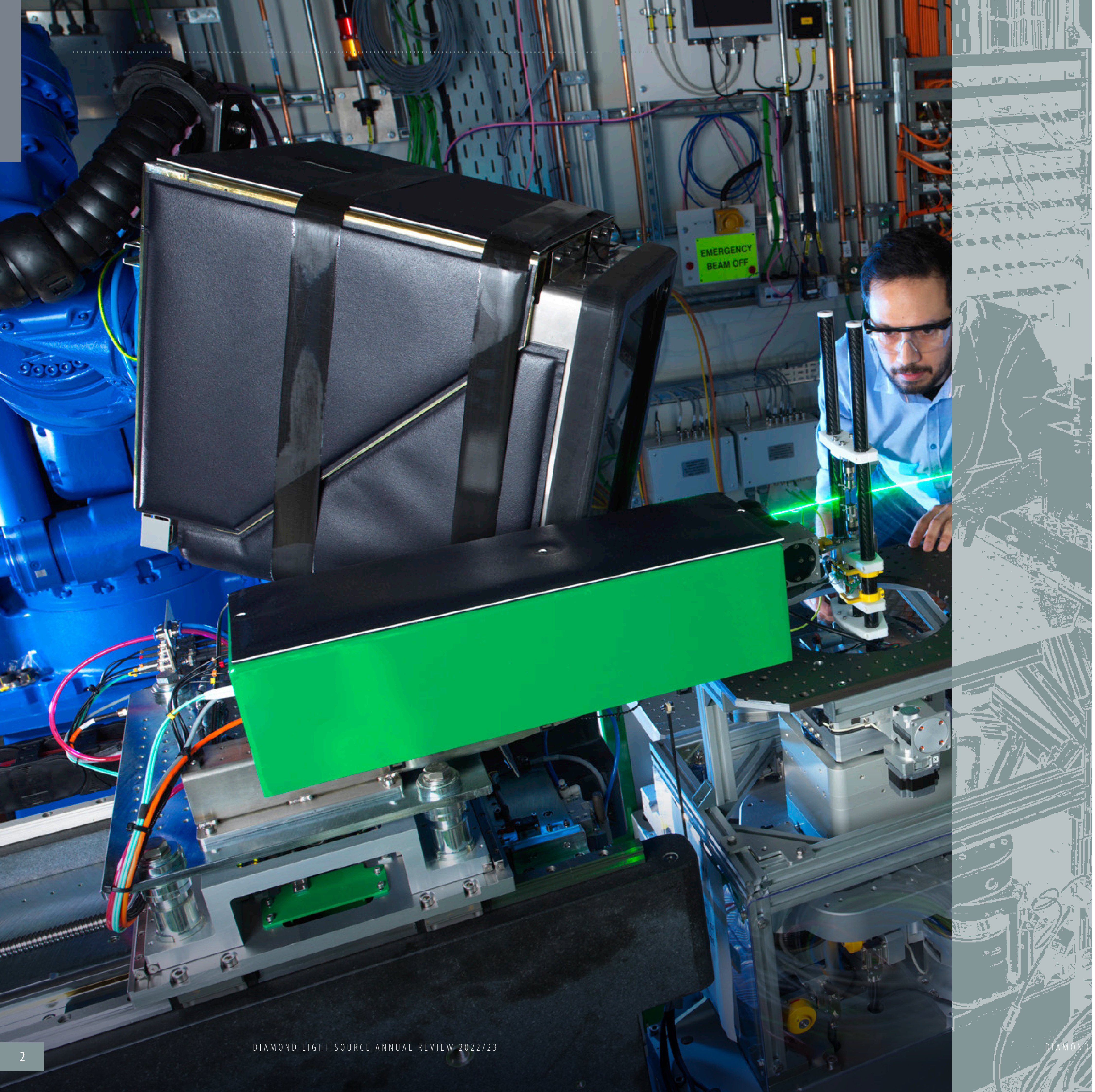
diamond

Diamond Light Source Ltd

2022/23



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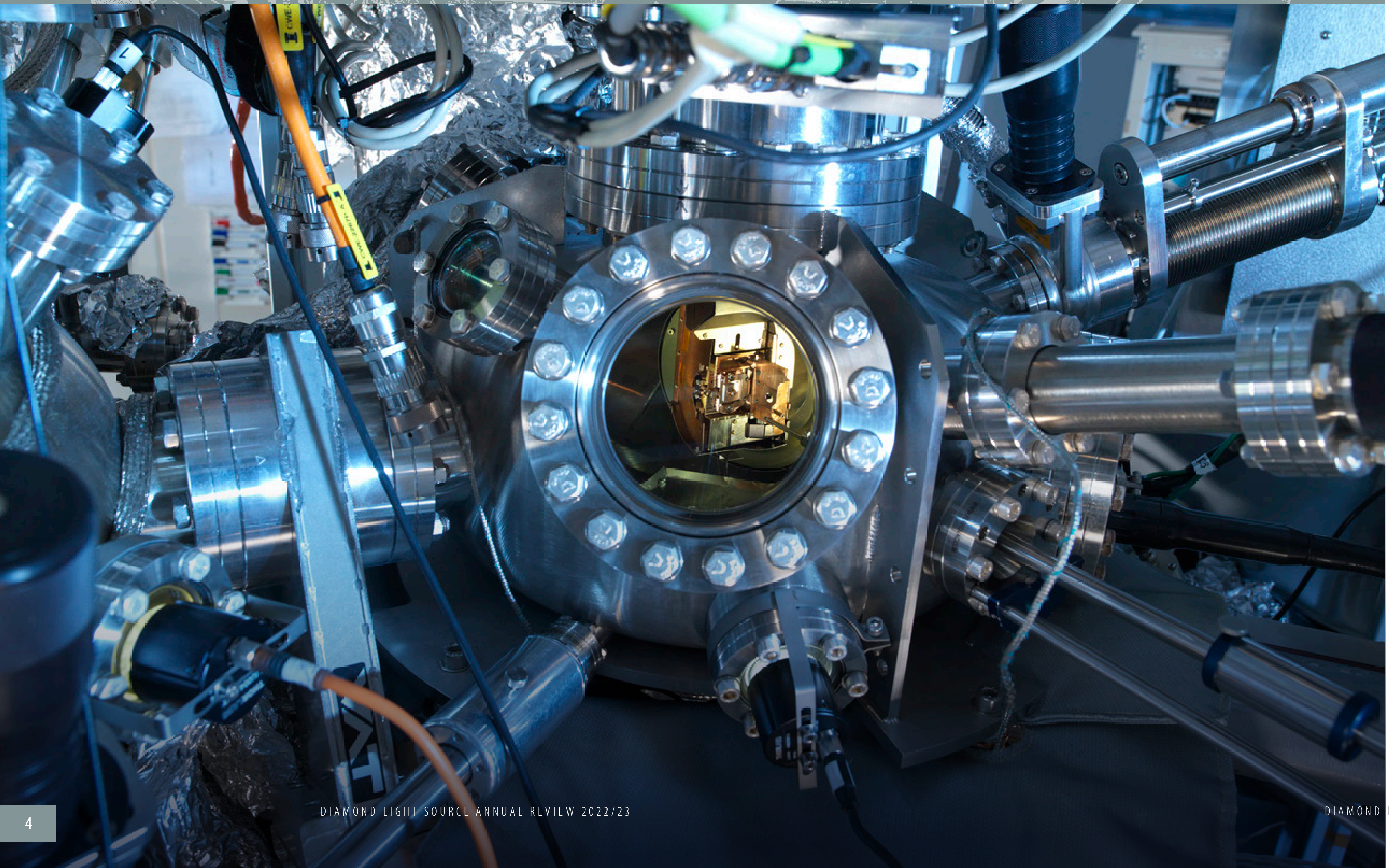
“let me end by extending on behalf of the Board our gratitude and admiration to all of you who contribute to the success of Diamond.”



Foreword

As I enter my 9th year of involvement with Diamond, it remains a privilege to continue to be the Chair of the Board of such a world class research facility. The Board and I will continue to seek to support in all possible ways the Shareholders, the Executive and all the workforce in driving the organisation forward and maintaining our outstanding national and international reputation. In June 2022, we all welcomed the funding announcement confirming the first phase of investment for Diamond-II, reflecting the importance of this project to the UK and signalling a bright future for the organisation.

However, there continue to be challenges. In particular, recruiting and retaining appropriate talent against the background of pay constraint policies, inflation and a competitive jobs market is becoming a major issue.

This issue will remain at the forefront of the Board's priorities going forward and we will continue to share our concerns and argue our case at the highest levels with our funding and policy colleagues in UKRI, Wellcome and Government. With that assurance, let me end by extending on behalf of the Board our gratitude and admiration to all of you who contribute to the success of Diamond.

Professor Sir Adrian Smith
Chairman of the Board of Directors

CEO Welcome

2022 has been a year filled with many changes. As CEO, for an interim period, I took over from Professor Andrew Harrison last November to navigate the transition whilst Shareholders look for a long-term appointment. I have been on Diamonds Board as an Executive Director since April 2019.

Diamond has been delivering excellent science in collaboration with its user community, fostering knowledge that is addressing many of our global challenges.

