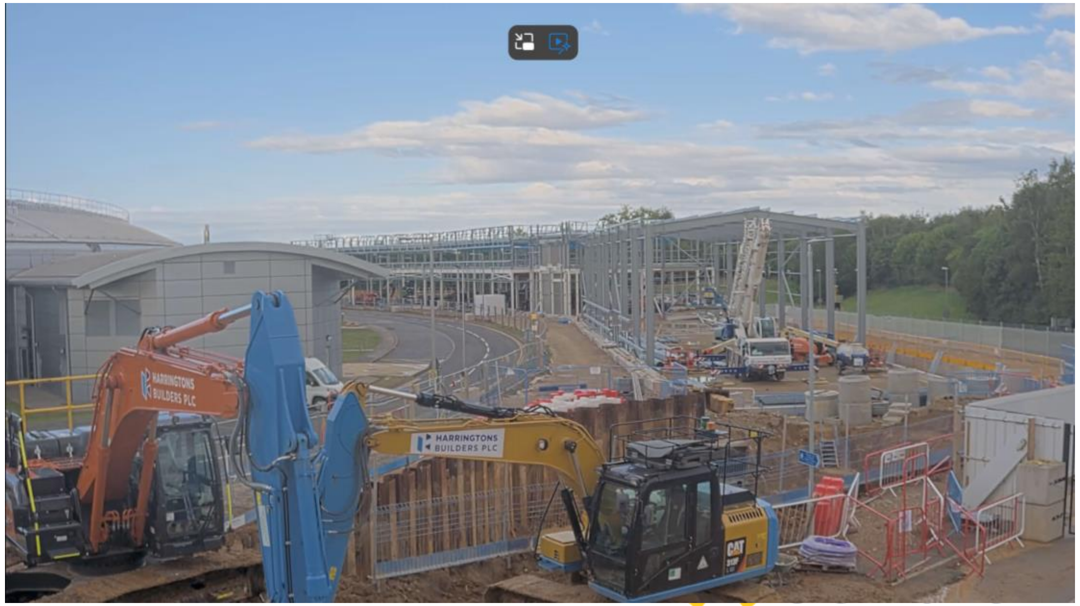
All of these have been relocated and now ready to start hutch construction

Diamond Extension Building



Architect's view

Web-cam view 24/8/24

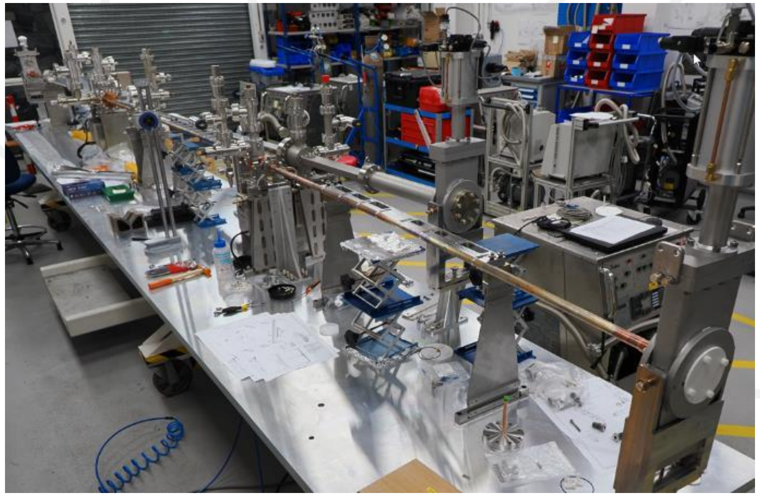


Diamond-II Status: Prototyping (some examples)

Girder with dummy magnets for vibration and alignment tests

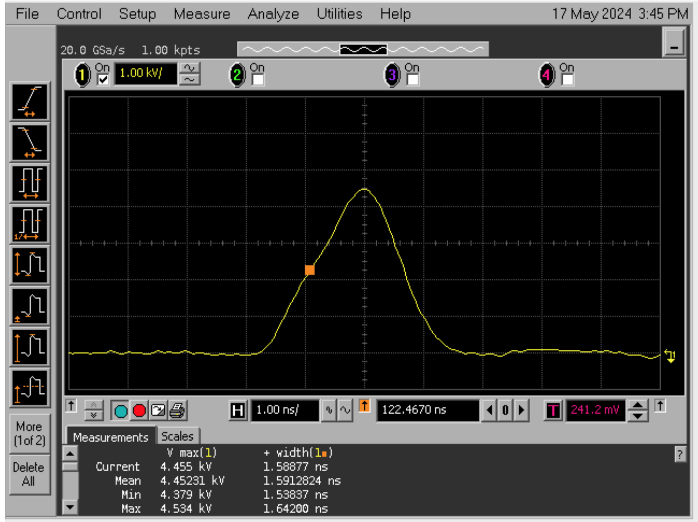
Transverse gradient dipole magnet (DQ)

Longitudinal gradient dipole magnet (DL)



Full girder vacuum vessel string

Ceramic kicker magnet vacuum vessels



Stripline pulser (±4 kV, < 4 ns 95% width)

Diamond-II Status: Procurement

- **Machine: 32% of budgeted £133.2m committed, includes**
  - 120 kW solid-state amplifiers
  - 3rd harmonic cavity
  - quadrupole magnets
  - sextupole magnets
  - DQ dipole magnets (imminent)
  - NEG coated copper vessels (first batch)
  - booster girder assemblies

- **Beamlines: 5.5% of budgeted £48.1m committed, includes**
  - lead hutches for CSXID and SWIFT flagship new beamlines

All active tenders published on
https://tenders.diamond.ac.uk/Home.aspx
as well as on official UK government websites.

Key Project Milestones

Milestone	Date
Project approval	Jul. 2023
Completion of the Diamond Extension Building	Mar. 2025
Start of the Diamond-II shutdown (“dark period”)	Dec. 2027
Start of machine commissioning	Dec. 2028
Start of regular beamline X-ray commissioning	Jun. 2029
First phase of operational beamlines	Sep. 2029
First User on a flagship beamline	Jan. 2030
Diamond-II Project completed	Mar. 2030

diamond

Brighter Times Ahead !

Thanks for Your Attention

diamond