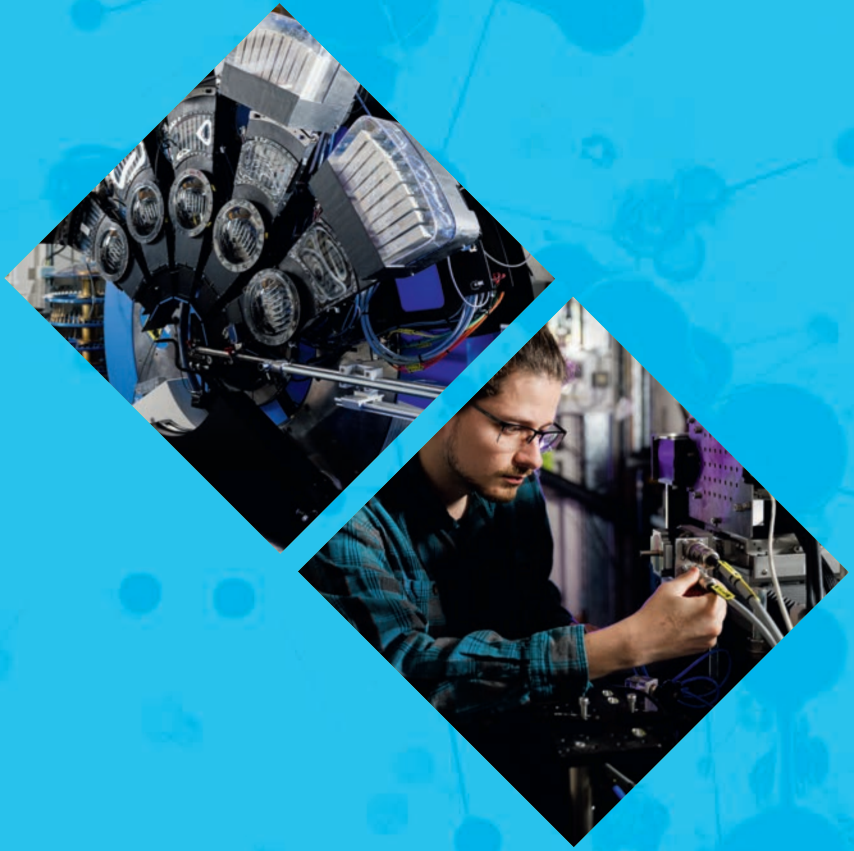

Diamond Light Source Ltd
Harwell Science & Innovation Campus
Didcot, Oxfordshire OX11 0DE

Tel: **+44 (0) 1235 778000**

www.diamond.ac.uk

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Annual Review

Diamond Light Source Limited

2024
2025

Contents

CEO Welcome

In my CEO report last year, I reflected on my first six months in post and noted that the real journey to tackle the many challenges ahead had already begun. In the last year, we have made progress against a number of my key priorities.

Over the past year, we completed an analysis of our current standing that brought together insights from across the organisation, our user community, and key stakeholders. This process was instrumental in defining the "Big Dream" for Diamond which helped define the core of our new long-term strategy and aligning our priorities with the evolving needs of science, industry, and society.

As a result of this new long-term strategy, we emphasise world-class science and innovation, world-class support of users, all this through world-class operations and working as one engaged Diamond team. The increased emphasis on innovation is delivered not only through our strong industrial science programme but also through measurable impact and by enhancing our support for translational research and industrial partnerships. This will ensure that Diamond's capabilities are more accessible and responsive to the needs of UK industry and global collaborators. These efforts also include the development of new mechanisms for collaboration with industry and expanding our innovation pipeline.

We are also embedding impact more deeply into our more unified scientific strategy—ensuring that our work not only advances fundamental discoveries but also contributes to solving real-world challenges that are at the core of the UK Government priorities in health, energy, environment, and economic growth through advanced manufacturing and industry support. This renewed focus will guide our decisions, shape our investments, and strengthen Diamond's role as a national asset delivering value across the UK's innovation landscape.

To deliver this strategy, the Diamond management, in partnership with its advisory committees, is undertaking a thorough portfolio review to ensure that our capabilities are aligned with our strategic goals, with the users' needs and can deliver maximum impact.

Over the past year, we have also initiated an organisational examination of how Diamond operates. This initiative, titled "Shaping our Future", aims to review the structure and processes in place at Diamond and how we can adapt these to what Diamond is today, over 20 years after the facility was built, and now in the delivery phase of the Diamond-II project. This review will help Diamond better deliver its long-term strategy.

Over the same period, significant progress has been made on the Diamond-II project. This ambitious upgrade aims to enhance the capabilities of Diamond, ensuring that we remain at the forefront of scientific research and innovation. A key sign of progress in this project includes the construction of the new 5,000m^2 Diamond Extension Building. The construction of this new space is well underway, with completion expected in July 2025. The new space will be used to build and store many new machine components. Significant progress has also been made in the procurement of major components of the new machine and in building the hutches for the new flagship beamlines. Progress has also been made in completing several of the technical design reports of the beamlines and initiating the procurement of optical components for these beamlines.

This progress made on Diamond-II is a testament of the collaborative efforts of the Diamond team, users, and committees. Their dedication and hard work have been instrumental in achieving these milestones.

In the past year, Diamond, in partnership with its user community, has delivered many examples of high impact science drawn from across the broad range of areas of fundamental science that Diamond serves, and the societal challenges it helps address. UK strategic priorities include enhancing public health and wellbeing, advancing environmental sustainability, and addressing the evolving challenges of transport and energy systems. A key enabler of these goals is the development of next-generation functional materials—such as those supporting quantum technologies, novel medical therapeutics, high-performance engineering alloys, and advanced manufacturing processes. Research carried out at Diamond supports these innovations which not only drive economic growth but also support national objectives in life sciences, climate resilience, energy security, and technological leadership.

In the last financial year, we delivered over 16,000 shifts across 35 beamlines and nine electron microscopes to our user community via peer reviewed access.

We welcomed 6,596 onsite user visits from academia across all instruments, with an additional 4,617 remote user visits. The machine continues to perform to the highest standard with 97.2% uptime.

Finally, the past year has also seen significant changes in the composition of our Board of Directors and Diamond committees. We welcomed new members to the Board, including a new Chair Prof Sir Leszek Borysiewicz, Prof Roger Eccleston and Victoria Grant. We also welcomed the new Chair of the Diamond Science Advisory Committee (SAC), Dr Kristina Djinovic-Carugo, a new Chair of the Diamond Industrial Science Committee (DISCo), Dr David Brown and a new Chair of the Diamond User Committee (DUC), Prof Silvia Ramos. Their insights and leadership will be invaluable as we continue to navigate the challenges and opportunities ahead. We also bid farewell to some long-serving members whose contributions have been instrumental in shaping Diamond's success, in particular Prof Tom Hase, former Chair of the SAC, Dr Malcolm Skingle, former Chair of DISCo and Prof Andrea Russell, former Chair of the DUC. We extend our deepest gratitude for their service and dedication.

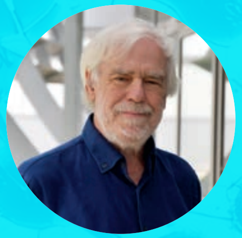
In closing, while we continue to have budgetary challenges affecting our operations, and the recruitment and retention of our staff, I remain committed to seek solutions to these challenges and to ensure that Diamond remains a priority with our funding agencies. I am humbled by the engagement and trust from Team Diamond in these times of change. With our new strategy, the support from our staff and stakeholders, we are preparing Diamond to face the next 10 years with ambition, confidence and excitement.

Prof Gianluigi Botton
CEO

Management Team

Prof Gianluigi Botton
CEO

Andrea Ward
CFO and Deputy CEO



Prof Sir David Stuart
Director of Life Sciences

Dr Richard Walker
Technical Director

Dr Adrian Mancuso
Director of
Physical Sciences

Board of Directors

Prof Sir Leszek Borysiewicz (Chair)
Prof Gianluigi Botton
Andrea Ward
Victoria Grant
Prof Michael Fitzpatrick
Dr Morag Foreman
Prof Keith S. Wilson
Dr Alan Partridge up to 31.03.25
Dr Roger Eccleston from 01.04.25

Company Secretary

Sean Hird

As of April 2025

Chair's Report

As I have taken on the role as Chair of the Diamond Board in the last few months, I want to convey my excitement in seeing the outstanding scientific impact that Diamond has produced since it became operational and the growth of the facility over the last few years. I also want to acknowledge the outstanding talent and remarkable innovative efforts of Diamond staff who support the success of this facility, enabling in many different ways the fantastic scientific output of our academic and industry users from the UK and around the world.

I arrive as new Chair of the Board in a period of significant challenges and opportunities. The operational funding continues to be a major risk for the facility, with resulting pressures, as in other UK national facilities, to support our staff with better pay, prioritise the activities and improve the efficiency of the delivery of the science. I also see great opportunities ahead with work leading to the Diamond-II upgrade project, enabling new experiments and new discoveries. I recognise that we have a short window of opportunity ahead of us, once the project is complete, to take advantage of the improvements in performance of the instrumentation at Diamond and for the facility to maintain its leadership as one of the best facilities in the world. We need therefore to ensure Diamond will be in the best position to take advantage of this major project. It has been a privilege to meet and engage with the leadership team at Diamond, especially Gianluigi but also I hope to be able to meet many more of our staff and students throughout the next year. Facilities matter but it is our amazing workforce that enables the magic to happen.

As Chair of the Board, I am committed to working closely with stakeholders, the Research Councils, the UK Government and the Wellcome Trust to support the evolving needs of Diamond. I am deeply honoured by the trust our shareholders have placed in me, and I look forward to leading the Board in the years ahead with dedication and integrity.

Prof Sir Leszek Borysiewicz
GBE DL FRS FMedSci FRCP FLSW

Chair of the Board

Advisory Bodies

The Scientific Advisory Committee (SAC)

Prof Kristina Djinović-Carugo, EMBL (Chair)
Dr Paul Adams, Lawrence Berkeley National Laboratory
Dr Steve Aplin, European XFEL
Dr Elke Arenholz, NSLS-II, Brookhaven National Laboratory
Prof Rohit Bhargava, University of Illinois Urbana-Champaign
Dr Dina Carbone, MAX IV
Prof Peter Dowding, Infineum (DISCo Representative)
Prof Chris Hardacre, University of Manchester
Prof Phil King, University of St Andrews
Dr Sylvia Ramos-Perez, University of Kent (Chair of the DUC)
Prof Matt Rosseinsky, University of Liverpool
Prof Andrea Russell, University of Southampton
Prof Christian Schroer, DESY
Prof Stephen Skinner, Imperial College London
Prof Xiaodong Zhang, Imperial College London
Prof Elizabeth Wright, University of Wisconsin-Madison

Diamond User Committee (DUC)

Dr Silvia Ramos-Perez, University of Kent (Chair) - Spectroscopy
Dr Colin Levy, University of Manchester - Macromolecular Crystallography
Dr Matthew Derry, Aston University - Soft Condensed Matter
Dr Hariom Jani, University of Oxford - Magnetic Materials
Dr Gary Nichol, University of Edinburgh – Crystallography
Dr Rosa Arrigo, Salford University - Structures and Surfaces
Dr Anna Regoutz, University College London – Structures and Surfaces
Dr Simon Kondrat, University of Loughborough – Spectroscopy
Dr James Everett, University of Keele - Imaging and Microscopy
Dr Alexander Lunt, University of Bath – Imaging and Microscopy
Benjamin Nash, University of East Anglia – Student Biological and Life Sciences
Dr Reshma Rao, Imperial College London – Early Career / Postdocs Physical and Chemical Sciences
Dr Josie Ferreira - University College London - Biological Cryo-Imaging
Dr Richard Collins - University of Manchester - Biological Cryo-Imaging

Diamond Industrial Science Committee (DISCo)

Prof Dave Brown, Vertex (Chair)
Dr Andrew Barrow, Rolls-Royce
Dr Helen Blade, AstraZeneca
Dr Jonathan Booth, Johnson Matthey
Dr Cheryl Doherty, GSK
Dr Andrew Doré, Charm Therapeutics
Prof Peter Dowding, Infineum
Prof Jonathan Hyde, NNL
Dr Andrew Johnson, Vital Chemical
Dr Olga Kazakova, NPL
Dr Jenny Moore, Syngenta
Dr Ellen Norman, RSSL
Dr Pamela Williams, Astex Pharmaceuticals

Scientific Software Advisory Committee (SSAC)

Steve Aplin, EU-XFEL (Chair)
Yves-Marie Abiven, Soleil
Stuart Campbell, NSLS-II
Vincent Favre-Nicolins, ESRF
Andrew Richards, Imperial College
Hanna Griffin, ISIS Neutron and Muon Source

Machine Advisory Committee (MAC)

Andreas Jankowiak, BESSY (Chair)
Eshraq Al Dmour, MAX-IV
Jean-Claude Biasci
Dieter Einfeld
Pedro Fernandes Tavares, MAX-IV
Gaël Le Bec, ESRF
Amor Nadji, SOLEIL
Montse Pont, CELLS
Vadim Sajaev, APS
Volker Schlott, SLS
Christoph Steier, ALS
Christian Schroer, DESY
Andy Wolski, University of Liverpool

Key facts and figures for 2024-25

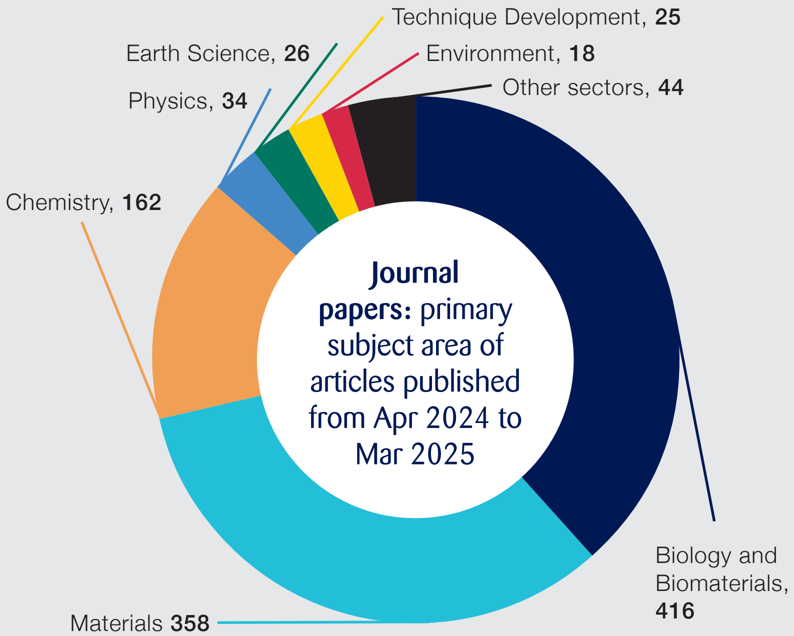
*calendar year 2024

820+
People are employed by Diamond

1,083
Journal articles published*

35
Beamlines

66
PhD theses published*



1,422
Structures deposited in the Protein Databank*

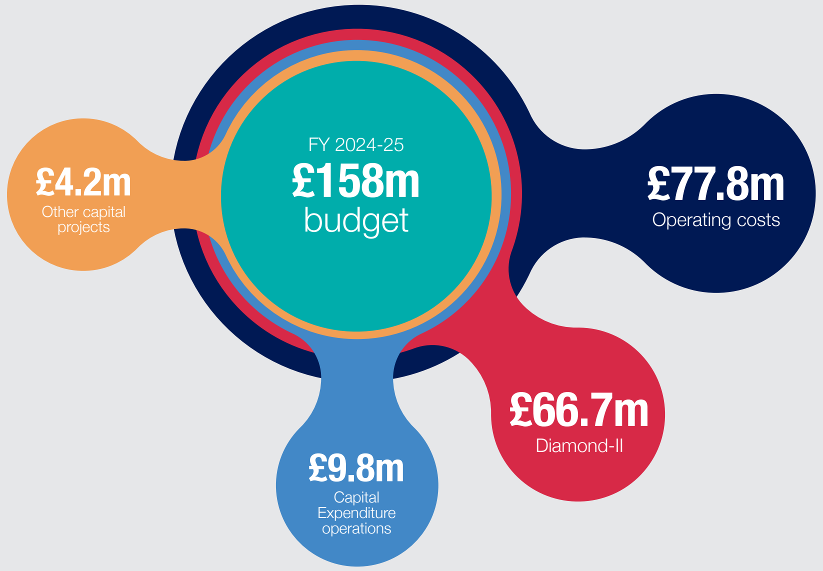
128,000+
Hours of beamtime delivered to facility users

4,000+
Scientific researchers

1,410
Proposals awarded

16,057
Shifts delivered

9
Electron Microscopes



Over 12PB
Of data added to the archive

184
Events and visits

10,300+
Members of the public visited Diamond

45
Scientific and technical events organised

97.2%
Machine uptime

77.9h
mean time between failures (MTBF)

Photovoltaics
Skyrmions
Lithium-ion
COVID-19
Crystallography
Magnetism
Bacteria
Viruses
Enzymes
Ferroelectricity
Additive Manufacturing
Crystal structure
Semiconductors
Alloys
Spintronics
Photocatalysis
Batteries
Data Storage

Top keywords from Diamond's publications database

Biological Cryo-Imaging Group

The Biological Cryo-Imaging Group brings together dedicated facilities for X-ray, light, and electron microscopy at Diamond.

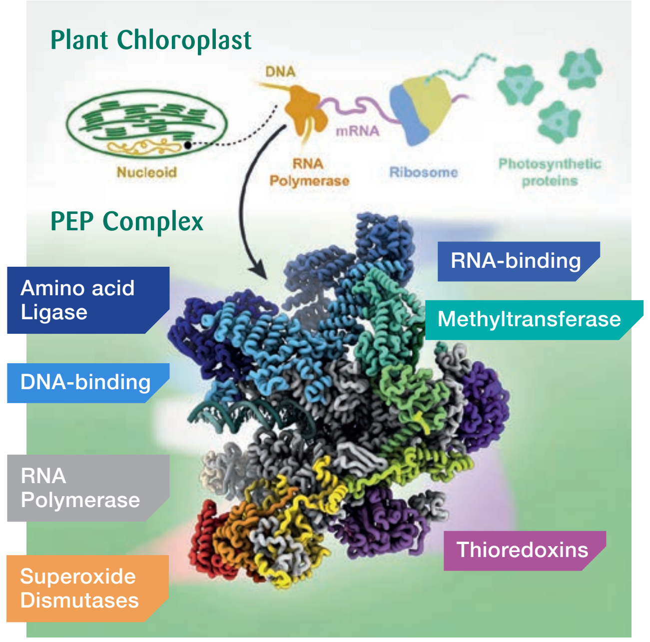
The electron Bio-Imaging Centre (eBIC) is a CryoEM centre providing scientists with state-of-the-art experimental equipment and expertise in the field of cryo-electron microscopy, for single particle analysis, electron tomography and electron diffraction. The location of eBIC enables scientists to combine their techniques with many of the other cutting-edge approaches that Diamond offers. Currently eBIC houses five Titan Krios microscopes, a Talos Arctica, two Glacios microscopes, Scios and Aquilos cryo-FIB/SEMs, and a Leica CryoCLEM.

Beamline B24 hosts a full field cryo-transmission X-ray microscope dedicated to biological X-ray imaging and has also established a cryo super resolution fluorescence microscopy facility, which is a joint venture between Diamond and the University of Oxford. It provides a unique platform for correlative light and X-ray microscopy, and cryoEM. A recent external beamline review rated the B24 facility as excellent and world leading. In particular, the panel commended the beamline team on establishing an internationally unique correlative platform combining two high-end 3D cryomicroscopy techniques (Cryo Soft X-ray Tomography (CryoSXT) and Cryo Structured Illumination Microscopy (CryoSIM) with user friendly protocols.

Jigsaw puzzle: Deciphering the chloroplast transcription machinery

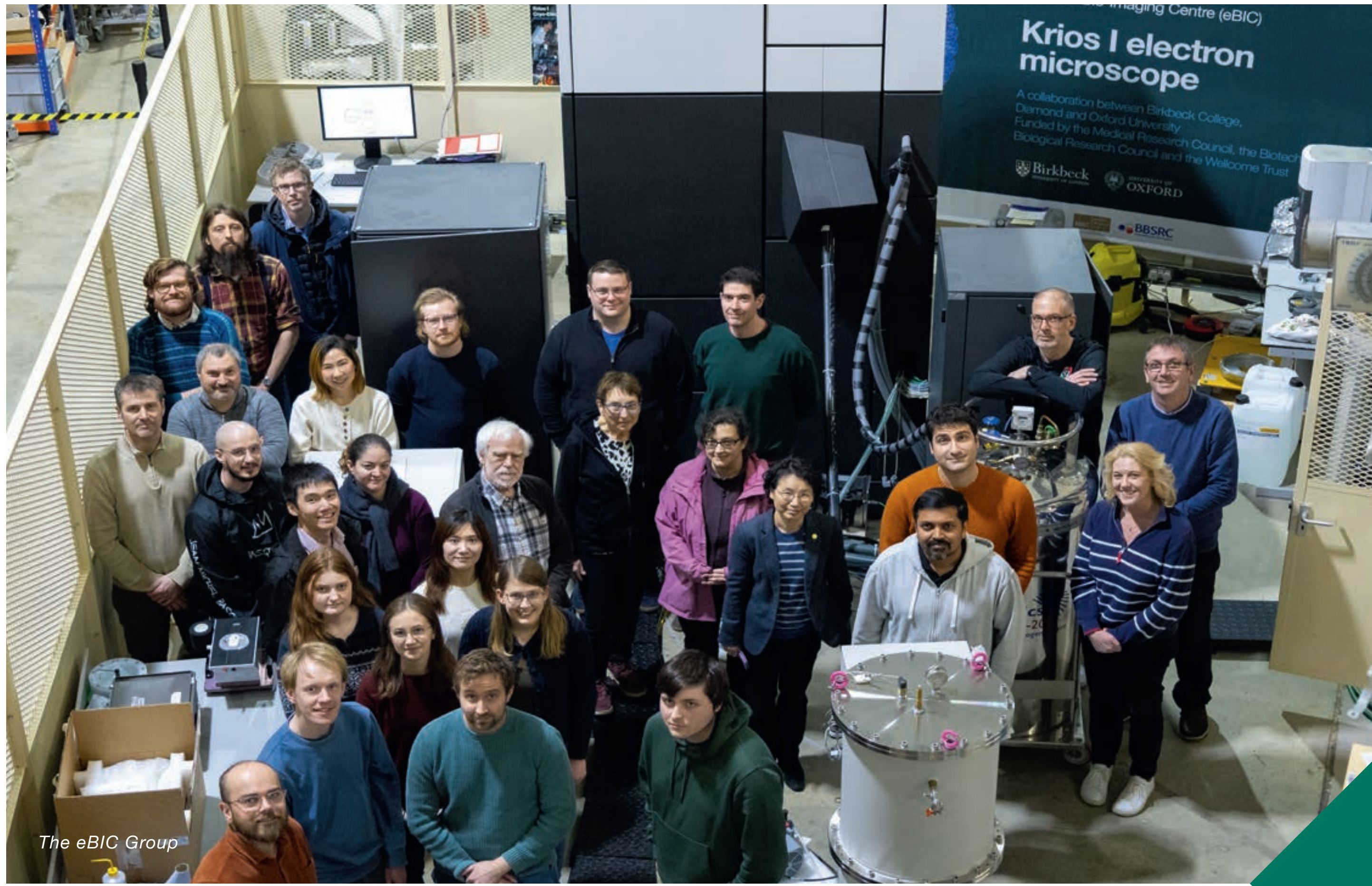
Chloroplasts are specialised organelles found in plant cells and some algae. Chloroplasts have a unique transcription machinery that is more complex than their cyanobacterial ancestors. The plastid-encoded RNA polymerase (PEP) is a multi-subunit complex crucial for transcribing chloroplast genes, which are essential for photosynthesis and plant growth. Despite its importance, the roles of many PEP-associated proteins (PAPs) are poorly understood.

In this study, researchers from the John Innes Centre purified PEP complex using chromatographic separation. It showed that the PEP is a huge complex of 1.1 MDa, more than twice the size of its bacterial counterpart. To visualise the PEP complex at high resolution, the researchers used cryoEM at eBIC. CryoEM is ideal for studying large protein complexes in their native state, allowing the researchers to capture the intricate details of PEP and its associated proteins.



The PEP complex in chloroplasts.

They discovered that the core polymerase of the PEP shares structural similarities with the cyanobacterial RNAP. Also, PAPs encase the core polymerase, forming extensive interactions that likely promote complex assembly and stability. The PAP subunits add new capability to the core polymerase. PAP1 and PAP2 add DNA binding and RNA binding, and several PAPs add enzymatic functions. Interestingly, if any single PAP subunit is missing, the polymerase will not function efficiently.



The eBIC Group

This research paves the way for further studies on the functional roles of PAPs and their contributions to chloroplast transcription. The potential applications of this research are vast. Understanding the structure and function of PEP can lead to advancements in agricultural biotechnology. For instance, manipulating the PEP complex could enhance photosynthetic efficiency and stress tolerance in crops, leading to higher yields and better resilience to environmental changes.

DOI: 10.1016/j.cell.2024.01.036

Unveiling magnetosome formation: insights from CryoSXT on iron uptake dynamics

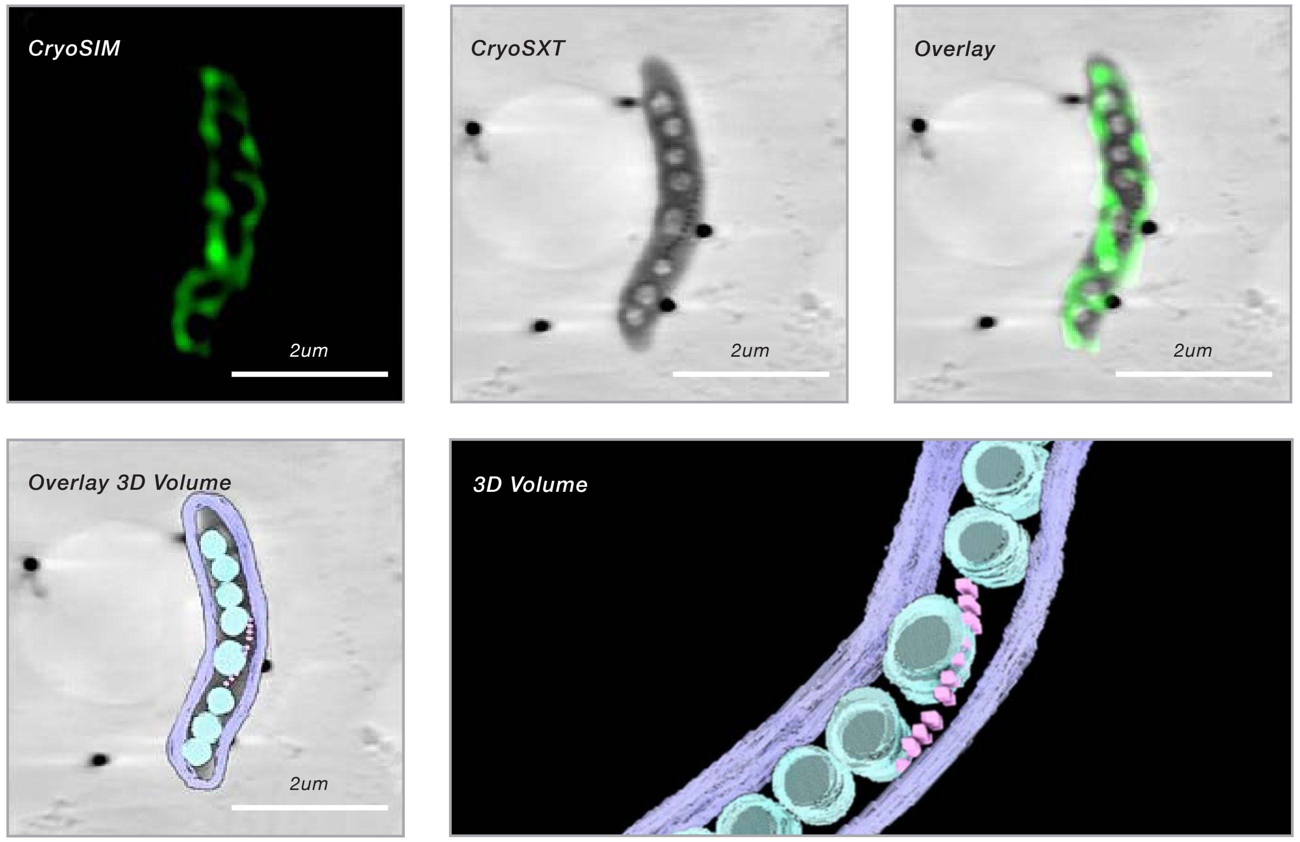
Iron plays several essential roles in bacteria, making it a crucial element for their survival and function. In magnetotactic bacteria like Magnetospirillum gryphiswaldense, iron plays a central role in the formation of magnetosomes. These peculiar bacteria possess the capability to orient themselves along the Earth's magnetic field lines, thanks to very specific type of intracellular magnetic nanoparticles called magnetosomes. These magnetosomes are mainly composed of magnetite crystals. Some mechanisms such as the internalisation and the transformation of iron into magnetite crystals are still poorly understood. To study the formation of these magnetosomes in bacteria, researchers from Aston University performed CryoSIM and CryoSXT experiments on the B24 beamline at Diamond.

CryoSXT is a powerful technique used to observe the internal structure of biological samples in a near-native state. In this study, it was instrumental in providing three-dimensional (3D) tomograms of individual bacterial cells. The technique allowed for high-resolution imaging without the need for traditional sample preparation that could damage cellular structures. On B24, the team was able to observe internal compartment including magnetosomes using the preferential absorption of carbon atoms in the cell. With cryoSIM, they stained the cell with PG-SK, a green fluorophore that reacts with the intracellular iron. The strength of the B24 beamline is that scientists were able to analyse the same region of interest in the same samples with Both CryoSIM and CryoSXT and correlate the data.

This approach provided compelling evidence of a correlation between the intracellular iron concentration and the number of magnetosomes. By modifying the oxygen concentration during the bacteria growth, the researchers demonstrated that these bacteria can tolerate high extracellular iron concentrations.

Understanding how magnetotactic bacteria and magnetosomes grow is essential as there is a growing interest into using magnetosomes for biotechnological and biomedical applications due to their unique properties such as narrow iron distribution and biocompatibility.

DOI: 10.1021/acsami.4c15975



Representative tomogram slices of the MSR-1 magnetosome producing cell grown under microaerobic conditions imaged by cryoSIM and cryoSXT, including a 3D volumetric representation of this cell using a SuRVos2 workbench. Magnetosomes are coloured in pink, PHA granules in blue and the cell membrane in purple. In the cryoSIM image, the intracellular iron is indicated by the Phen Green SK fluorophore (PG-SK)

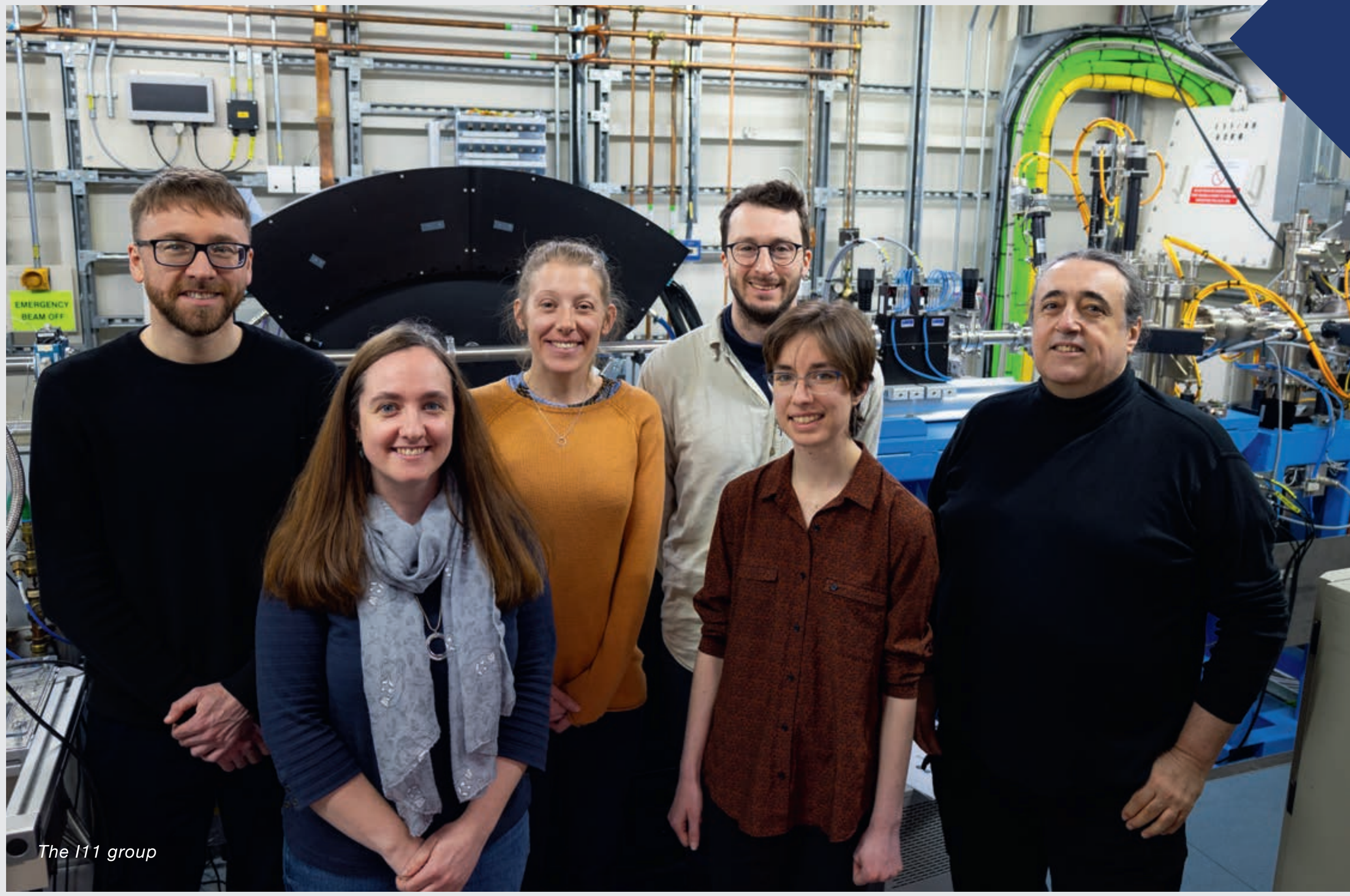
Crystallography Group

The Crystallography Group comprises the High-Resolution Powder Diffraction beamline (I11), the Extreme Conditions beamline (I15), the X-ray Pair Distribution Function (XPDF) beamline (I15-1), and the Small-Molecule Single-Crystal Diffraction beamline (I19).

Having these beamlines together in one science group allows us to fully exploit the technical and scientific expertise within the teams to provide the basis for future development and pioneering experiments. The Crystallography Group's beamlines use single crystal diffraction, powder diffraction and total scattering techniques to study structural properties of crystalline, amorphous, and liquid materials in different conditions. These powerful facilities are used in a wide range of science disciplines, including Condensed Matter Physics, Chemistry, Engineering, Earth Sciences and Materials, and Life Sciences.

I11 is a high-resolution powder diffraction beamline for structural crystallography. This beamline specialises in investigating the structure of complex materials, including metal-organic frameworks, high temperature superconductors, ceramics, alloys, zeolites and minerals under non-ambient, time-resolved, and long duration conditions.

I15, the extreme conditions beamline, is a high energy diffraction and scattering beamline used to



The I11 group

explore planetary interior conditions, as well as other experiments requiring high pressures and non-ambient temperatures including porous materials and engineering applications.

I15-1 is a dedicated X-ray Pair Distribution Function beamline. The pair distribution function allows researchers in fields as diverse as materials chemistry, solid-state physics, Earth science and pharmaceuticals to gain insight into the local structure of crystalline, amorphous, and liquid materials both *ex situ* and *in situ*.

I19 is a high-flux tuneable-wavelength facility for the study of small-molecule systems by single-crystal X-ray diffraction techniques. The beamline supports high throughput analysis of challenging samples as well as a variety of techniques to map structural change of systems under the influence of an external effect (such as pressure, temperature, photoexcitation or gas exchange).

Solid electrolytes: a breakthrough for safer, high-performance batteries

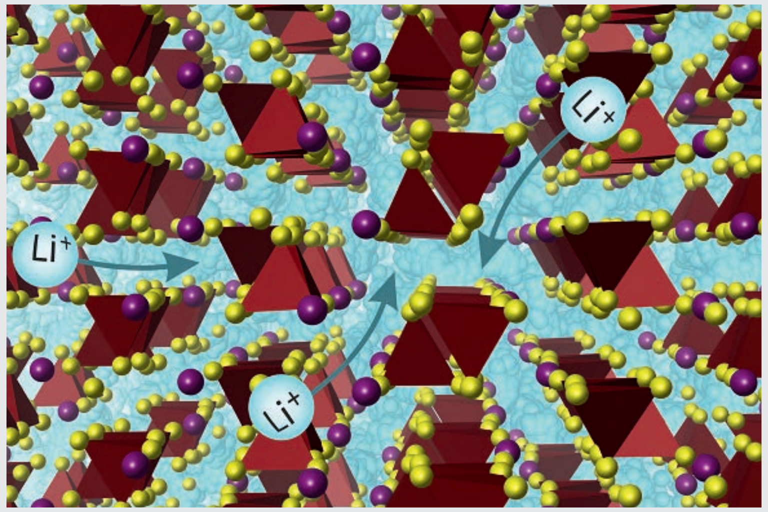
Batteries are a critical technology for the transition to a sustainable energy economy. Most Li-ion batteries rely on a liquid electrolyte to conduct ions between the anode and cathode. However, liquid electrolytes can leak and are flammable, which can lead to fires. One solution to this issue is to use a solid electrolyte. A team of researchers from the University of Liverpool have discovered a solid material with high enough Li-ion conductivity to replace the liquid electrolytes in current Li-ion battery technology, improving safety and energy capacity.

The team opted for a design strategy using multiple anions to construct suitable pathways, supported by AI and physics-based calculations. The material they synthesised, $Li_7Si_2S_7I$, is a pure Li-ion conductor created by an ordering of sulphide and iodide with many different cation coordination environments that combine to create superionic conductivity. Created from non-toxic earth-abundant elements, the new material operates in a new way and achieves a high enough Li-ion conductivity to replace liquid electrolytes.

After suitable crystals for single-crystal diffraction were grown, the team used high resolution single-crystal X-ray Diffraction (SCXRD) on beamline I19 to solve the crystal structure. Measurements on these initial crystal samples - using both SCXRD on the I19 beamline, and Powder X-ray Diffraction (PXRD) on I11 - showed that the material has a lot of disordered lithium sites. Operando studies confirmed that the high conductivity of $Li_7Si_2S_7I$ arises from a combination of Li-ion sites of widely varying geometry and anion coordination. This diversity offers multiple rapid transport pathways by providing many different low-barrier site-to-site connections.

The team is now exploring ways to optimise the chemistry of $Li_7Si_2S_7I$ to further enhance the properties of the material. The new understanding provided by the study will also allow the identification of other materials that are well suited to exploratory synthesis.

DOI: 10.1126/science.adh5115



The figure represents the lithium ions (in blue) moving through the structure (Credit: Liverpool University)

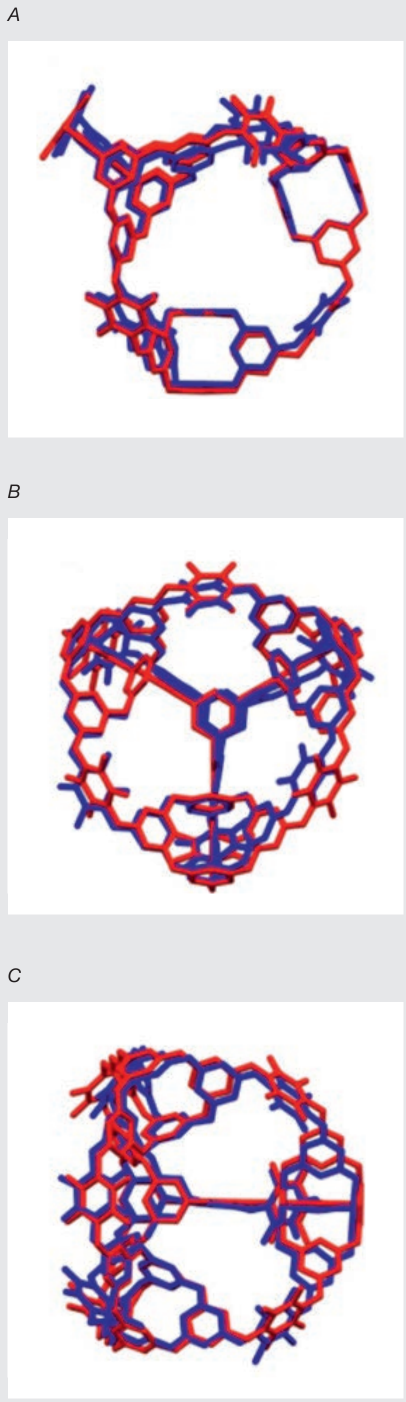
Hierarchical self-assembly: unlocking new functional materials

Pushed and pulled by competing interactions, molecules can self-assemble into complex structures. Using supramolecular self-assembly, we can synthesise materials with unique structures and function. However, predicting how molecules will assemble themselves, and controlling the reaction conditions to nudge them into forming a desirable structure, is challenging. Using porous cage molecules as building blocks for larger structures is an attractive prospect.

A team of researchers led by the University of Liverpool, Imperial College London and Heriot-Watt University has developed a hierarchical cage molecule that can adsorb other molecules, like carbon dioxide and sulphur hexafluoride. A key aspect of the project was using computer modelling to accurately predict how the precursor molecules would self-assemble into a new material. In order to validate the accuracy of the computer predictions, they performed diffraction experiments at I11 and I19.

This hierarchical cage molecule has a high storage capacity for gas molecules like carbon dioxide and sulphur hexafluoride. In the future, complex hierarchical structures could be used to perform challenging molecular separation, such as filtering toxic volatile organic compounds (VOCs) from the air or have applications in medical science.

DOI:10.1038/s44160-024-00531-7



A-C, The predicted structure (red) overlaid with the single-crystal X-ray diffraction structure (blue) is shown as viewed along the a (a), b (b) and c (c) crystallographic axes, highlighting the close structural similarity between the predicted and experimental structures.

Some of the I13-1 beamline team (clockwise from back left) Darren Batey, Tim Ardern, Silvia Cippia (UCL, Diamond Visiting Scientist), Kudakwashe Jakata

Imaging and Microscopy Group

The Imaging and Microscopy Group brings together eight experimental facilities (I08, I08-1, DIAD, I12, I13-1, I13-2, I14 and the electron Physical Science Imaging Centre [ePSIC]), which use electrons and X-rays to image samples under different experimental conditions across a diverse range of length scales and time scales.

The ability to image material properties in minute detail lends itself to a wide range of scientific applications, from chemistry and catalysis to environmental science, materials science, biology, medicine, and cultural heritage.

The DIAD (Dual Imaging and Diffraction) beamline is a pioneering facility designed to provide simultaneous imaging and diffraction capabilities for advanced material and biological research. The beamline features a unique dual-beam setup, where one beam is optimised for high-resolution imaging, allowing for detailed visualisation of internal features and defects, while the other beam is tailored for diffraction, providing insights into the crystalline structure and phase composition.

I13-1 coherence beamline is a hard X-ray beamline, operating in the 6-20 keV range. The beamline specialises in high-speed, multiscale and multimodal coherent diffraction imaging and ptychography in both transmission and Bragg geometries. These methods provide nanoscale resolutions with a quantitative phase contrast and can often be combined with other methods, such as tomography and X-ray Absorption Near Edge Structure (XANES), and complementary signals, such as fluorescence and diffraction mapping.

The I13-2 Diamond Manchester Imaging beamline is focused on micro-and nano-tomography and provides, in connection with the I13-1 Coherence beamline, multiscale imaging capabilities over three orders of magnitude in resolution. The beamline operates in the 8-30 keV energy range, offering a variety of imaging capabilities including in-line phase contrast imaging, full-field microscopy and grating interferometry.

I14, the Hard X-ray Nanoprobe beamline, provides a focused beam of 50 nm for high resolution imaging of a diverse range of samples using multiple techniques including X-ray fluorescence, diffraction, XANES, differential phase contrast imaging and ptychography. With a strong emphasis on spectral imaging and provision of environments for nanoscale in situ studies under liquid, gas and electrochemical environments, I14 welcomes users from fields across physical and life sciences.

The Scanning X-ray Microscopy beamline (I08) is for morphological, elemental and chemical speciation on a broad range of organic-inorganic interactions in a 250 - 4400 eV photon energy range, and sample investigations under ambient conditions. The second branch, I08-1, is designed for soft X-ray ptychography offering exciting possibilities for imaging higher spatial resolutions for spectral and dichroic imaging.

I12 is a high energy beamline principally for material science, engineering and processing science. The instrument's main focus is to allow in situ studies of samples in environments as close as possible to real world environments using imaging, tomography, diffraction and small-angle scattering. I12 is particularly well suited to study large or dense objects and offers a unique sample and environment installation facility for weights up to 2000 kg.

ePSIC provides scientists with state-of-the-art experimental equipment and expertise in the field of physical sciences electron microscopy and characterisation. Currently ePSIC offers beam time on two microscopes: (E01) A probe-corrected JEM ARM200F with EELS and EDX capabilities in collaboration with Johnson Matthey, and (E02) a probe and image corrected JEM ARM300F in collaboration with University of Oxford.

Bridging the thickness gap: advanced soft X-ray imaging unlocks magnetic textures

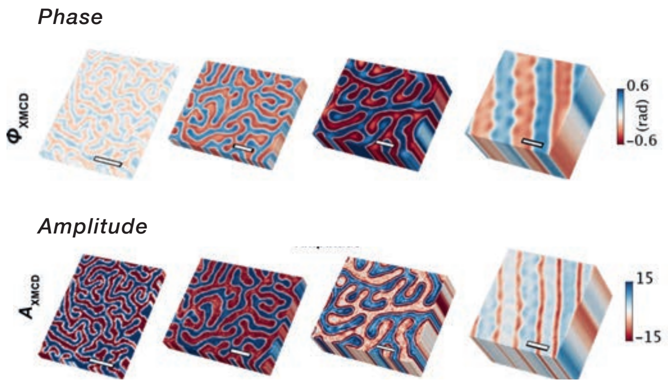
Magnetic materials underpin our high-tech lifestyles and will play key roles in the production of clean energy and next generation computing technologies. The behaviour of magnetic materials is governed by their underlying magnetisation configuration, including magnetic domains (local areas of uniform magnetisation) and defects such as domain walls.

However, while using a combination of high spatial resolution soft X-ray imaging and electron microscopy allows the analysis of thin samples (≤300 nm) and surfaces, investigation of thicker samples has been limited to hard X-ray dichroic imaging, limiting studies to thin films for most materials, including transition metal magnets. A team of researchers, led by Claire Donnelly of the Max Planck Institute for Chemical Physics of Solids, have used I08-1 to develop a soft X-ray coherent imaging technique for thicker magnets, closing this "thickness gap".

X-ray phase dichroism exists for a much wider range of X-ray energies than the absorption dichroism, traditionally used to probe magnetic systems, and at energies where the sample is less absorbing. Phase dichroism therefore extends soft X-ray magnetic imaging to samples beyond the capabilities of conventional techniques.

The research team tested this technique with magnetic samples up to 1.7 µm thick and were able to demonstrate that thick samples of a chiral magnetic material host unconfined states, which opens exciting prospects for studying knot-like magnetic textures.

DOI: 10.1103/PhysRevX.14.031028



ϕXMCD and AXMCD imaging of magnetic films of increasing thickness. The XMCD projections with highest SNR of the 100-nm-thick CoPt are measured at 780 and 779.4 eV for AXMCD and ϕXMCD, respectively. The XMCD projections with highest SNR for the 400 nm, 1 µm, and 1.7 µm FeGd films are measured at 709, 708.5, and 708 eV, respectively, for both AXMCD and ϕXMCD.

A greener route to gold nanoparticles

Gold nanoparticles (NPs) are used in a variety of applications including catalysis, drug delivery, biosensing, and electronics. Traditional methods for producing gold NPs often involve harsh conditions and tend to produce larger NPs (10-200 nm). Smaller gold NPs (less than 10 nm) are more desirable for catalysis, because their higher surface area to volume ratio offers a higher number of catalytically active surface sites, and hence greater reactivity. There is a need to develop more sustainable methods of synthesising metal nanoparticles that allow precise control over their size and shape. In addition, there is a lack of sustainable methods for synthesising core-shell NPs, which are composed of two or more materials.

Researchers from the University of Oxford developed a more sustainable method for synthesising metal nanoparticles using an isolated enzyme, NAD+ reductase (NRase), to achieve better control over size, shape, and catalytic activity. They used NRase to reduce gold (Au) salts, in a process that involves the oxidation of NADH at the enzyme's active site, which releases electrons used for the reduction of the metal salts. The new process resulted in the formation of highly uniform, spherical gold nanoparticles.

The team was also able to use the process to synthesise core-shell NPs. After forming a gold NP, they found that adding platinum salts and more NADH resulted in the deposition of a platinum (Pt) shell over the gold core. Using HR-STEM at ePSIC allowed them to confirm the core-shell structure of Au@Pt NPs, with the results showing a higher ratio of platinum in the outer layers and gold (Au) in the centre. The ability to simultaneously acquire atomic resolution images - which tells us where the atoms are - with energy dispersive X-ray spectroscopy - which tells us what the atoms are - is a powerful tool. This enables researchers to develop a fundamental understanding of the chemistry that is occurring during a catalytic process, which in turn can help us to develop increasingly efficient catalyst materials.

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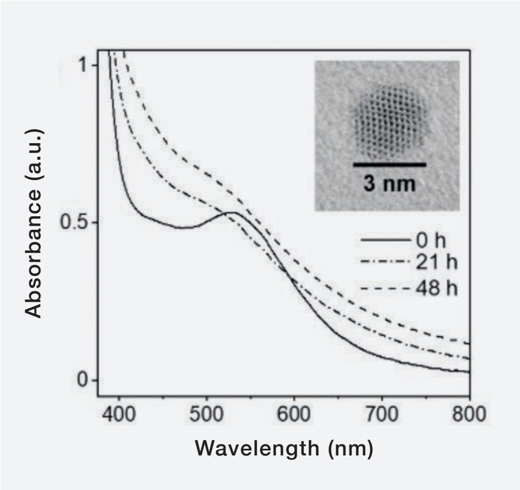

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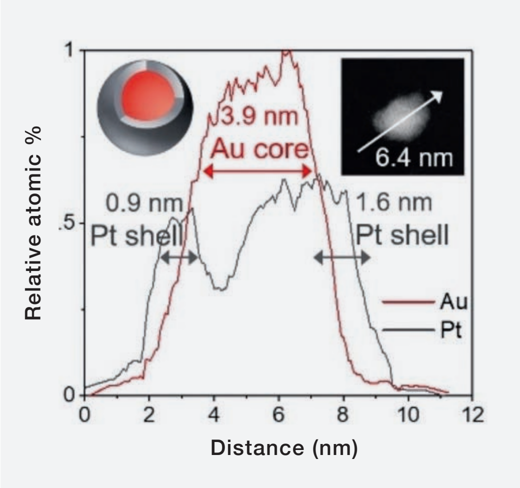


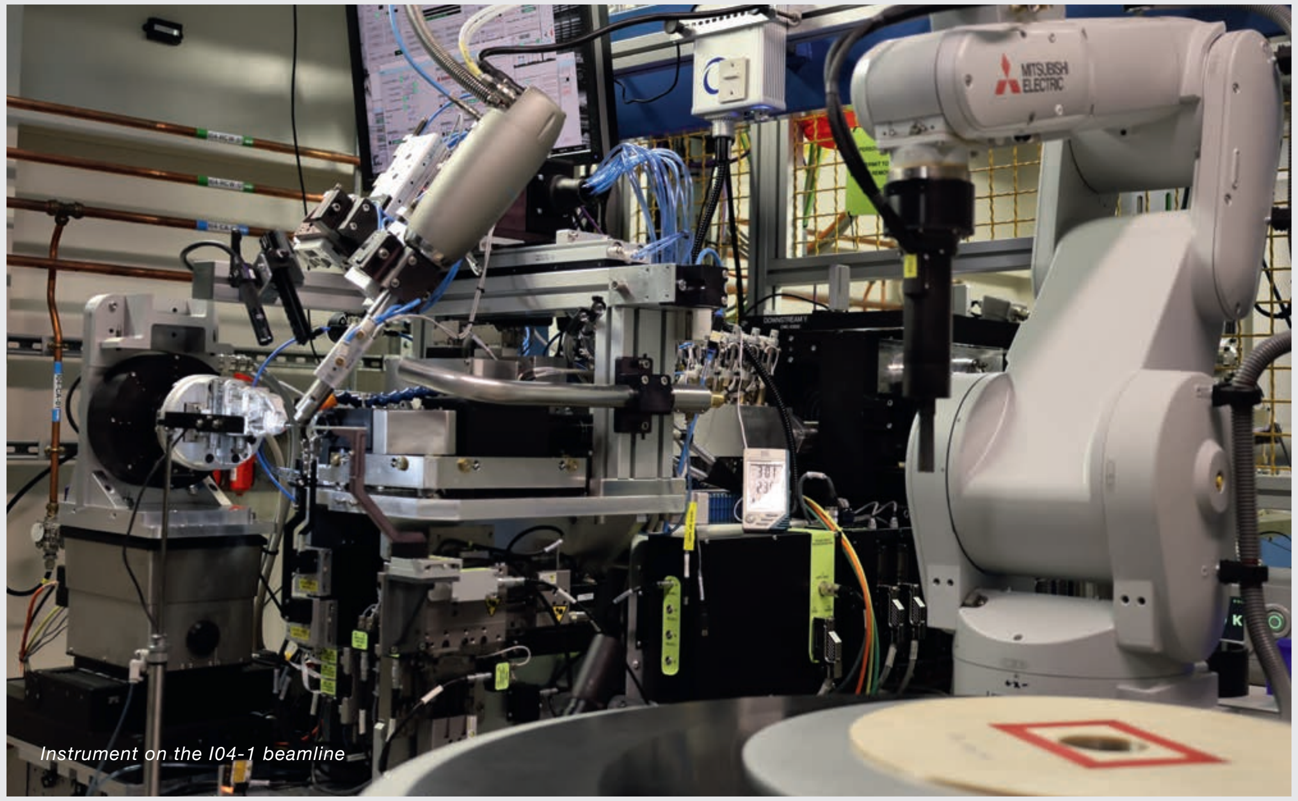
B

Synthesis of core-shell Au@Pt NPs using NRase to reduce Au(III) followed by Pt(IV). A) UV/Vis spectra recorded after addition of K_2PtCl_6 and NADH to a solution of NRase and Au NPs (0 h) and after 21 and 48 h. Inset is a HR-STEM (BF) image of a NP after 48 h. B) EDX data of the line scan shown in the inset HR-STEM (HAADF) image, of sample after 48 h, showing a Pt shell and gold core, as depicted in the inset diagram (top left).

Macromolecular Crystallography Group

Macromolecular crystallography (MX) exploits the high flux X-rays created at Diamond to enable our large international academic and industrial user community to investigate the structure and function of biological macromolecules at atomistic resolution and up to millisecond timescales. This provides deep insight into the details of biological activity key to our understanding of the processes of life.

MX is a core activity at Diamond with seven beamlines (I03, I04, I04-1, I23, I24, VMXi and VMXm) dedicated to the technique alongside the XFEL Hub, Membrane Protein Laboratory, Crystallisation Facility and XChem fragment screening facility for the extensive UK structural biology community as well as researchers in Europe and beyond. The beamlines cover a very broad range of capabilities from high throughput, micro- and nano-focus beams, extremely long wavelengths, room temperature in situ collection from crystallisation plates and (time-resolved) serial synchrotron crystallography (SSX). The staff of the MX group are recognised as innovative world leaders in MX, moving the goalposts of what is feasible for 'conventional' MX as well as developing techniques and beamlines that transform MX to the next level, enabling new experiments and methodologies. One new future capability will be the exploitation of high energy electrons with the electron diffraction instrument HeXI currently in development following funding from the Wellcome Trust. Additionally, as part of the Diamond-II upgrade, XChem fragment screening will be transformed into a fully automated pipeline at the new K04 beamline, providing the capability to deliver larger campaigns while also investigating more challenging protein targets.



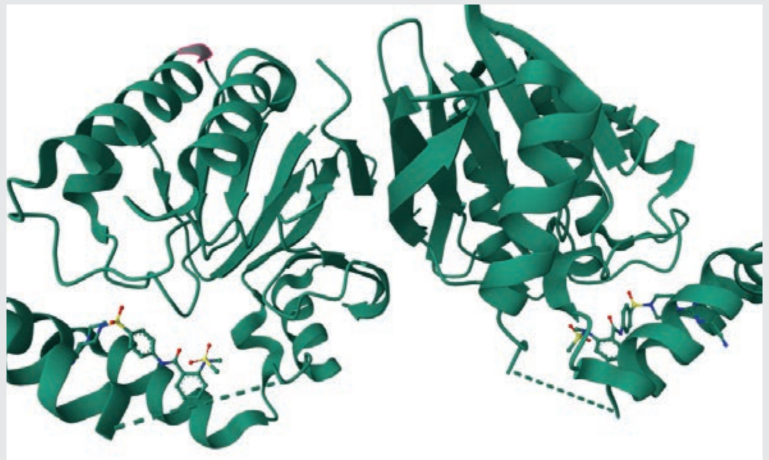
Instrument on the I04-1 beamline

Tearing down bacterial membranes with new antibiotics

According to the UN Environment Programme, bacteria resistant to existing antibiotics cause approximately one million deaths each year. Some bacteria, including strains of the gut pathogen Escherichia coli or the lung pathogen Klebsiella pneumoniae, are resistant to multiple antibiotics, limiting treatment options. These bacteria possess two bacterial membranes, the outer of which is studded with fatty carbohydrates called lipopolysaccharides (LPS) that play an essential role in reinforcing the membrane's integrity. Researchers at Uppsala University in Sweden are designing compound series that obstruct LPS synthesis. They merged a compound previously developed by AstraZeneca with a new compound and found a potent blocker that inhibits an essential enzyme called LpxH by binding to part of the active site. Since this enzyme is conserved in many species, drugs that target it could potentially have broad-spectrum use, much like the cephalosporin drugs used to treat many Gram-negative microbes.

Their newly fashioned molecule, which they called JEDI-1444, worked in bacteria with functioning efflux pumps, suggesting it is potent enough to kill bacteria even if they expel some of the compound from the cell. By further refining the compound's structure, they ended up with two new molecules called EBL-3647 and EBL-3599 bearing corrections that improved the stability and solubility of the compounds and reduced their interactions with serum proteins. Finally, they administered both compounds to mice and found that neither induced side effects, suggesting these compound series might be safe. Testing them out on mice infected with K. pneumoniae showed that a single dose of either compound could partially lower bacterial numbers. Infections with E. coli were more promising: the same treatment cleared the infection to undetectable levels. In the next steps, researchers will continue assessing the compounds' safety and efficacy with further animal tests and subsequent human trials.

DOI: 10.1073/pnas.2317274121

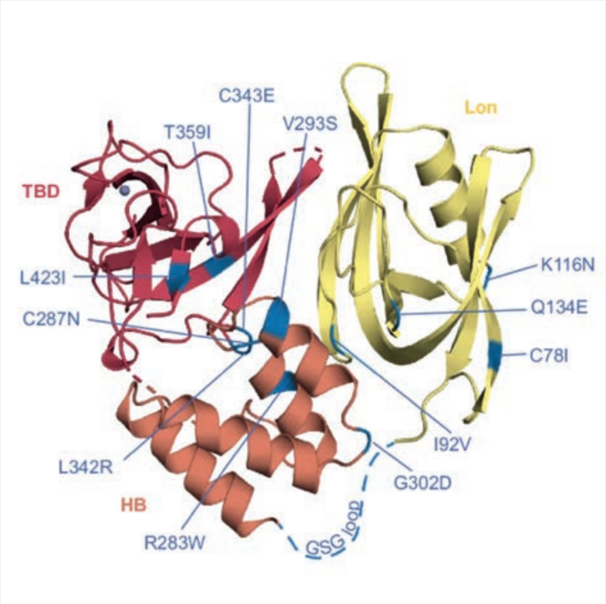


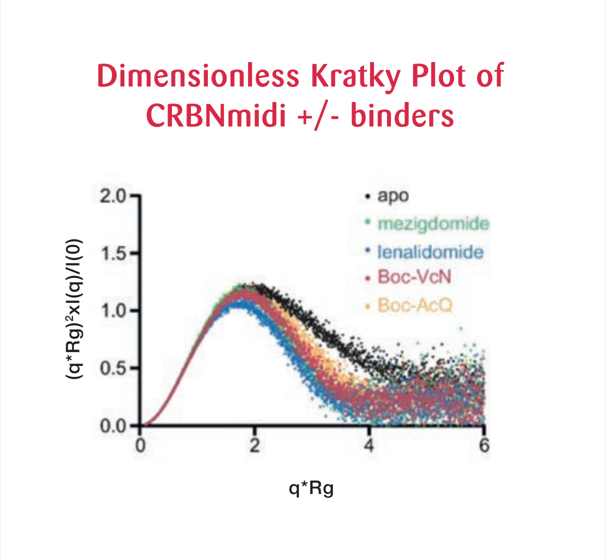
X-ray crystallography experiments at Diamond's I04-1 beamline revealed that the new compound, JEDI-1444, binds to the LPS-synthesising enzyme in the same place as substrates, suggesting it may interfere with the active site. Image credit: Douglas Huseby; adapted from the PNAS publication in accordance with CC-BY 4.0 license.

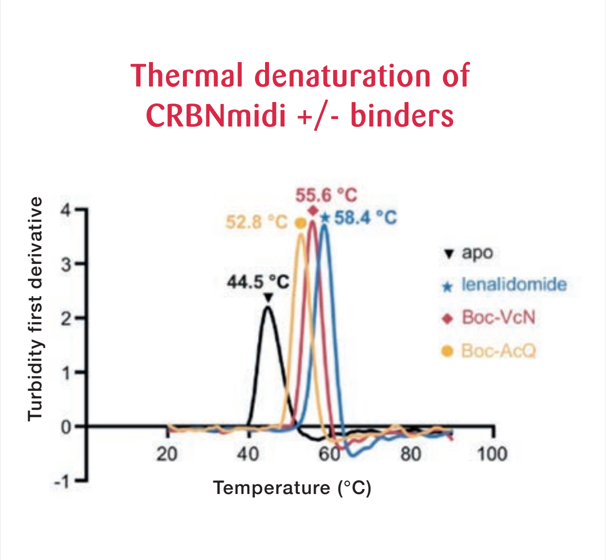
Targeted destruction of disease-related proteins

While most conventional drugs work by inhibiting proteins, not all proteins are easy to block in this fashion. Drug developers are investigating new classes of drugs that mark proteins for degradation in the cell. A large, barrel-shaped structure called the proteasome drives this breakdown process, and a protein called Cereblon behaves as an usher, delivering proteins to the proteasome for destruction. Some drugs act as "molecular glue", sticking to Cereblon and altering its structure so that it binds to target proteins. Other drugs called proteolysis targeting chimeras (PROTACs) bind to target proteins and Cereblon, bridging the two together. Thus, an in-depth understanding of Cereblon's morphology is crucial for drug investigations. However, scientists have struggled to determine high-resolution structures of this protein in the past due to complications with its synthesis and stability. Researchers from the University of Dundee developed a highly stable, easily purified Cereblon variant. Combining X-ray crystallography data collected using Diamond's I04 and I24 beamlines, they demonstrated that the structure of their Cereblon variant matched ones previously collected by other groups, but the new crystals achieved higher resolution. Cereblon changes shape when bound to different drugs, and the team also collected Small-Angle X-ray Scattering (SAXS) data at beamline B21 to study how shapeshifting varies between different drug candidates. Together, these findings reveal that the new Cereblon variant is amenable to structural analysis, which could facilitate future research into this promising class of protein-degrading drugs.

DOI: 10.1038/s41467-024-52871-9





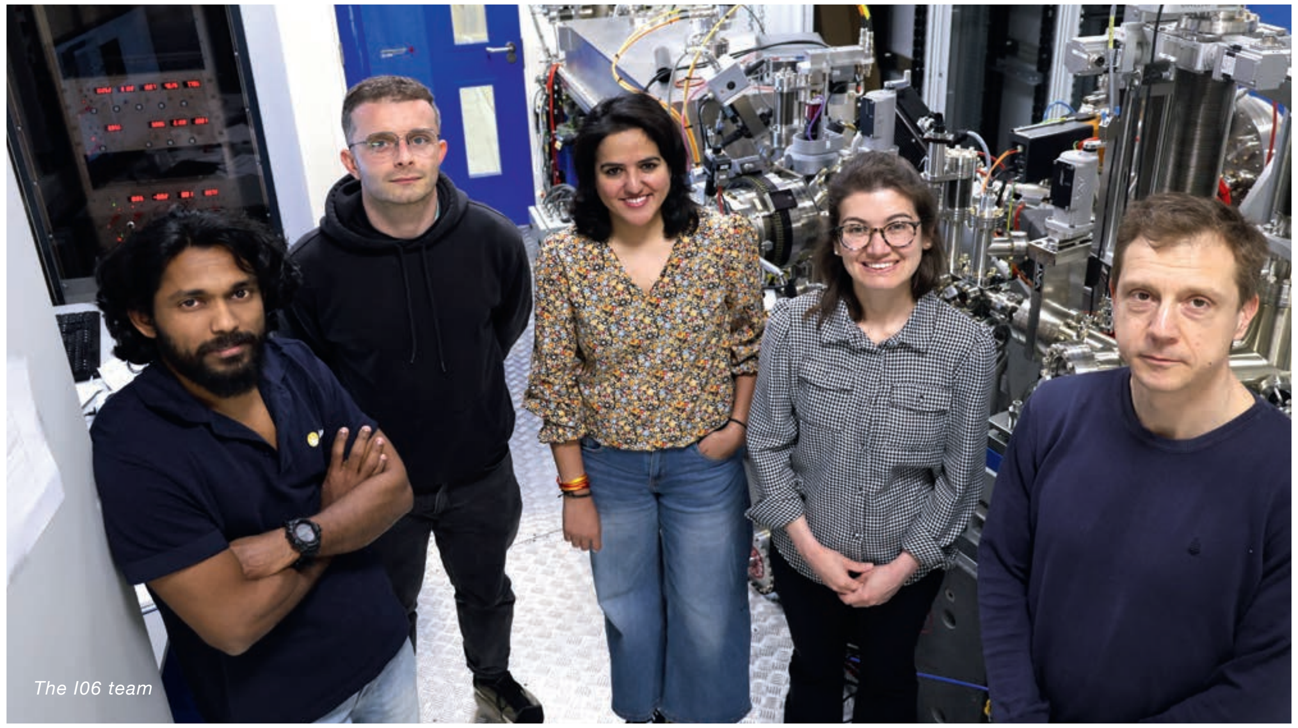


Above: Crystal structure of CRBNmidi in the apo state, containing Lon (yellow), HB (orange) and TBD (red) domains. The mutated residues are indicated (blue), the unresolved region containing the GSG linker is shown as blue dashed line, and Zn2+ is shown as a purple sphere. Bottom: Dimensionless Kratky Plot generated from SAXS data of apo CRBNmidi (black) and CRBNmidi bound to mezigdomide (green), lenalidomide (blue), Boc-VcN (red), or Boc-AcQ (orange). First derivative of turbidity of thermal denaturation for CRBNmidi in the absence (black) or presence of binders lenalidomide (blue), Boc-VcN (red), or Boc-AcQ (orange).

Magnetic Materials Group

Diamond's Magnetic Materials Group (MMG) concentrates on emergent phenomena in quantum materials using the capabilities of beamlines I06, I10, I16 and I21. The research encompasses a variety of challenges and opportunities at the frontiers of condensed matter physics and materials science ranging from topological states of matter, superconductivity, spintronics, two-dimensional systems, skyrmions and multiferroics.

The key insights made by the research community exploit the high sensitivity of polarised X-ray spectroscopy, microscopy and scattering available across the beamlines. For instance, polarised soft X-rays combined with the PhotoEmission Electron Microscope (PEEM) on beamline I06 have visualised the domain dynamics underpinning antiferromagnetic spintronics while the resonant soft X-ray scattering on beamline I10 has been used to understand the topological properties of skyrmions. On beamline I16, interference effects in hard X-ray scattering have led to a deeper understanding of long-range magnetic ordering in canted antiferromagnets. Inelastic X-ray Scattering on beamline I21 has been used in groundbreaking experiments measuring orbital excitations, magnon dispersion and electron-phonon coupling in several highly-correlated systems. I17 is in the planning stages as a flagship Diamond-II beamline and will be a unique facility for performing polarised X-ray imaging from quantum and functional materials. The MMG also runs the Materials Characterisation Laboratory (MCL), to characterise and align samples. The MCL houses a Supernova X-ray diffractometer, SQUID, AFM and sputtering and wire bonding facilities. The research output from the MMG beamlines demonstrates how polarised X-ray science can uncover dramatic changes in the magnetic properties of materials from subtle changes to the geometric and electronic structure.


The I06 team

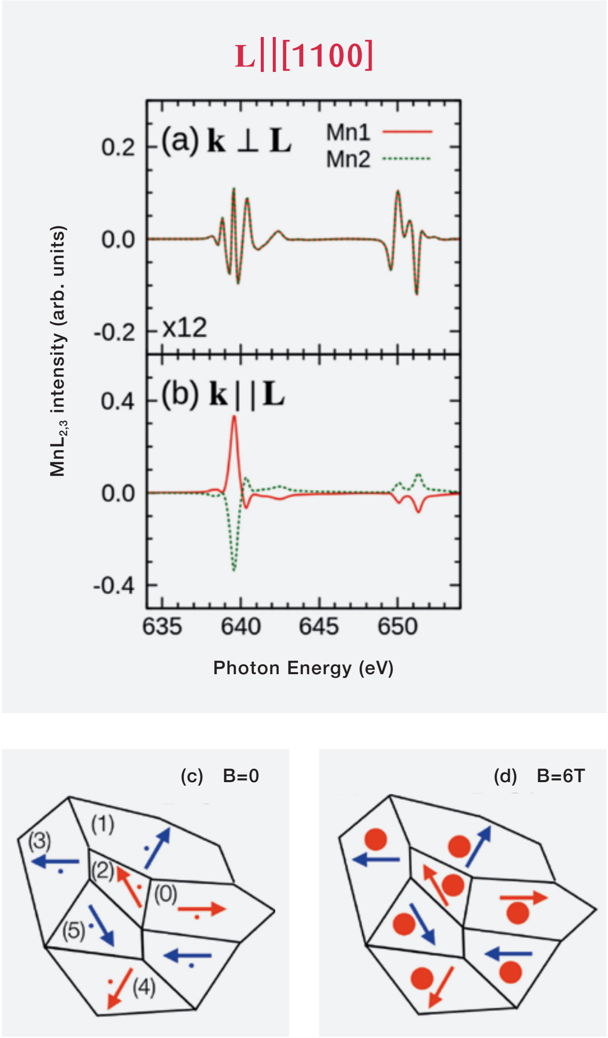
XMCD fingerprints expose altermagnetism

Traditionally, collinear magnetic materials have been classified as ferromagnets or antiferromagnets. Magnetism arises from electron spin, and in ferromagnets the spins all point in the same direction. In antiferromagnets, they point in opposite directions, cancelling each other out. Altermagnets are a new class of magnetic materials that possess the useful properties of both ferromagnets and antiferromagnets, potentially making them very useful in future electronic devices based on spintronics – technology that uses the spin-state of electrons to carry information. However, identifying altermagnetism is challenging.

X-ray Magnetic Circular Dichroism (XMCD) is a standard way for investigating ferromagnetic materials, which shows the difference in absorption between left- and right-circularly polarised light. In a non-magnetic sample, and in antiferromagnets, no difference is observed. However, if the spins in an altermagnet are aligned, a signal is observed.

A team of researchers from the UK, Japan, Austria, Germany and the Czech Republic theoretically predicted an altermagnetism fingerprint in manganese telluride (α-MnTe). They used XMCD on Diamond's I06 beamline to detect it experimentally. If you cool down altermagnetic α -MnTe, the magnetic moments align in one of six different directions, and regions in which the moments align in one particular direction are called domains. Using XMCD, researchers are now able to detect the domains and visualise their location in the sample, things that previously have been extremely difficult. Their results demonstrate that XMCD is an effective method of identifying altermagnetic materials, a discovery that could accelerate the use of these new properties in next-generation electronic devices.

DOI: 10.1103/PhysRevLett.132.176701



The Mn site-resolved contributions to XMCD calculated by the LDA+DMFT AIM for the Néel vector L*//*[1⊠1¯⊠00] and the light propagation vector k*//*L (a) and k*//*L (b). (c) A cartoon view along the c-axis of the possible domain structure with the six easy-axis orientations of ***L***. The domains with even labels (red) contribute Δ⊠F⊠(ω) with positive prefactor, the odd ones (blue) with negative prefactor. The red and blue dots indicate the positive and negative orientation of the out-of-plane magnetisation ***m***. (d) The out-of-plane canting of the moments in 6 T applied field does not strongly depend on the domain's ***L*** (The domain sizes and shapes were chosen randomly and are not intended to have physical meaning.)

RIXS shows why Li-rich batteries fade

The net zero transition necessary to limit the effects of climate change requires dramatic cuts to carbon emissions. One of the cornerstones of the UK's transition will be switching to fossil-free transport, with electric vehicles (EV) one of the most developed options. However, the cathode is a critical limiting factor in efforts to increase the energy density of lithium-ion (Li-ion) batteries for EV applications. Cathodes have layered structures with alternating layers of transition metal oxide and lithium ions.

Lithium-rich cathodes are next-generation materials which have higher concentrations of lithium within the cathode structure, replacing some of the transition metals. They have a higher capacity because they store energy via oxidation of the oxygen in the structure as well as the transition metal. However, a long-standing question has been how the oxygen undergoes charge storage.

Using high-resolution resonant inelastic X-ray scattering (RIXS) spectroscopy on beamline I21, researchers from the Faraday Institution and the University of Oxford followed the oxygen redox reaction in Li-rich cathodes over cycling and quantitatively measured the O2 trapped within the material. Their results show that a gradual increase in electrochemically inactive O2 and the loss of O2 from voids near the cathode surface leads to a reduction in the O redox capacity and the observed voltage fade. These important insights could lead to innovations in cathode chemistry and aid the transition to low-carbon energy sources.

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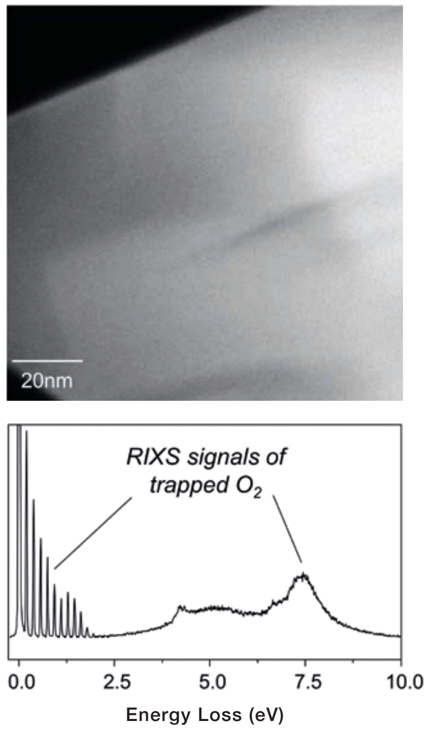
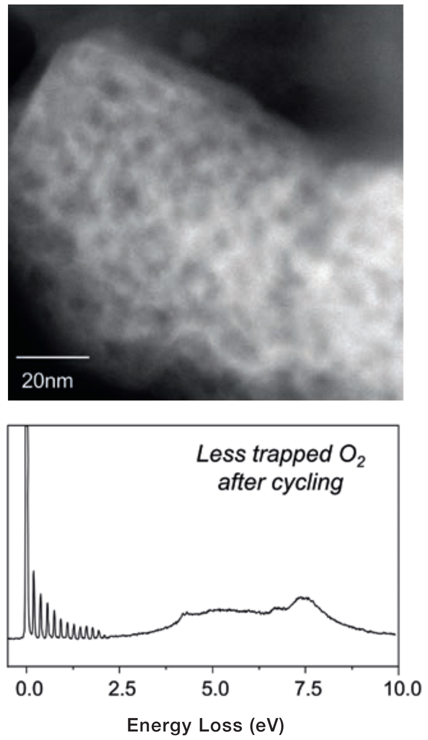
2nd Charge



100th Charge



Imaging and measurements demonstrated the battery fade.

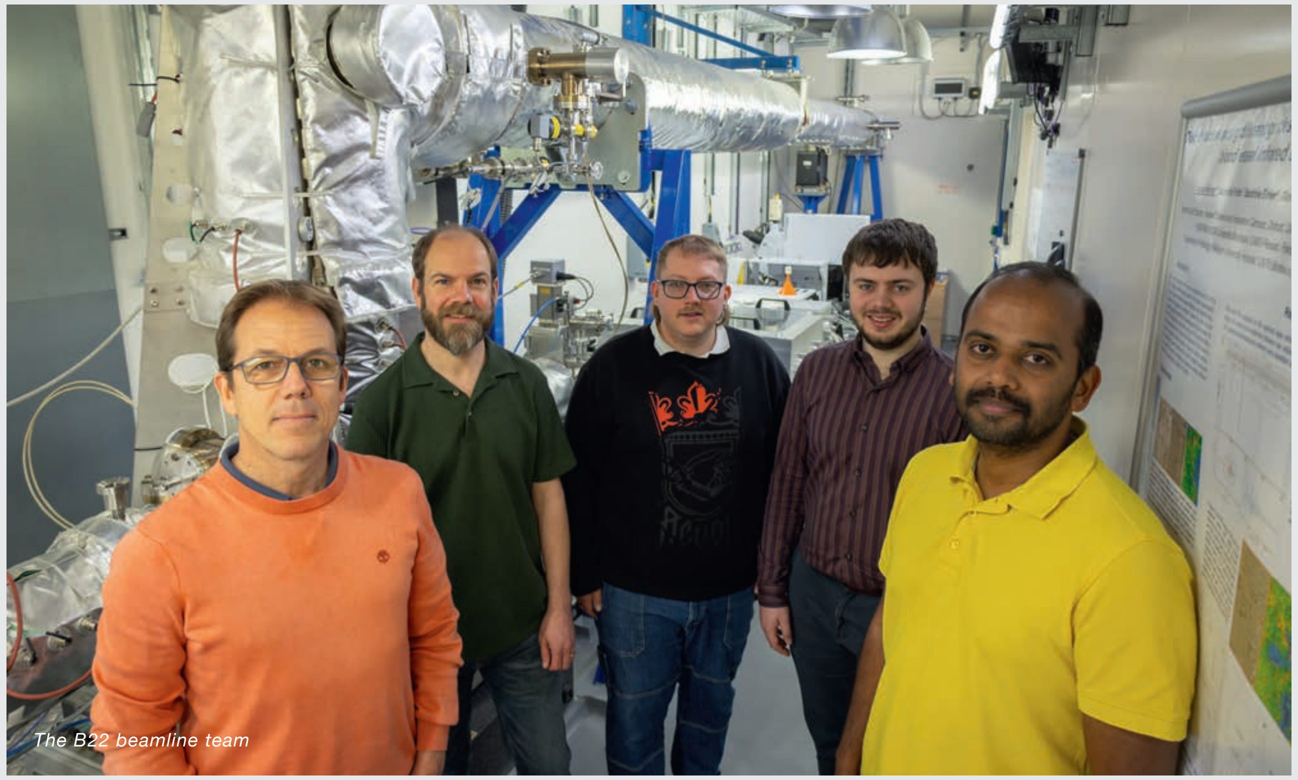
Soft Condensed Matter Group

The Soft Condensed Matter Group provides the infrared (IR) and ultraviolet Circular Dichroism (UV-CD) spectroscopy and, both Small and Wide Angle X-ray Scattering (SAXS and WAXS) imaging capabilities of Diamond.

The Soft Condensed Matter Group comprises four beamlines B21, B22, I22 and B23 and the Offline SAXS Instrument, labSAXS (P38). This unique portfolio of beamlines can analyse a range of samples that include two-dimensional thin films (photovoltaics), living mammalian cells, three-dimensional matrices (metal-organic frameworks) and nano-particles in non-crystalline states. The Soft Condensed Matter Group also maintains a dedicated laboratory space for our visiting users. The laboratory houses vital equipment for sample preparation and analysis such as centrifuges, a small tissue-culture facility, spectroscopy equipment (including CD, standalone IR and UV spectroscopy, multi-angle and quasi-elastic light scattering) and the ability to work with different gases. Both B21 and B23 offer mail-in services for solution-state SAXS and CD measurements. labSAXS now offers the same facility for solid, liquid and gel SAXS samples.

I22 is a multifunctional SAXS/WAXS beamline for the physical and life sciences providing essential information on the structure and dynamics of large molecular assemblies in low ordered environments. Working in both transmission and grazing incidence with full and microfocus beam I22 provides a working platform for studying the full range of soft matter systems. B21 is a bending magnet SAXS beamline primarily focused on dilute solution state systems.

B22 provides a brilliant and versatile microprobe across the whole IR range, for the highest spatial resolution of molecular structures via highest



The B22 beamline team

sensitivity vibrational spectroscopy in Fourier Transform IR (FTIR) mode, plus TeraHertz (THz) spectroscopy. Since 2022, a nanoIR endstation couples an Atomic Force Microscope to the B22 beamline and uniquely measures photothermal (AFM IR) and scattering (s-SNOM) nanospectroscopy at sub-wavelength resolution.

B23 is a life sciences, chemistry and material science beamline for investigating and observing structural, functional and dynamic interactions in proteins, nucleic acids, nanoparticles and polymers using UV-CD. B23 is a world-leading instrument in Muller Matrix polarimetry for studying chiral materials which can detect the emergence of chirality from achiral particles.

Unveiling the subcellular impact of metallo-drugs by infrared nanospectroscopy

New treatments are urgently required for osteosarcoma, a type of cancer that mainly occurs in children and teenagers. Current treatments mostly rely on DNA-damaging agents such as cisplatin, which was the first platinum-based anti-cancer metallodrug, introduced in the clinics in the 1970s. However, the in vivo anticancer activity of cisplatin is severely limited by low bioavailability, serious side effects and acquired resistance.

Researchers from the University of Coimbra in Portugal carried out synchrotron nano-FTIR measurements on cisplatin-exposed human osteosarcoma cells as well as on drug-free (control) cells. This method allows topography, mechanical response and optical images to be obtained simultaneously, in this case revealing a high sub-cellular heterogeneity at the nanometre scale. The data show well resolved cell topography and organelle contours, and the nano-FTIR spectra revealed the impact of cisplatin on cellular proteins, lipids and DNA.

The new information gathered during these experiments adds to data previously obtained on different scales using micro-FTIR and THz spectroscopies, together with micro-Raman and neutron scattering methods (both inelastic and quasi-elastic). By adding subcellular-level insight on the effect of the drug on specific cellular regions and biochemical components, it goes a step further, demonstrating the potential for using synchrotron nano-FTIR as a suitable nanospectroscopy probe in biomedical research. This new approach to studying the mode of action of metallodrugs at a molecular and subcellular level will be a key tool in the development of improved anticancer agents, potentially leading to improved clinical outcomes and a better quality of life for oncology patients.

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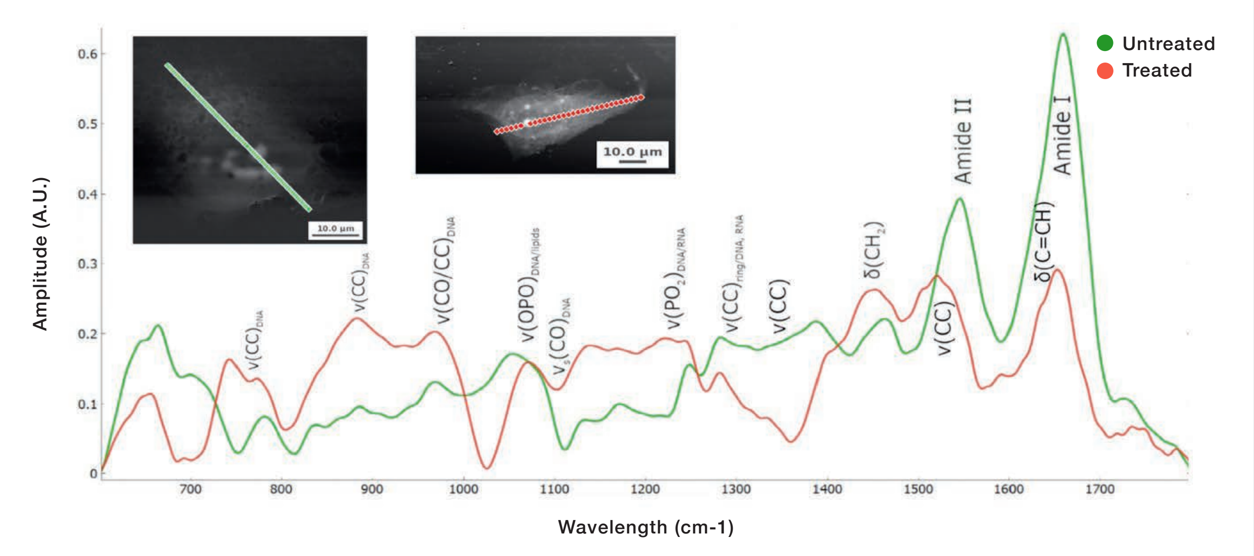

Synchrotron-radiation nano-FTIR spectra, for human osteosarcoma cells (MG-63, formalin-fixed) both untreated and treated with cisplatin, averaged over all the points of the line-scans shown in corresponding top graphic images (inset).

Ending the cold chain: novel hydrogel set to improve access to vital medicines

The storage and distribution of vital protein therapeutics presents several complex challenges. Many medicines and vaccines need stable, temperature-controlled environments and chemical additives such as preservatives to keep them effective and safe for use. This requires cold storage infrastructure and reliable energy sources which causes accessibility and affordability challenges, especially in developing countries where resources are limited.

A multidisciplinary team led by a team of researchers from the University of Glasgow have designed the world's first hydrogel technology for the storage and distribution of crucial medicines and other biopharmaceuticals without the need for refrigeration or chemical additives. The new hydrogel system has been designed to stabilise proteins, protecting their properties and functionality under stresses such as vibration and temperatures as high as 50 degrees centigrade. Key to this breakthrough is the hydrogel's mechanical structure. The unique gel was developed using a Low Molecular Weight Gelator (LMWG) and a chemical trigger that prompts the gelator molecules to self-assemble into very long, three dimensional fibres. When the proteins are added, they become lodged in the spaces between the fibres, where they are unable to mix and aggregate.

During the initial stages of the research the gels were explored with time-resolved experiments on Diamond's beamline I22 using small angle X-ray scattering (SAXS) techniques. The resulting scattering patterns revealed several structural parameters in the gels, which were then analysed using mathematical models. Further experiments were conducted at Diamond's B21 beamline to confirm that the protein which entered the gel was the same after it was expressed.

With a patent-pending, different market segments are being explored where the novel hydrogels can make impact, including vaccines for low-resource environments, therapeutic proteins and enzymes, and antibody therapies.

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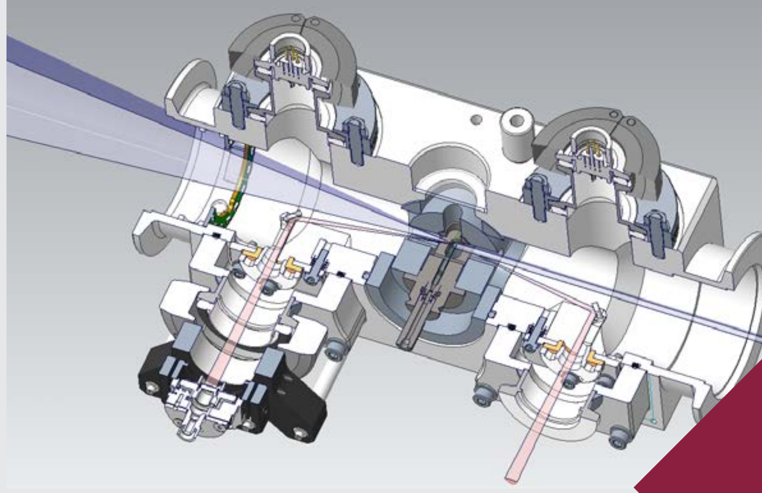
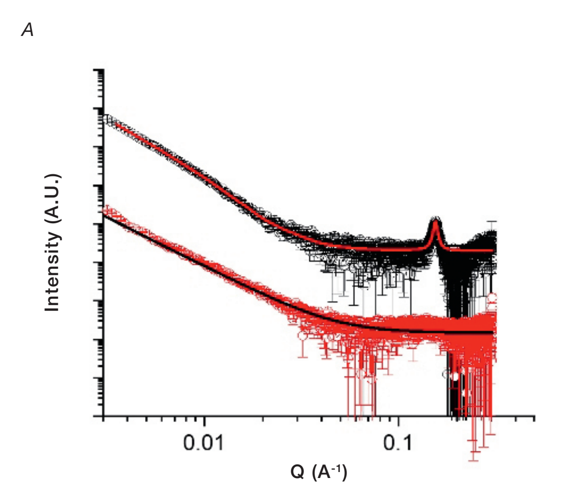
B21 Sample Environment Unit (SEU) designed by Diamond's Engineering group. The SEU provides direct heating and cooling of samples from 0 to 150 oC, with an in-line, on axis camera for visualization of the sample. There are added ports for lasers for photo-activation of the sample. In addition, the SEU minimizes air gaps with the sample windows forming the windows with the beamline vacuum system. This unit is optimized for weakly scattering samples. X-rays (from right-to-left) scatter as a cone (purple) whilst the incoming laser light (red) is transmitted through the sample. Modular sample cells (dark grey) can be adapted to hold a variety of sample types (e.g., semi-solids, liquids, gels, solids). The SEU is compatible with geometry for WAXS measurements.





Initial gel studies. SAXS patterns of gels made in presence of calcium chloride (black) and without CaCl2 (red). The fits obtained through model fitting are overlayed on each spectrum. The plotted data show the averaged scattering pattern obtained from five measurements across the sample.

The spectroscopy group

Spectroscopy Group

The Spectroscopy Group consists of three operational beamlines; the Microfocus Spectroscopy beamline (I18), the Core EXAFS beamline (B18), and the Versatile X-ray Absorption Spectroscopy beamline (I20-Scanning).

An additional beamline, SWIFT, is being built as part of the Diamond-II programme. The three operational spectrometers are complementary in the energy ranges they cover, the size of their focused beam spots delivered to the sample, and the time resolutions they reach. This complementarity means that they can support research across many different scientific disciplines, from chemistry and catalysis through materials science, condensed matter physics, environmental and life science, energy materials and cultural heritage. The addition of SWIFT to the portfolio of beamlines will enhance the fast-scanning capabilities of the Spectroscopy Group, pushing the achievable time resolution towards the millisecond timescales.

I18 is optimised for the 2D and 3D study of heterogenous samples using a variety of experimental techniques such as X-ray Fluorescence (XRF) and X-ray Diffraction (XRD) imaging, micro X-ray Absorption Spectroscopy (microXAS), and XRF and XRD micro-tomography (microCT).

B18 is a general-purpose beamline optimised for the efficient collection of XAS over a wide energy range. The optical design, including the continuous scanning capabilities of the monochromator, together with the flexible experimental space and the large range of sample environment equipment available, make this beamline ideal for experiments that are performed under in situ and operando conditions.

I20-Scanning is a high-flux wiggler beamline optimised for both, absorption and emission spectroscopy (XAS and XES). The XAS end-station is equipped with a multi-element germanium detector that enables the structural study of low concentration samples in fluorescence detection mode. The XES end-station is based on a 1m Rowland circle point-to-point spectrometer and is used to perform High-Energy-Resolution Fluorescence Detection XAS (HERFD-XAS) and resonant and non-resonant X-ray Emission Spectroscopy (RXES and XES) to study the electronic structure of materials.

SWIFT (Spectroscopy WithIn Fast Timescales) will be a wiggler-based, quick-scanning EXAFS beamline dedicated to operando studies, also at micrometric scale. The construction of the SWIFT hutches is progressing well, some of the main optical components have already been ordered, and the design of the challenging fast monochromator is well advanced. The beamline will become operational on Diamond-II after the upgrade period.

Modelling glass long term corrosion using naturally altered archaeological glasses

Lead silicate glass ingots from the East Indiaman sailing vessel the Albion, sunk off Margate UK in 1765 and recovered from the wreck in 1985, were studied to ascertain the chemistry and mineralogy of alteration products after exposure to seawater for 220 years. The results were compared to those of the same glasses exposed to short-term, high temperature, laboratory dissolution tests in synthetic seawater. The research team from the Universities of Sheffield, Bristol, Essex and Cologne used X-ray Absorption Near Edge Structure (XANES) spectroscopy on beamline I18 to study the local coordination environment and speciation of elements within these layers, particularly iron (Fe), calcium (Ca), and phosphorus (P).

The XANES results highlighted significant differences between natural and laboratory-altered samples. In natural samples, Fe accumulated to form Fe-silicates, while in laboratory tests, Mg-silicates predominated due to limited Fe availability. Similarly, natural samples showed the formation of Pb-substituted apatite phases, influenced by the continuous supply of PO_4^{3-} from the open seawater system, unlike the Pb-sulphate phases formed in laboratory conditions.

These findings underscore the importance of considering minor elements and biological activity in long-term corrosion studies, as they significantly impact the alteration processes and the resulting mineral phases. The study demonstrates the challenges in replicating complex natural systems in laboratory settings and the need for more realistic simulations to predict the long-term behaviour of materials.

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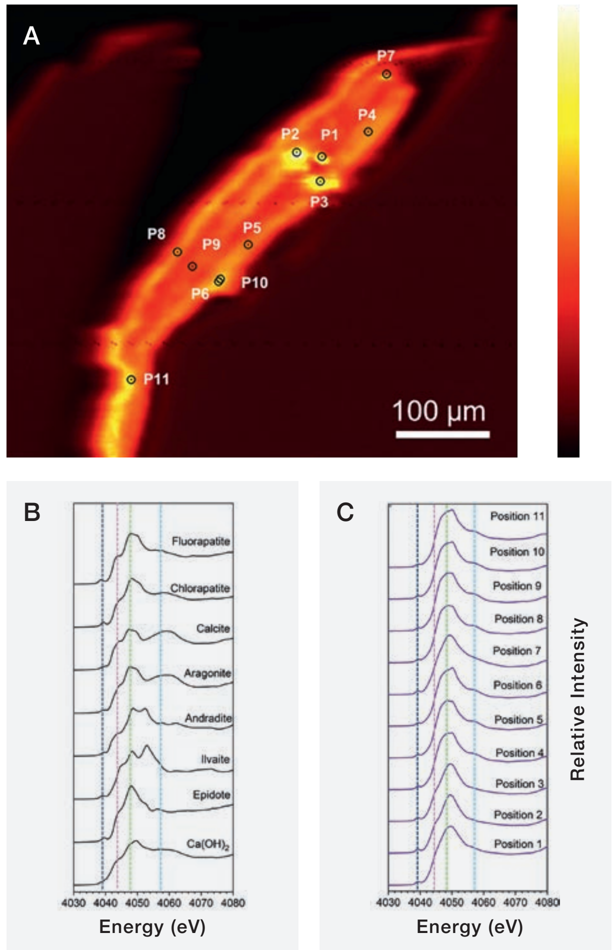


A) Location of Ca K-edge XANES spot analysis on µXRF map of Ca. B) Ca K-edge XANES spectra of Ca-bearing mineral phases and C) Ca K-edge XANES spectra of Ca rich spots.

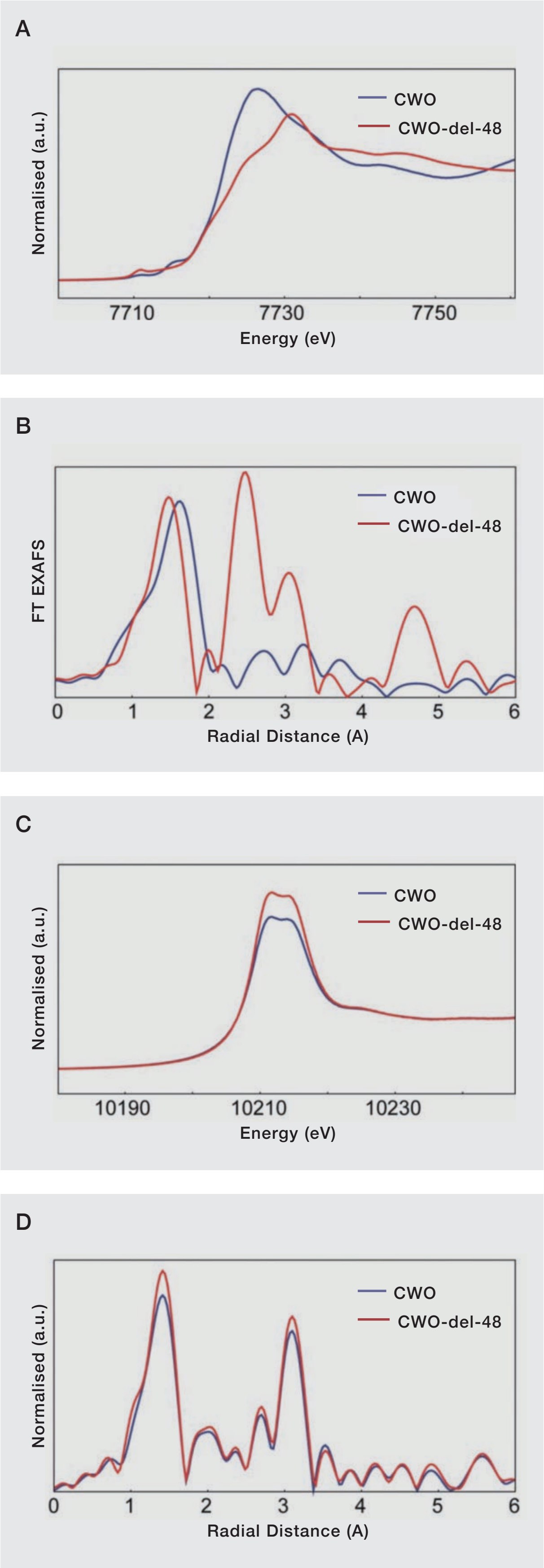
A novel catalyst design for green hydrogen production harnesses the power of water

Hydrogen has the potential to play a key role in building low-carbon economies, yet today it is mostly obtained from methane, which releases significant amounts of CO_2. "Green hydrogen," by contrast, is generated cleanly: renewable electricity drives water electrolysis, splitting H_2O into hydrogen and oxygen. Among the electrolysis methods, proton-exchange-membrane water electrolysis (PEMWE) stands out for its high energy efficiency and fast hydrogen output. Although industrial electrolysis is usually carried out under alkaline conditions, operating in acid can boost efficiency even further. However, most alternatives to the very expensive iridium catalysts break down rapidly in acidic environments.

In this work, the research team led by The Barcelona Institute of Science and Technology proposed a solution to acid degradation by stabilising a cheaper and more abundant cobalt catalyst through the deliberate introduction of tungsten. In their work, they demonstrated control over the oxygen evolution reaction (OER) by modulating the interfacial water structure and intermediate species in a delaminated CoW oxide lattice. This is achieved through a delamination strategy where the tungsten is selectively eliminated in a water-hydroxide anion exchange process, as observed by XAS studies, stabilising water and hydroxide species in the cobalt oxide defected network. This water-hydroxide "shielding" prevents cobalt ion dissolution, making the catalyst highly stable and active in PEMWE.

The cobalt-based catalyst achieved a threefold improvement in activity, remaining stable for up to 600 hours. While this does not yet match current industrial iridium catalysts, it is a big step forward in the search for cost-effective alternatives. The team is currently working on scaling the synthesis of the material to industrial levels and has applied for a patent.

DOI: 10.1126/science.adk9849



Co K edge (A) and W L3 edge (C) XANES spectra for CoWO before (red line) and after (blue line) delamination, and corresponding radial distribution fuctions for Co (B) and W (D).

Distinguishing bulk and surface degradation of lithium nickel oxide cathodes in lithium-ion batteries using multidisciplinary X-ray spectroscopy techniques

Layered transition metal (TM) oxides such as lithium nickel oxides ($LiNiO_2$) are the cathode materials of choice for commercial high energy density lithium-ion batteries as these materials can endure thousands of lithium intercalation cycles to increase their capacity. Furthermore, there is a growing preference for nickel-rich compositions to maximise capacity while minimising cobalt content. However, the role of the different redox centres in $LiNiO_2$ remains a topic of debate, and the connections between these processes and structural instabilities, along with the associated degradation, are not yet fully understood.

In this work the authors from the UK, France and Canada have conducted extensive investigations into the oxygen redox processes occurring in these cathode materials using various multidisciplinary spectroscopy techniques. Their research emphasises the importance of combining bulk and surface-sensitive spectroscopy techniques, and HERFD-XAS on I20-Scanning was utilised to investigate the detailed electronic states of bulk nickel in pristine and charged $LiNiO_2$.

This work has demonstrated that the molecular oxygen redox processes in cathode materials are primarily bulk phenomena that contribute to reversible charge compensation, and that the surface instability of $LiNiO_2$ is linked to rehybridisation at high states of charge (Figure 1). This research underscores the importance of employing strategies such as cathode coatings, composition gradients, and tailored electrolyte formulations to stabilise nickel-rich cathode surfaces in contact with the electrolyte, rather than relying solely on bulk stabilisation methods to enhance the capacity of lithium-ion batteries.

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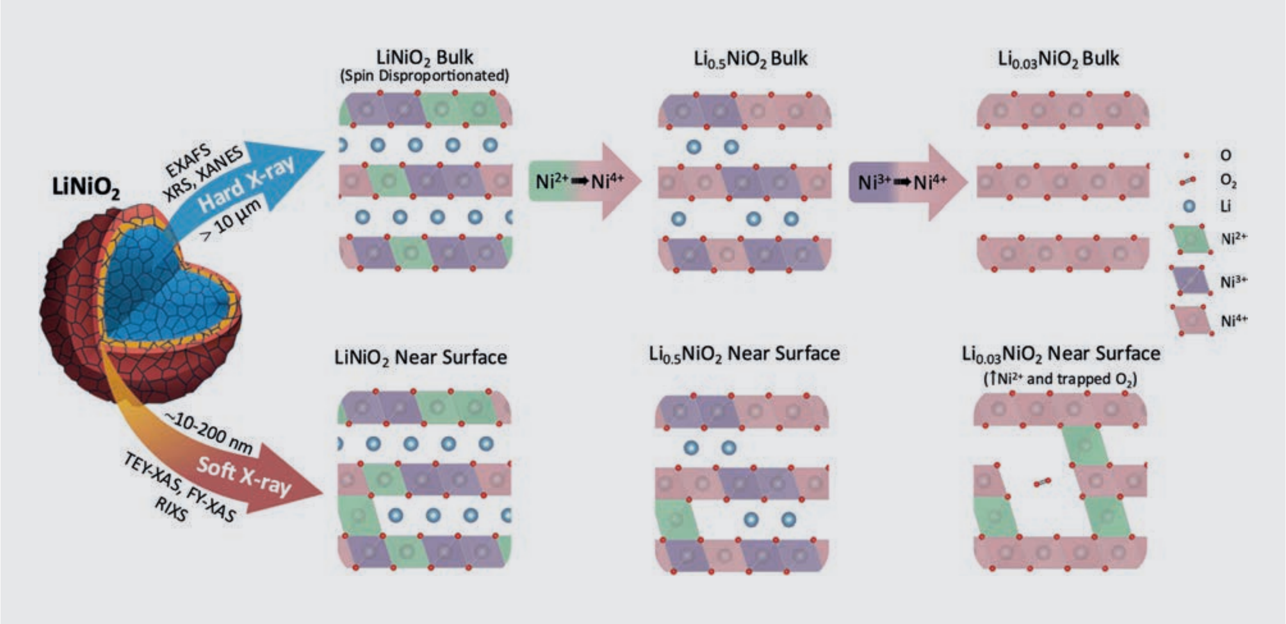

Schematic representation of $LiNiO_2$ bulk charge compensation mechanism and surface degradation processes probed by different X-ray spectroscopy techniques.

The structures and surfaces group

Structures and Surfaces Group

The Structures and Surfaces Group includes four beamlines, each consisting of multiple end-stations that are optimised for a specific type of experiment: I05 (Angle Resolved Photoelectron Spectroscopy – ARPES), I07 (Surface and Interface X-ray Diffraction), B07 (Versatile Soft X-ray Scattering – VERSOX) and I09 (Surface and Interface Structural Analysis – SISA). They offer a variety of techniques to examine the atomic scale structure, chemical nature and electronic state at buried interfaces or the surfaces of materials.

I05 provides an intense and highly monochromatic beam of vacuum ultraviolet radiation. Photoelectrons emitted from the sample are analysed by a high-resolution angle-multiplexing electron analyser. A cryogenic sample manipulator is used to rotate the sample to cover different emission angles above the surface and thus different electron momenta.

I09 is designed for high-resolution studies of atomic and electronic structures of surfaces and interfaces using Photoelectron Spectroscopy (PES), Near Edge X-ray Absorption Fine Structure (NEXAFS), X-ray Standing Waves (XSW), Photoelectron Diffraction (PhD) and X-ray Reflectivity (XRR). I09 offers a unique opportunity for probing the electronic structures of buried layers and interfaces in either an angle-integrated or angle-resolved mode.

I07 is a high-resolution X-ray diffraction beamline for investigating the structure of surfaces and interfaces under different environmental conditions, including harsh and real-world environments. The design of beamline I07 includes the capacity for Grazing Incidence Small Angle X-ray Scattering (GISAXS) and X-ray Reflectivity (XRR) techniques in addition to Grazing Incidence X-ray Diffraction (GIXD).

B07 is designed to provide soft X-rays between 50 and 2800 eV for studying atomic structures and electronic/chemical properties of surfaces and interfaces by Photoelectron Spectroscopy (XPS) and Near-Edge X-ray Absorption Spectroscopy (NEXAFS).

Advances in seawater electrolyte-assisted photocatalysis

The photocatalytic process of water-splitting uses sunlight to break down water molecules into hydrogen and oxygen gases with a light-absorbing catalyst. Using seawater has so far been limited by poor energy conversion efficiencies, instability, and the negative effects of electrolytes in seawater at room temperature. In addition, high electricity consumption and desalination capital costs have impaired technological advancements.

The focus of research led by a team from the University of Oxford was to understand how electrolyte-assisted charge polarisation could influence the photocatalytic performance of nitrogen-doped titanium dioxide (N-TiO$_2$) in seawater (N-TiO$_2$ is a semiconductor and a versatile photocatalyst). This type of polarisation could increase the lifetime of charged species on the surface of the photocatalyst for splitting water into hydrogen and oxygen.

The results demonstrate that N-TiO$_2$, under electrolyte-assisted polarisation, can achieve a higher solar-to-hydrogen conversion efficiency of 15.9% at 270°C, surpassing previous conversion efficiencies of <5% using other photocatalysts.

Ionic species in seawater were also found to prolong the charge-carrier lifetime, significantly enhancing photocatalytic activity.

Diamond's B07-C beamline was used to study charge separation and distribution on the photocatalyst's surface at an atomic level. B07-C is ideal because it specialises in providing gas delivery systems that deliver the well-defined compositions of gases a catalyst might be exposed to, using a computer-controlled environment that can be managed remotely. The surface-sensitive Near-Ambient Pressure X-ray Photoelectron Spectroscopy (NAP-XPS) technique and trimethylphosphine (TMP) as the surface probe were deployed to investigate the surface charge transfer/accumulation on different crystal facets of the photocatalyst at different temperatures, ranging from 150 to 270°C.

Concept plans have been drawn up for a commercial scale solar farm to produce green hydrogen from thermal assisted photocatalytic splitting of seawater. Ultimately, the goal is to promote energy security through decentralised, local production facilities, paving the way for exploration into scaling up the technology for industrial applications.

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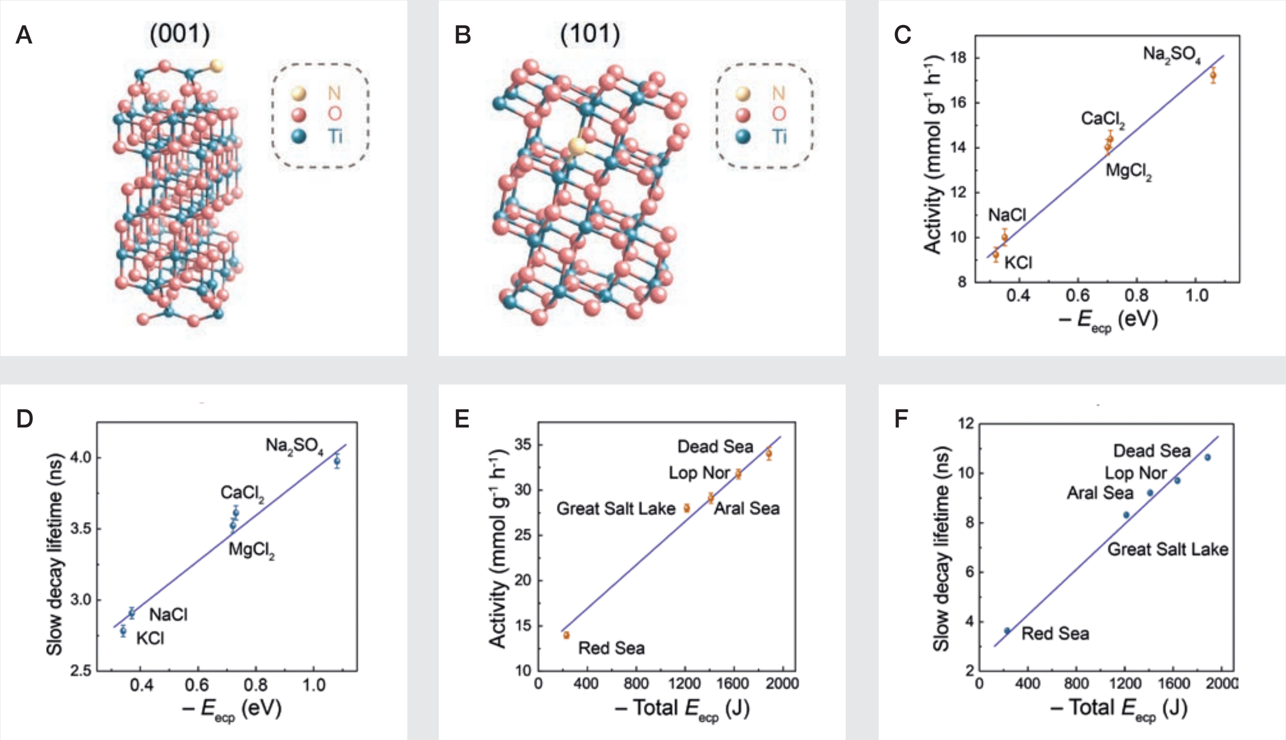

Computational study of the electrolyte-assisted photocatalytic overall water splitting (POWS) system.

Unlocking the secrets of hafnia: a new era in ferroelectric materials

Ferroelectric materials exhibit a unique property called spontaneous polarisation. Their built-in electric dipole moment can be switched between different directions by applying an external electric field. This makes them incredibly useful for a wide range of applications, including memory storage devices, sensors, and energy harvesters. Hafnia displays unusual behaviour in that its ferroelectricity becomes stronger as the material gets thinner, and one theory suggests that the electrochemical state within the hafnia film is directly linked to its polarisation and responsible for the unique size-dependent properties.

A research team from the University of Cambridge focused on two specific compositions, $Hf_{0.5}Zr_{0.5}O_2$ (HZO) and $Hf_{0.88}La_{0.04}Ta_{0.08}O_2$(HLTO), both in the form of single-phase epitaxial films. The first step was to meticulously characterise the structure and ferroelectric properties of the HLTO and HZO films using a combination of techniques. They used X-ray Diffraction (XRD) to determine the crystallographic phase and orientation of the films, Piezoresponse Force Spectroscopy (PFS) and Microscopy (PFM) to confirm the presence of ferroelectricity. These initial characterisations confirmed the presence of the desired ferroelectric phases in both HLTO and HZO and identified 24 areas on the samples, two sets of each specific polarisation state (P-up, P-down, or as-grown), to analyse using depth-resolved XPS on the I09 beamline.

During the XPS experiments, the researchers discovered a surprising difference in the electrochemical behaviour between HLTO and HZO. These findings suggest that the polarisation state is not solely responsible for the changes in oxygen electrochemistry in these materials. Instead, the electric field used to switch the polarisation plays a crucial role.

As irreversible electrochemical changes that occur within ferroelectric materials are a significant factor in device degradation, leading to performance decline over time, understanding and controlling the electrochemical processes in these materials is crucial for improving device performance and longevity. The study's findings, therefore, have significant implications for the future development of hafnia-based ferroelectric devices.

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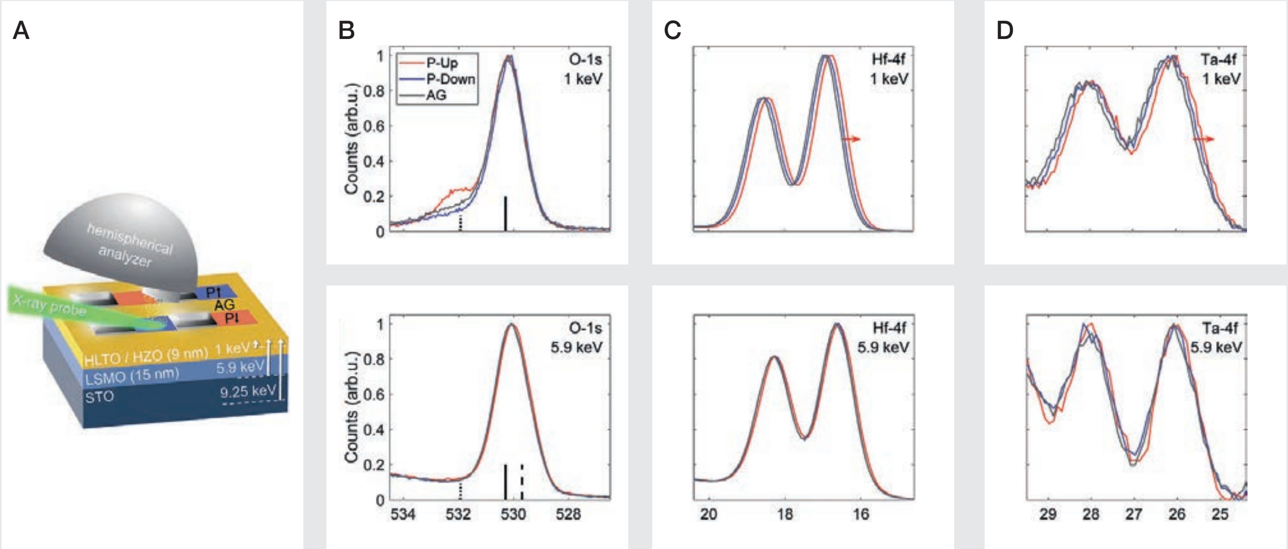


Variable energy XPS for HLTO/HZO stacks. a) Schematic of XPS measurement and HLTO device stack with a focused X-ray probe aligned between W markers (grey) to probe PFM-poled regions of the HLTO/HZO. b) O-1s spectra for P-up (red line), P-down (blue line), and as grown (grey line) PFM conditions, c) Hf-4f and d) Ta-4f spectra for P-up, P-down, and AG conditions. O-1s peaks marked: (Hf/Ta)-O (solid line), NL-O (dotted line), and La-O (dashed line). Core-level shifts are highlighted by red arrows.

Optics and Metrology

The Optics & Metrology (O&M) group's preparations for Diamond-II are now well advanced. The versatile optics test beamline B16 was reopened to users in September 2024 after remodelling to accommodate the new Diamond-II CSXID beamline at I17.

The rebuilt optical metrology laboratory OML2, which had been moved to make room for CSXID, has also resumed operation. The recently established in-house multilayer fabrication lab and ion-beam figuring machine have been fully commissioned and have started to produce niche optics to go on to Diamond beamlines. The upgrade of B16 for Diamond-II has moved to the implementation phase after the successful completion and sign-off of the B16 Technical Design Report and a new double multilayer monochromator and double crystal monochromator are being designed. O&M continues its active involvement in the design and procurement of new optical components for Diamond-II. This includes the development of new software tools for simulations, such as PGMweb for plane-grating monochromators and MLgrating for multilayer gratings, as well as more streamlined procedures for writing tender documents for optical systems.

Development of a high-performance multilayer grating in the tender X-ray regime

Laminar and blazed gratings are commonly used in plane-grating monochromators (PGM) for soft X-ray beamlines. However, the efficiency of conventional single-layer coated gratings is poor in the tender X-ray range. Multilayer-coated gratings offer significantly higher efficiency for tender X-rays. We have designed and developed a multilayer grating for the B07 beamline (Figure 1a) in our recently established multilayer fabrication facility. After installation on the beamline, the grating demonstrated an efficiency in the energy range 1500 to 2800 eV that was significantly superior to that of a grating coated with a single layer.

A comparison of the flux transmitted through the PGM using the ML-coated grating or a single-layer Pt-coated grating shows up to a 14-fold intensity enhancement in X-ray photoelectron spectroscopy (XPS, Figure 1b) and near-edge X-ray absorption fine structure (NEXAFS) measurements. In addition, the PGM with the multilayer stripe exhibits high flux transmission, even when it deviates from the Bragg equation. This suggests that, in some cases, strict adherence to the Bragg equation may not be necessary to achieve high flux transmission. The improved spectral resolution and flux demonstrate the potential of such gratings to enhance the performance of beamline monochromators. By extending the photon energy range, it will help many soft X-ray beamlines address additional scientific applications.

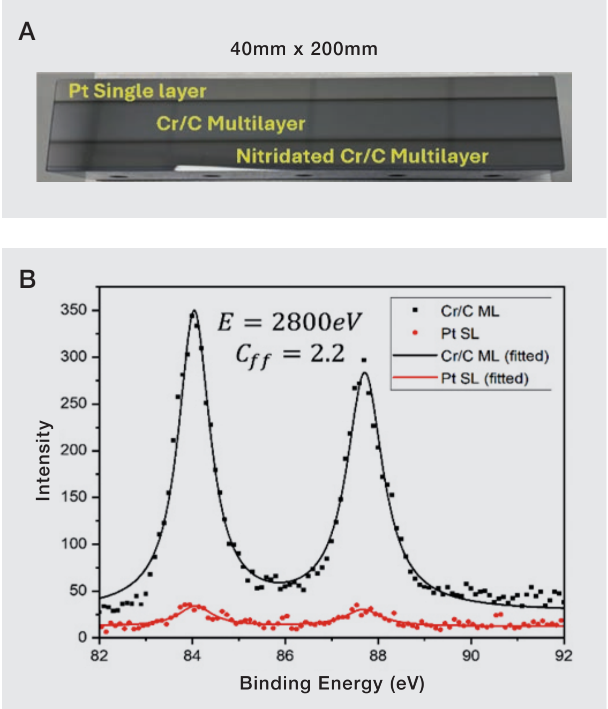


Figure 1: (a) Photo of multilayer grating with Pt-coated grating stripe and Cr/C multilayer-coated grating stripes. (b) The measured photoelectron spectral intensity (Au 4f) with the Cr/C multilayer stripe (black) and Pt-coated stripe (red) at a photon energy of 2800 eV.

Additive manufacturing of X-ray mirrors for synchrotron beamlines

Additive Manufacture (AM) in metals, colloquially known as 3D-printing, is increasingly used to create novel engineering components and light-weighted optics for astronomy and space applications. Compared to traditional "subtractive" techniques, such as drilling and cutting, AM can create intricate internal structures and fuse multiple components into a single piece. X-ray mirrors in silicon with slope errors < 100 nanoradians are becoming commercially available. However, "real world" performance on the beamline is limited by distortion under opto-mechanical clamping, localised heat-bumps induced by photon-beam illumination, and strain caused by differential expansion when dissimilar materials are cooled. To investigate if AM could solve such problems, a prototype X-ray mirror (Figure 2) was designed and fabricated together with the engineering group. The optical substrate, beamline mount and internal cooling pipework were combined into a single, monolithic piece. AM unlocks exotic internal cooling designs, including promoting turbulent flows, reduced coolant vibrations, and conformance to the X-ray heat-load distribution. The mirror was 3D-printed in an aluminium alloy over which the usual polishing processes were applied. Optical metrology demonstrates that surface quality is comparable to a traditional silicon mirror and is virtually immune to clamping deformations. Having demonstrated basic technology feasibility, the next step is determining how AM mirror technology can benefit Diamond-II beamlines.

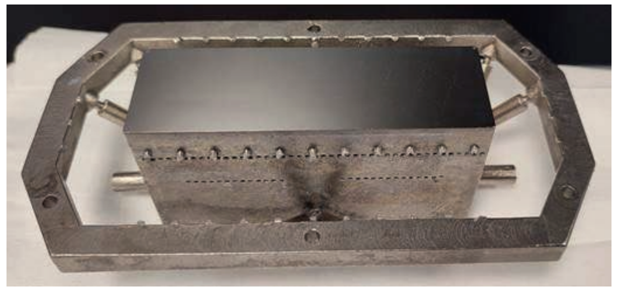


Figure 2: X-ray mirror produced by additive manufacturing.

Cryo-cooled silicon crystal monochromator: measurement of flux versus power

In-house designed cryo-cooled double crystal monochromators (DCMs) ensure delivery of highly stable X-ray beams. Temperature sensors confirm that indirect side cooling using liquid nitrogen via copper plates and indium foil interfaces is highly effective. The resilience of several existing crystal monochromators under higher power density beams on the Diamond-II machine was assessed using FEA and analytical models. A simple equation formulated earlier by the optics group scientists predicts critical power levels, above which the optics deformation increases steeply and diffraction efficiency decreases (Figure 3a). An experiment was carried out on several Diamond beamlines (I04, I07, I18 and I19) on a machine day to test the model: different amounts of power were deposited on the monochromator while the storage ring current was varied from 50 to 300 mA. At each ring current value, flux was measured in static and identical accelerator conditions on all beamlines. Excellent flux linearity was measured on all the beamlines under normal power operation conditions. On one beamline (I04) (Figure 3b) the power load was excessively increased by collecting the entire fan from the Front End custom aperture. Then, the flux levelled off, as predicted by our model (settings 1 & 3), because of the decreased efficiency of the DCM due to thermal distortions. The thermo-mechanical analytical deformation model in Figure 3a therefore is very effective and can be used to predict deformation caused by Diamond-II power quickly, making time-consuming FEA simulations unnecessary.

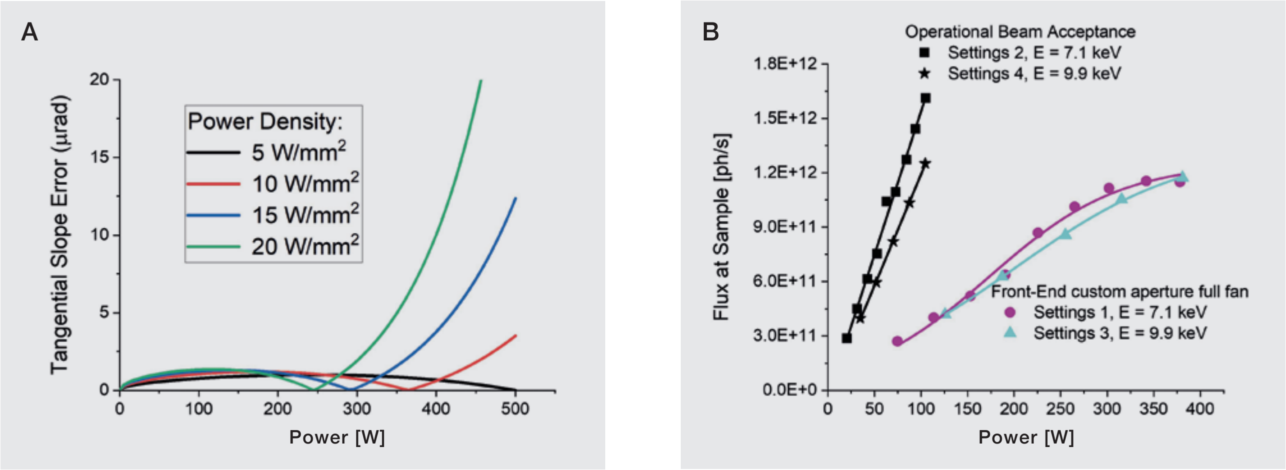


Figure 3: (a) Model of cryo-cooled Si tangential deformation. Threshold power levels are defined as values at which deformation starts to increase steeply. (b) Measured flux on I04 versus incident power.

Estimation of Compton and Rayleigh scattering from white-beam optics

Diamond's beamlines I12, I15 and I20 and the future SWIFT rely on wigglers to produce X-rays with a smooth spectrum up to energies of 80 keV. The increase in electron energy from 3.0 GeV today to 3.5 GeV in Diamond-II will not only increase the power load on the first optic but also increase the portion of the power emitted at higher photon energies (Figure 4a). First beamline optics are normally made from silicon because of its favourable thermal properties. For X-rays of energy over 57 keV, the cross section for Compton scattering in silicon exceeds that for photoelectric absorption, while the cross section for Rayleigh scattering is not much less. These processes scatter X-rays into the components surrounding the first optic. Since the scattered power is estimated to be 3 times greater in Diamond-II than currently, proper Compton shielding must be planned based on the spatial distribution of scattering estimated on various planes around the first optic (Figure 4b & c). A cooled copper "roof" should be within 10 mm of the first optic's active surface. A cooled copper mask should protect the upstream end of the second optic. No mechanical or electrical components should be placed within 200 mm of the reflected beam. This guidance has been included in the procurement specifications for the first beamline optics.

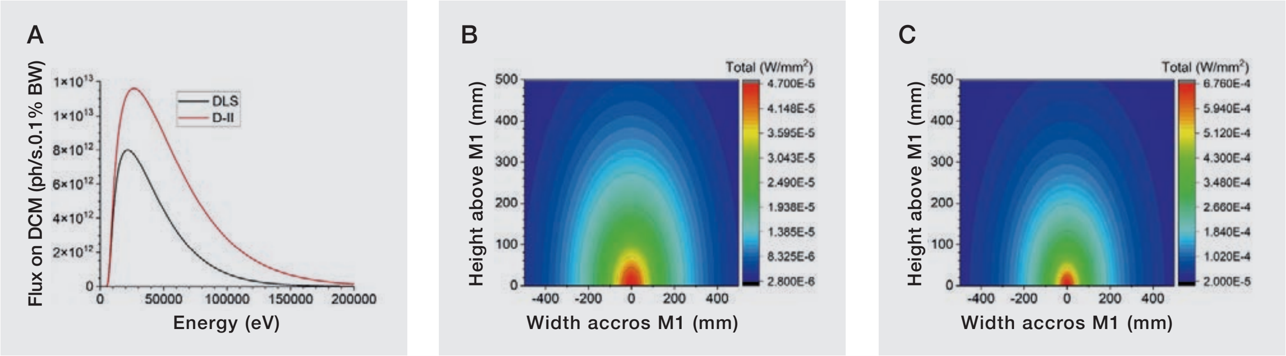


Figure 4: (a) Current ("Diamond") and Diamond-II ("D-II") spectrum of I15 wiggler through the primary slit aperture. (b) Diamond I20, 20 mm wiggler gap: Total power density (Compton + Rayleigh) scattered onto the plane perpendicular to the reflected beam and centred 1 m downstream of the centre of M1. (c) Diamond-II I20, 11 mm wiggler gap: Scattered power density on the same plane as in (b).

Industrial Liaison Group

During 2024-2025 the Industrial Liaison team has played a crucial role in advancing scientific research and fostering industry partnerships.

Our team has been instrumental in driving a wide range of projects that leverage Diamond's cutting-edge synchrotron technology to address complex challenges across various sectors. From healthcare and pharmaceuticals to cultural heritage and materials science, our collaborative efforts have led to significant breakthroughs and innovations.

By connecting industry with Diamond's unique capabilities, we continue to enhance the impact of our research, support economic growth, and contribute to the global scientific community.

Cancer Research Horizons Partnership

In December 2024, Diamond announced a groundbreaking partnership with Cancer Research Horizons, the innovation arm of Cancer Research UK. This collaboration aims to establish a world-leading fragment-based drug discovery programme.

Leveraging Diamond's advanced synchrotron technology and Cancer Research Horizons' expertise, the partnership focuses on accelerating the drug discovery process to bring new cancer treatments to patients faster. The initiative includes funding for two postdoctoral research assistants and early access to proprietary developments, enhancing the appeal of Diamond's XChem Fragment Screening platform to pharmaceutical and biotech partners.

The partnership is expected to significantly impact the field of oncology by identifying novel drug candidates more efficiently. By combining the strengths of both organisations, the programme aims to overcome current limitations in drug discovery, such as the time-consuming and costly nature of traditional methods. The use of Diamond's synchrotron technology allows for high-throughput screening of drug fragments, providing detailed insights into their interactions with biological targets. This approach not only speeds up the discovery process but also increases the likelihood of finding effective treatments for various types of cancer.

Malcolm Skingle's retirement

November 2024 marked the retirement of Malcolm Skingle, Chair of Diamond's Industrial Science Committee (DISCo). Over his 20-year tenure, Malcolm witnessed significant advancements at Diamond, from its early days in portacabins to Diamond's contribution to Nobel Prize-winning research. His leadership helped drive industry engagement, making Diamond's capabilities accessible and beneficial for industrial research, particularly in drug design and material science. Malcolm's reflections upon retirement highlighted the growth and streamlined capabilities of Diamond, emphasising its role in advancing scientific innovation.

Malcolm's contributions to Diamond have been instrumental in fostering collaborations between academia and industry. Under his guidance, Diamond has developed a reputation for excellence in industrial research, attracting partnerships with leading pharmaceutical companies and research institutions. His efforts have ensured that Diamond remains at the forefront of scientific discovery, providing cutting-edge facilities and expertise to support a wide range of research projects. As he steps down, his legacy will continue to influence Diamond's future direction, with a strong foundation in place for continued success.

Uncovering ancient texts

In February 2025, Diamond's Industrial Liaison Group played a pivotal role in uncovering ancient texts from the Oxford Herculaneum scroll. Using the I12 beamline, researchers scanned the 2,000-year-old scroll, revealing its contents through advanced X-ray imaging and machine learning techniques. This project is part of the Vesuvius Challenge, a global effort to decipher the texts of scrolls buried by the Mount Vesuvius eruption in 79AD. The first word revealed, διατροπή (disgust), marks a significant milestone in understanding these ancient artefacts.

The discovery of the word διατροπή is just the beginning of what promises to be a fascinating journey into the past. The use of synchrotron technology has allowed researchers to examine the scrolls in a non-invasive manner, preserving their integrity while uncovering their secrets. This breakthrough has the potential to shed light on the literary and cultural heritage of the ancient world, providing valuable insights into the lives and thoughts of people who lived over two millennia ago. The Vesuvius Challenge continues to inspire researchers and historians, with Diamond playing a crucial role in this exciting endeavour.

Hazel Aitkenhead loading samples for cryo-EM experiments

Scientific Software, Controls and Computation

Scientific Software, Controls and Computation (SSCC) department manages all software, computing and control systems to facilitate and support the science programme of Diamond.

The department functions as seven groups: Scientific Computing, Data Analysis, Data Acquisition, Beamline Controls, Accelerator Controls, Electronic Systems, and Scientific Information Management Systems. The overall structure and function of these areas recognises the importance of, and is optimised to provide, the best possible delivery and support for software, computing, and control systems.

Over the past year there has been an increasing emphasis on planning for Diamond-II. SSCC will deliver new software, control systems and computing as part of the machine upgrade and beamline developments for Diamond-II. In addition, it was recognised that there needed to be developments in the underlying software and computing capabilities to prepare for the substantial increase in data rates that will come with Diamond-II.

Advances in toolkits for applying Artificial Intelligence and Machine Learning (AI and ML) techniques have evolved considerably in recent years. They now provide an important opportunity to automate data reduction and analysis as part of the science programme but also to support business functionality.

Diamond has an extensive scientific IT landscape, extending from high performance computing and storage solutions through to classic IT services. These systems have to be maintained and periodically updated to ensure they are fit for purpose. In doing so, the changes must not impact operation of the facility. This presents many challenges in running what can be complex technological projects. An update to the provisioning of Identify and Access Management services is an example of a complex IT project that SSCC has managed.

Diamond produced more than 12 PB (a PB of data is equivalent to 213,000 DVDs) of data last year from photon beamlines and electron microscopes. It is recognised that provisioning all computing services within Diamond is a key enabler to the operation of the facility.

Update on the development of the new software for Diamond-II

Significant advancements in Diamond's software and computing capabilities are essential to fully leverage the Diamond-II upgrade and maximise scientific opportunities. Key developments required include:

- handling faster detectors and delivering rapid data processing and reduction;
- supporting greater automation of experiments, data reduction, and analysis;
- introducing new data processing techniques, including AI and ML exploitation;
- providing a more open software environment to enable development by scientists;
- addressing obsolescence and modernising the beamline experiment management software stack;
- adapting to changing needs and expectations of Diamond's users.

The Diamond-II core software and computing project focuses on the following areas:

- high performance sample stages;
- detector readout, data compression, and reduction;
- modernisation of data acquisition software framework;
- science-specific data analysis software developments;
- data archiving;
- post-visit data analysis services;
- user administration and information management.

This project, one of the five pillars of the Diamond-II programme, is described in terms of six work streams: Hardware Infrastructure, Software Infrastructure, Data to Information, Real-time Data, Experiment Management, and Information Management. These are divided into over thirty detailed work packages. A phased delivery plan has been developed to prepare for the improved brightness of the Diamond-II machine and enable new flagship capabilities. This project will provide incremental benefits to Diamond, reducing technical debt, addressing obsolescence, and deploying new capabilities with greater flexibility and extensibility.

Early successes include the rollout of a new web-based engineering user interface to the accelerator control system and the development of a new experiment orchestration platform. For the latter initial core services are being developed and deployed onto a simulated beamline. In addition a range of "opportunity projects" are being used to thoroughly test new capabilities examples being live data streaming for ptychography, and live analysis of X-ray diffraction data for experiment feedback, proving the viability of GPUs to reduce image processing times.

Preparing for new opportunities coming from Artificial Intelligence

Artificial Intelligence and Machine Learning (AI & ML) techniques are now foundational enabling technologies in data science. Recent advances in areas such as Large Language Models (LLMs) are also having a science impact and have the potential to unlock new capabilities for the science programme, operation of the accelerators, and business functionality.

Looking forward to Diamond-II three key AI & ML themes have been identified as driving improvements in the science programme. These are Making Experiments Easier; Making Experiments Better; and Understanding Experiments Better. Each of these themes are aimed at opening new capabilities to Diamond's users and so enabling new science to be conducted as well as enhancing our existing science programme. We hope that the early adoption and integration of these technologies not only helps with the 'data deluge' but also assist in making experiments conducted at Diamond more dynamic and easier for the facility's users.

An example of improving operation of the accelerators is our machine stability project. This is a multi-year collaboration with STFC's SciML Group, that has the potential to benefits to all the beamlines across Diamond through improved electron beam characteristics.

In addition to science-focused AI and ML initiatives, the application of Generative AI tool using Retrieval Augmented Generation (RAG) is being tested across Diamond to support business functions. This enables secure access not only to business data within LLMs, but also to Diamond's corporate information.

Delivering challenging IT projects IAM as an example

A recent IT transformation project involved replacing Diamond's Identity and Access Management system (IAM) from a historical database, the Corporate Data Repository (CDR), with a commercial cloud service. Successfully delivering this project was a significant milestone for our team, given that the project faced challenges such as complex scope definition, tight deadlines, and managing a complex rollout.
Risks about readiness were mitigated by extensive testing, and so the final transition was seamless.

Careful planning around key resources was essential to the success of the project. Diamond's core team collaborated closely with development partners whose expertise was crucial for aligning the technical changes with the existing IT infrastructure. Diamond's project team built strong relationships with those managing Scientific IT and Corporate IT services, and coordinating planning between them.

The final rollout had the potential to significantly impact Diamond's operations, as facility operations depend on IAM's functionality and reliability. Diamond was comfortable with the level of testing undertaken, and so final migration from CDR to the new product was able to proceed with an acceptable risk. The result was a smooth transition from the old to new systems. Feedback from a lessons-learnt process indicated satisfaction with Diamond's management of the project.

The project's success from Diamond's perspective was due to the team's hard work, a good communication plan, strong project governance, and a shared commitment to delivery. Despite being a demanding project, it was highly satisfying, showcasing commitment and perseverance from all parties involved.

Development of a roadmap for Scientific Computing

In today's data-driven research landscape, the pace of scientific discovery is closely tied to the effectiveness of computational methods and infrastructure. At Diamond, we are seeing an exponential increase in scientific data production, exceeding 12 PBs (petabytes) annually, due to increased automation, experiment complexity, and the use of photon imaging techniques and electron microscopy.

The arrival of Diamond-II and the launch of upgraded beamlines will significantly boost data production and scientific discovery. Some experiments, like beamline K04, could generate hundreds of terabytes of data per day. This necessitates evaluating our current computing model to handle the increased data volume and velocity. A review of our scientific computing infrastructure began in 2024, leading to a strategic technology and delivery roadmap for scientific computing infrastructure, ensuring support for current operations and new Diamond-II capabilities.

Key areas of focus include:

- data centres: developing new data centre capacity to replace end-of-life provisions and accommodate next-generation of computer hardware. The 1 MW Data Centre project will start construction in late 2025;
- storage: moving from monolithic high-performance file systems to hybrid storage tiers to meet performance and capacity needs;
- networking: upgrading network infrastructure with high-bandwidth links and advanced routing protocols to support seamless data transfer;
- compute and cloud: transitioning from monolithic compute infrastructure to cloud-based research.

This roadmap will provide a framework to deliver the scientific computing infrastructure to realise Diamond-II's potential and enhance current facility performance.

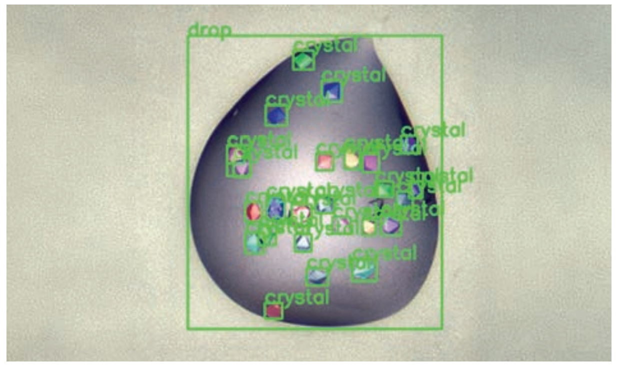


Figure 1: Output of a deep learning network trained to detect the location of drops and crystals in images.

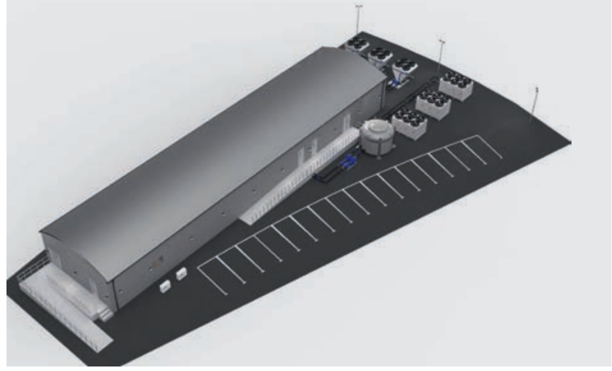


Figure 2: Development of the design for 1MW Data Centre project for first-level data storage and initial processing.

Machine, Buildings and Infrastructure

2024/25 was our 18th year of operation, and was carried out in normal operating mode: 6-day running per week, from 09:00 Wednesday to 09:00 Tuesday interspersed with Machine Development days.

A total of 204.5 days (4,910 hours) were scheduled for User Mode operation, including 5 beamline start-up days. All scheduled operation was in standard multibunch mode (900 bunch train) with total current of 300 mA, apart from two periods of 6 days of "hybrid" mode in February/March 2025, consisting of a 686 bunch train with a high charge (3 nC) bunch in the middle of the dark gap. Unfortunately several periods of 200 and 250 mA running were required in Runs 3, 4 and 5 in 2024 due to RF cavity problems.

The annual operating statistics are shown in Figure 1. The overall Mean Time Between Failures (MTBF) was disappointing at 77.9 hrs, but still above the target minimum of 72 hrs. The 97.2% uptime was slightly below the target of 98%.

Various challenges were faced during the year particularly with the RF system. Superconducting cavity SCC#1 had to be removed in Shutdown 2 (June 2024) due to a leak of the insulation vacuum and replaced with SCC#2, which however needed time to condition with beam and which forced us to have to reduce beam current. Unfortunately SCC#2 then developed a waveguide flange vacuum leak and so had to be removed in Shutdown 3 (August 2024). Due to a simultaneous failure of one of the back-up normal conducting cavities we could only reliably provide a beam current of 200 mA. SCC#2 was repaired in the RAL Space clean-room and re-installed in Shutdown 4 (October 2024), and 300 mA operation was reinstated in Run#1 2025.

Other significant problems that occurred during the year were:

- load arc trips on one of the Normal Conducting Cavities (NCC), eventually traced to broken ferrite tiles in the load;
- a fire alarm-induced shutdown of the machine cooling;
- two mains brown-outs;
- a fast valve on a front end repeatedly disarming, losing the SR Machine Protection System;
- absorber temperature trips on 3 front ends at narrow ID gaps;
- major water leak on the DIAD beamline, losing water pressure on the machine side, tripping multiple systems. A Helium compressor failure.

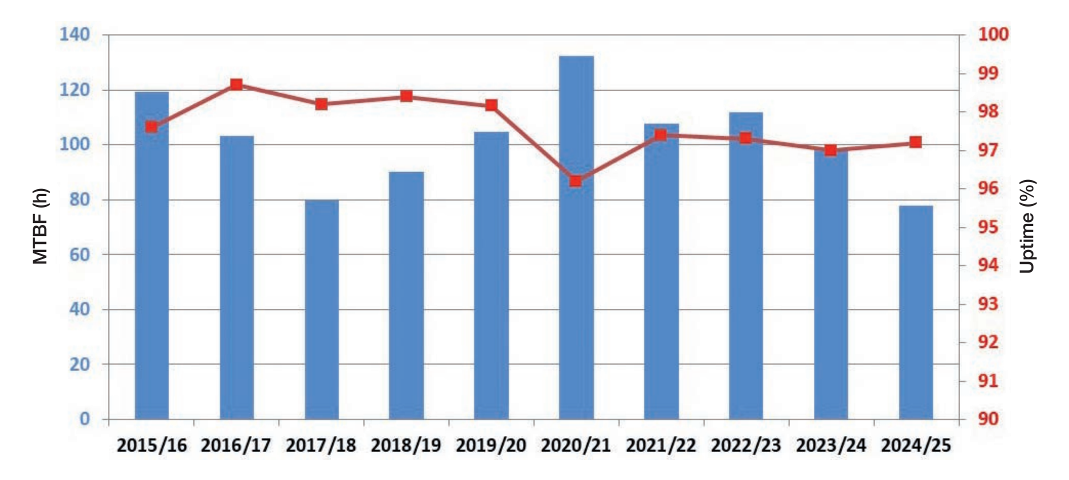


Figure 1. Mean Time Between Failures (blue bars, left axis) and Uptime (red curve, right axis) for the last 10 years.

Installation of CPMU-5

The 5th Cryogenic Permanent Magnet Undulator (CPMU) designed and built in-house was successfully installed in November 2024 (Fig. 2). This was the last Diamond insertion device (ID) upgrade to be carried out before commencing the preparation of new IDs for Diamond-II.

Figure 2. CPMU-5 installed in the storage ring, as viewed from the storage ring roof.

Testing the Diamond-II prototype injection stripline kicker and pulser

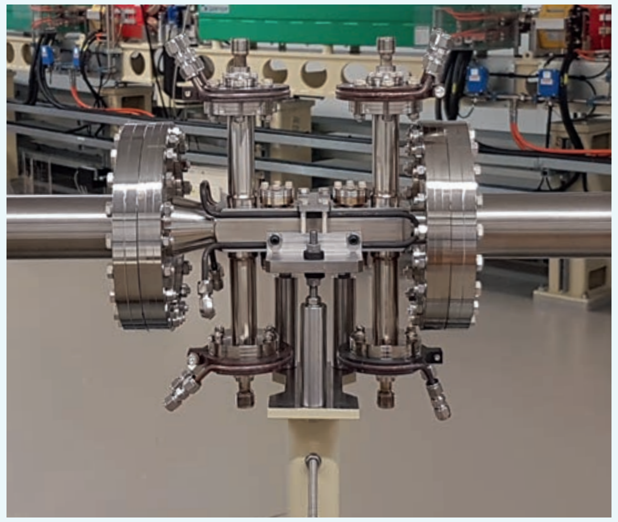


Figure 3. The prototype Diamond-II injection stripline kicker installed in the Booster-to-Storage Ring transfer line.

We are planning a fully transparent top-up injection in Diamond-II whereby the process of injecting additional charge does not materially impact on the quality of the beamline source points. This will be achieved using a novel single bunch "kick-and-cancel" injection scheme which requires the use of high voltage stripline kickers. As there was little in-house experience of designing such systems, a prototype stripline kicker and power supply were developed. These prototypes were tested using the existing test stand in the booster to storage ring transfer line (Fig. 3).

Electron bunches were sent through the kicker and then onto the last beam dump before the storage ring. Fluorescent screen detectors downstream of the kicker were used to measure the transverse location.
By measuring with and without power applied we were able to determine that the angular kick generated was 65 µrad. This compared well with the analytically calculated value of 54 µrad with the applied voltage of ±5.3 kV. Further testing in the storage ring is planned to assess thermal behaviour, impact on beam impedance and full ±20 kV operation. The results from this exercise will inform the final Diamond-II designs and reduce the risk of the overall injection kicker project.

Synchrotron roof solar panels

Following the energisation of the first 1 MWp of solar panels on the Synchrotron roof in May 2023, the second phase was energised in July 2024 making a total of 2.7 MWp installed solar panels (Fig. 4).

The design annual yield estimation for the installation was 2.3 GWh of electricity, being approximately 5% of Diamond's annual consumption. Whilst we have not completed a full operating year with the total installation, Figure 5 shows that we remain on target to realise the predicted yield with an actual generation of 1.6 GWh of electricity over the reporting period.

Figure 4. 2.7 MWp of solar panels installed on the synchrotron building roof.

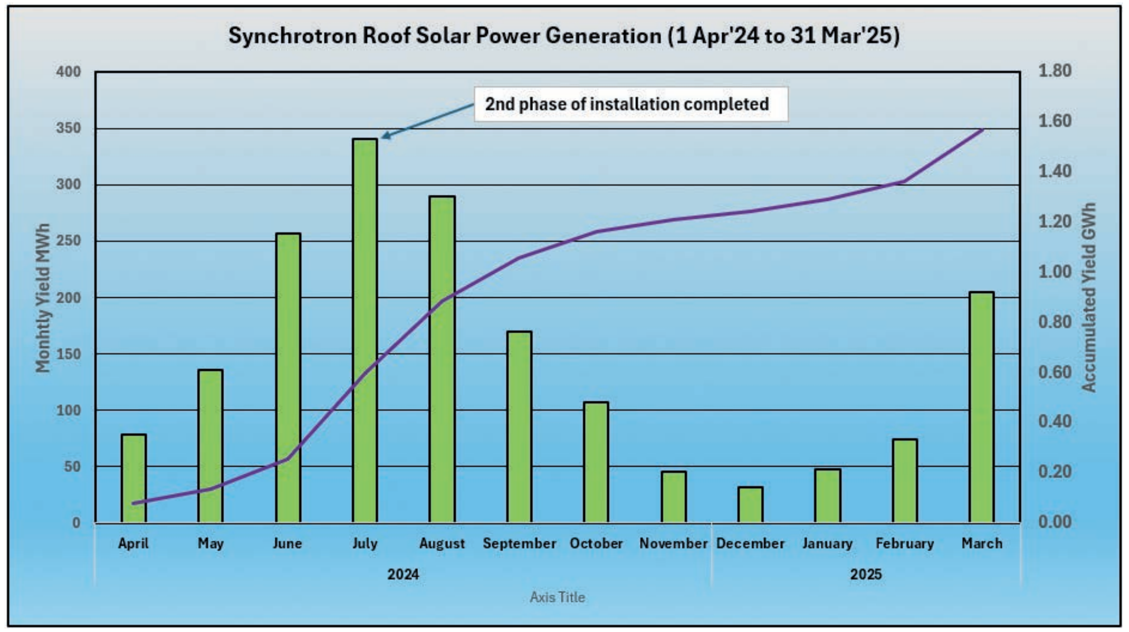


Figure 5. Electrical power generated by the solar panels on the synchrotron building roof per month (green bars, left axis) and cumulatively (curve, right axis) from April 2024 to March 2025.

Diamond-II update

The Diamond-II project has been making impressive progress over the last year, taking full advantage of shutdowns to de-risk the upgrade period.

Significant amounts of procurement have taken place, and in many cases budgets have proved robust; in conjunction with financial and risk management this has allowed the release of contingency scope into the project. So far £5m of additional scope has been added, mainly focused towards the 1 MW data centre and improving the operational resilience of the radiofrequency (RF) systems. Future releases of contingency scope are expected to occur through the life of the project assuming the budget and risk profile allows, which should allow us to maximise the scientific and operational benefits from Diamond-II.

The high-level plan for Diamond-II remains robust, with the only milestone moving so far being the completion of the Diamond Extension Building (DEB). This slight delay has not impacted the overall programme as there was contingency built within the plan along with the team working hard to look at options to mitigate any impact to the larger programme.

A major focus this year has been on procurement - completing designs and specifications, issuing Invitations to Tender, and subsequently placing contracts and monitoring the Suppliers' progress. 30 major orders were placed in the year, bringing the total committed cost to 53% of the total hardware budget for the machine.

Alongside this work, the team have been carrying out as much installation activity as possible before the shutdown for Diamond-II to minimise work during the "upgrade period". This has involved, for example:

- installation of penetrations in the shield wall, for later installation of waveguides to feed power to the new locations of the RF accelerating cavities. The first of 7 new penetrations was successfully installed in the March 2025 shutdown;
- installation of modifications to the demineralised water cooling circuit "Demin A": 11 of 24 cells have so far been completed;
- vacuum rack upgrades to overcome obsolescence and to reduce space requirements: 3 of 24 cells have so far been completed;
- 4 of the 18 front-end X-ray beam position monitor upgrades which are required for compatibility with Diamond-II and are planned to be carried out before the upgrade period have been completed;
- cable re-routing in the Control & Instrumentation Areas: 4 of 24 cells have so far been completed;
- installation of front-end patch panels: 9 of 31 front-ends have been modified so far;
- upgrading over 400 ADC cards used in the Magnet Power Supplies;
- upgrading and commissioning 650 units of 25 A Magnet Power Supplies to 50 A;
- upgrading and commissioning of one of the transformers in the Booster Quadrupole Power Supply, which will be repurposed as the BB Dipole Power Supply in Diamond-II.

Matt Fletcher
Head of Programmes

Construction of the first Diamond-II insertion device, a cryogenic permanent magnet undulator (CPMU) for the VMXm (K02) beamline, is underway (see Fig. 1). The design of this device is different to previous CPMUs constructed for Diamond. CPMU-6 will fit in a new mid-straight hence is shorter than CPMUs 1 to 5 which are located in standard straights. As a result, a new ID structure design was required, and we took the opportunity to incorporate lessons from the earlier IDs. The new structure is all-welded, rather than bolted together, making it stiffer and cheaper to manufacture. Magnet beams fit straight onto the new design in hours rather than several days for the older design.

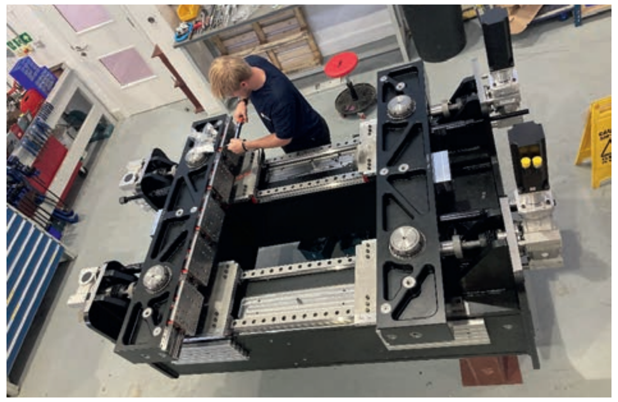


Figure 1: Start of assembly of the first Diamond-II insertion device. Initial assembly and first stage motion testing are carried out with the device 'on its back'.

The first pre-series magnets for Diamond-II have reached the factory acceptance testing stage to verify their performance before committing to the full series production. Figure 2 shows a sextupole magnet after its factory acceptance test.

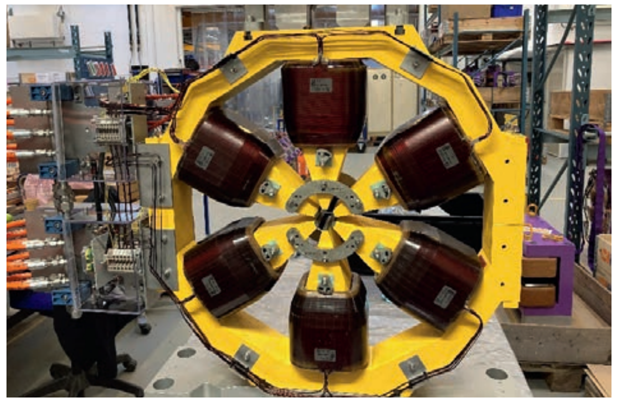


Figure 2: The first completed pre-series electromagnet for Diamond-II.

Buildings and infrastructure

The DEB is progressing as we work towards completion in the summer of 2025, followed by Diamond's own fit out of laboratories, offices and meeting rooms.

Figure 3: A view of the DEB from the synchrotron building

The DEB 20 tonnes crane has been installed, bridge connection works are well underway, external cladding is now complete, primary plant such as chillers/AHU's have been delivered.

The liquid nitrogen connection into Synchrotron main liquid nitrogen ring main has now been completed and awaits the second phase of installation to be run externally to the DEB.

The DEB and the future 1 MW Data Centre will have a new dedicated High Voltage (HV) Substation nestled into Diamond's HV Outer Services Ring circuit delivering in excess of 3 MW of power. The high voltage cables have been pulled across the synchrotron perimeter road to the DEB and the jointing was completed by the end of March 2025.

Figure 4: The high voltage substation

Engaging with Diamond Light Source

10,334
significant interactions

2,529
scientific and technical event attendees

4,300 +
visitors during Harwell Open Week

748
Stakeholder and VIP visitors

2,043
school pupils/university student visitors

4,759
members of the public visited Diamond

Significant interaction is defined as a talk, tour, activity or meeting of 30+ minutes, typically longer.

This year has been another successful period for engagement at Diamond. The large-scale, multi-facility event of Harwell Open Week in June 2024 was a particular highlight, contributing to a substantial increase in our total number of significant interactions, which rose from 7,638 in 2023-24 to 10,334 in 2024-25.

We also observed a shift back to predominantly in-person activities, although hybrid events continue to be a valuable part of our engagement strategy.

Public engagement

Our core public engagement programme, including partner events with STFC, continued to thrive. Notable highlights from this period include the site-wide Harwell Open Week in June 2024, our Schools/College Work Experience Week, which welcomed 57 students across 28 projects, and the Light Up Lancaster art-science festival. Light Up Lancaster was especially successful, attracting 19,000 visitors to our installation, which illustrated the intersection of art and science.

> **“What was clearly evident was the sheer pride and enthusiasm amongst the Diamond Light Source staff that we had the pleasure of meeting”**
>
> Public Inside Diamond open day attendee, October 2024.

Student engagement

This year we saw an increase in the number of externally funded PhD studentships and strengthened partnerships with institutions such as the Ada Lovelace Centre. The 2023 Year in Industry cohort completed their placements in September, showcasing their work to Diamond staff through a poster session and presentations. The 2024 cohort, though reduced to five students, began their journey with us in September. Additionally, we welcomed 441 university students throughout the year, a blend of undergraduate and postgraduate students, who visited to explore Diamond's capabilities and opportunities.

17
Diamond co-funded PhD students joined Diamond

12
Externally-funded PhD students joined Diamond

PhD Students joined Diamond **from 18** separate universities

114
Total number of active PhD students at Diamond

Scientific and technical events

Diamond continued to host a wide array of scientific and technical events, catering to the needs of our diverse staff and user communities. Highlights from this period include multiple successful user meetings including the Magnetic Materials User Meeting, Spectroscopy User Meeting, I15 Extreme Conditions User Meeting, and the Imaging and Microscopy User Meeting. Moreover, we were proud to host the 32nd European Synchrotron Light Workshop, which brought together leading scientists and engineers to share the latest developments within the accelerator physics community.

In conclusion, the 2024-25 period marked another year of robust engagement at Diamond, underpinned by a blend of in-person and hybrid events, a strong public engagement core programme, and significant contributions to student engagement and the wider scientific discourse. We look forward to building on these successes in the coming year.

45
Scientific and Technical Events

2,529
scientific and technical event attendees

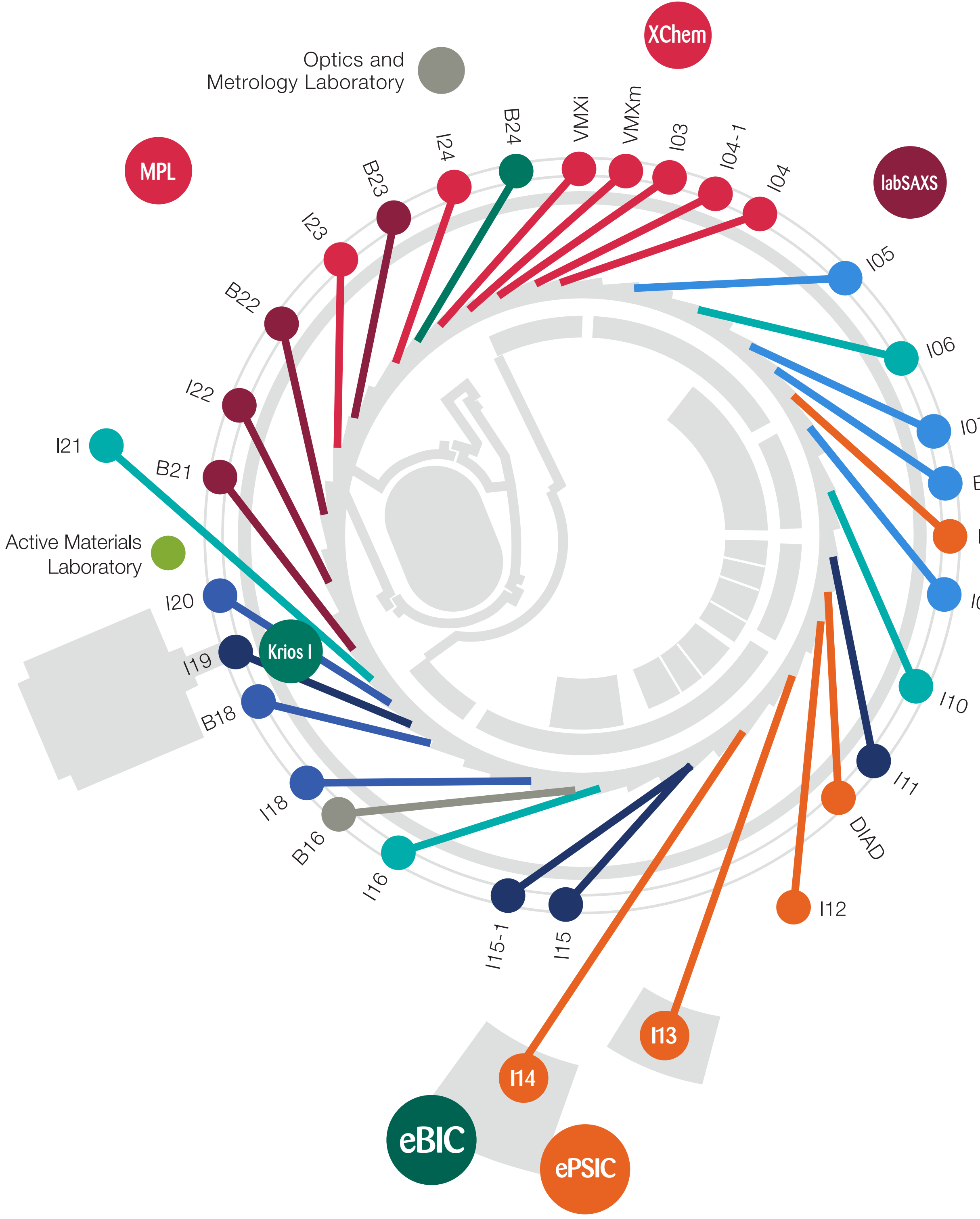
Instrument Development and Technical Summary

Diamond currently operates 35 beamlines and nine electron microscopes for user experiments. The microscopes make up eBIC (electron Bio-Imaging Centre) and ePSIC (electron Physical Science Imaging Centre).

Alongside the beamlines and microscopes, Diamond also houses the UK's life science X-ray Free Electron Laser (XFEL) Hub, the Membrane Protein Laboratory (MPL), the XChem fragment screening facility, and Active Materials Laboratory along with an extensive suite of offline instrumentation to support user experiments. For academic research, all of Diamond's instruments (beamlines and microscopes) are free at the point of access through peer review. For proprietary research, access can be secured through Diamond's Industrial Liaison team.

The instruments and beamlines are organised into science groups as described below.

Science groups around our facility



Key

- ● Macromolecular Crystallography
- ● Crystallography
- ● Structures and Surfaces
- ● Biological Cryo-Imaging
- ● Magnetic Materials
- ● Spectroscopy
- ● Imaging and Microscopy
- ● Soft Condensed Matter
- ● Optics and Metrology

Electron Microscopes

Microscope	Main Capabilities	Accelerating Voltages
Titan Krios I	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV
Titan Krios II	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV
Titan Krios III	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV
Titan Krios IV	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV
Titan Krios V	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV
Glacios	Cryo-EM, Cryo-ET	200 kV
Aquilos	Cryo-SEM, Cryo-FIB	3 to 30 kV
JEOL ARM200F	Atomic scale STEM imaging, EELS, EDX, electron diffraction	80, 200 kV
JEOL ARM300F	Atomic scale TEM and STEM imaging, electron diffraction, 4D-STEM, EDX	30, 60, 80, 160, 200, 300 kV

Beamlines

Beamline	Main Capabilities	Energy / Wavelength Range
Versatile MX micro (VMXm)	Micro- and nano-focus in vacuum cryo-macromolecular crystallography	7 - 28 keV
Versatile MX in situ (VMXi)	In situ microfocus, room temperature macromolecular crystallography, Serial Synchrotron Crystallography	10 - 25 keV
I03 - UDC MX	High Throughput (HT) Unattended Data Collection (UDC) Macromolecular Ccrystallography (MX), Multiwavelength Anomalous Diffraction (MAD)	5 - 25 keV
I04 - Microfocus MX	MX, MAD, variable and microfocus MX	6 - 2018 keV
I04-1 - Monochromatic MX	MX, XChem fragment screening	13.53 keV (fixed wavelength)
I05 - ARPES	Angle-Resolved PhotoEmission Spectroscopy (ARPES) and nano-ARPES	18 - 240 eV; 500 eV
I06 - Nanoscience	X-ray Absorption Spectroscopy (XAS), X-ray photoemission microscopy and X-ray magnetic circular and linear dichroism	80 eV – 2200 eV
I07 - Surface and Interface Diffraction	Surface X-ray diffraction (SXRD), Grazing Incidence X-ray Diffraction (GIXD), Grazing Incidence Small Angle X-ray Scattering (GISAXS), X-ray Reflectivity (XRR)	6 - 30 keV
B07 - VerSoX: Versatile Soft X-ray	Branch C: Ambient Pressure XPS and NEXAFS	110 - 2800 eV
	Branch B: NEXAFS and High-Throughput XPS	45 - 2200 eV
I08 - Scanning X-ray Microscopy	Scanning X-ray microscopy, NEXAFS/ XANES, X-ray fluorescence (XRF)	I08 branch: 250 eV - 4.4 keV
		I08-1 - Soft and Tender X-ray Ptychography branch: 250 - 2000 eV
I09 - Atomic and Electronic Structure of Surfaces and Interfaces	XPS (including HAXPES), X-ray Standing Waves (XSW), Near Edge X-ray Absorption Fine Structure (NEXAFS), energy-scanned photoelectron diffraction	Hard X-rays: 2.1 - 18+20 keV
I10 - BLADE: Beamline for Advanced Dichroism Experiments	Soft X-ray resonant scattering, XAS and X-ray magnetic circular and linear dichroism	Circular: 400-1600 eV; Linear Horizontal: 250- 1600 eV; Linear Vertical: 480-1600 eV
I11 - High Resolution Powder Diffraction	X-ray powder diffraction	7 – 25 keV (1.7 - 0.5 - 2.1 Å)
DIAD: Dual Imaging and Diffraction	Correlated X-ray computed tomography (XCT) and microfocus X-ray powder diffraction (XRD)	Imaging: 7 - 38 keV Diffraction: 7 - 38keV

Beamline	Main Capabilities	Energy / Wavelength Range
I12 - JEEP: Joint Engineering, Environmental and Processing	Time-resolved imaging and tomography (EH1 and EH2); phase contrast imaging (EH1); 2D detector for time-resolved monochromatic powder diffraction, single crystal diffraction and diffuse scattering; energy dispersive X-ray diffraction (EDXD);	53 keV - 150 keV monochromatic or continuous white beam
I13-1 - Coherence	Nano-tomography: Ptychography, X-ray fluorescence (XRF), X-ray diffraction (XRD). 3D Bragg mapping: Coherent diffraction imaging (CDI) and Ptychography	6 – 20 KeV
I13-2 X-ray imaging	Phase contrast imaging, Tomography, Ptychography, Bragg CDI, Full-field microscopy (TXM), grating interferometry, nano-tomography	8 – 30 keV
I14 - Hard X-ray Nanoprobe	Nanofocus X-ray fluorescence (XRF), X-ray Absorption Spectroscopy (XAS) and transmission diffraction (XRD) mapping and tomography. Differential phase contrast (DPC) imaging, ptychography and ptycho-tomography.	5 - 23 keV
I15 - Extreme Conditions	Powder diffraction, single crystal diffraction	Monochromatic and focused 20 - 80 keV
I15-1 - XPDF	X-ray Pair Distribution Function (XPDF)	40, 65, and 76 keV
I16 - Materials and Magnetism	Resonant and magnetic single crystal diffraction, fundamental X-ray physics	2.57 - 15 keV
B16 - Test beamline	Diffraction, imaging and tomography, topography, reflectometry	4 - 20 keV monochromatic focused; 4 - 45 keV mono-chromatic unfocused White beam
I18 - Microfocus Spectroscopy	Microfocus X-ray Absorption Spectroscopy (XAS), X-ray fluorescence (XRF) and X-ray diffraction (XRD) mapping and tomography	2.05 - 20.5 keV
B18 - Core XAS	X-ray Absorption Spectroscopy (XAS)	2.05 - 35 keV
I19 – Small Molecule Single Crystal Diffraction	Small molecule single crystal diffraction	5 to 25 keV / 0.5 to 2.5 Å
I20 - LOLA: Versatile X-ray Spectroscopy	X-ray Absorption Spectroscopy (XAS), X-ray Emission Spectroscopy (XES)	Scanning branch: 4.5 - 20 keV
I21 - Inelastic X-ray Scattering	Resonant Inelastic X-ray Scattering (RIXS), X-ray Absorption Spectroscopy (XAS)	250 - 3000 eV
B21 - High Throughput SAXS	BioSAXS, solution state small angle X-ray scattering	6 - 23 keV (set to 13.1 keV by default)
I22 - Small Angle Scattering and Diffraction	Small angle X-ray scattering and diffraction: SAXS, WAXS, USAXS, GISAXS. Micro-focus SAXS Tensor Tomography.. Micro-focus capability.	7 - 20 keV
P38 - labSAXS (Offline SAXS instrument)	SAXS/WAXS, GiSAXS/GiWAXS	9.2; 17.4 keV
B22 - MIRIAM: Multimode InfraRed Imaging And Microspectroscopy	FTIR microscopy & FPA imaging FTIR and THz spectroscopy FTIR nanospectroscopy s-SNOM and AFM IR	microFTIR: 5,000-500cm1 (2-20μm) FTIR/THz:10,000-10cm1 (1-1000μm) nanoFTIR: 5000-600cm1 (2-17μm)
I23 - Long Wavelength MX	Long wavelength macromolecular crystallography	2.1 - 11 keV (1.1 - 5.9 Å)

Beamline	Main Capabilities	Energy / Wavelength Range
B23 - Circular Dichroism	Circular Dichroism (CD)	Module A: 125-500nm for CD Imaging at 50 μm spatial resolution, and for 96-cell high throughput CD (HTCD). Module B: 180-700nm for MMP at 50 μm spatial resolution.
I24 - Microfocus and Serial MX	MX, MAD, Serial Crystallography, high energy MX	7 - 30.0 keV
B24 - Cryo Transmission X-ray Microscopy (TXM)	Cryo Structured Illumination microscope (CryoSIM) 3D cryo super resolution fluorescence microscopy /correlative microscopy	405, 488, 561, 647 nm

New beamlines in development for Diamond-II

Beamline	Main Capabilities	Energy / Wavelength Range
K04 - ultra-HT MX for XChem	Automated, integrated, ultra-high throughput crystal preparation and MX for accelerated chemical biology	10 – 27 keV
K14 - SWIFT	X-ray Absorption Spectroscopy (Quick-EXAFS), X-ray fluorescence (XRF) and X-ray diffraction (XRD) mapping and tomography	4-34 keV
I17 – CSXID	Ptychography, Tomography, Scanning Transmission X-ray Microscopy (STXM), X-ray Absorption Spectroscopy (XAS) and X-ray Magnetic Circular and Linear Dichroism (XMCD/XMLD)	250 eV – 2000 eV