Diamond now has 33 operational beamlines, which together with complementary facilities – eBIC, ePSIC, the MPL together with the XChem Fragment Screening service and the XFEL Hub - provide a truly integrated facility for virtually every field of science.

The switch from pandemic to endemic in the management of the coronavirus has meant a slowdown in our normal activities. The past year saw us increase our total of peer reviewed journal articles to some 12,384. This is a slower increase than expected as the effects of the lost measurements during the pandemic are starting to affect our numbers. Last year, there were 9,193 user visits to Diamond via academic access routes. In the last financial year, we received 1,906 proposals for experiments on beamlines and electron microscopes, which requested a total of 24,252 shifts. This resulted in 15,413 experimental shifts being awarded, spread across the 33 operational beamlines and seven of the electron microscopes. Within academia, 5,279 of our user visits were on-site visits, while the remaining 42% (3,914) were done via remote access.

We have seen reassuring signs of recovery with more beamtime to users being delivered but not yet to the full levels we reached prior the start of the pandemic. As new challenges emerge like the heightened threat of industrial action, the path to full recovery will take time. Recruitment and retention of our staff is now a major issue. With turnover levels increasing, I am working closely with our chairman to raise these issues at the highest levels with our shareholders. Like many other STEM institutes; we are faced with this issue, but we are working tirelessly to bring this issue to the attention of the UK Government to help us address this challenge.

In autumn 2022 we presented an update of our socioeconomic impact report at the International Conference of Research Infrastructures in Czech Republic. The report was initially published in May 2021 and undertaken by Technopolis together with representatives from our funding agencies. The report has become an influential piece of work within the research infrastructure community with many learning from its methodology and approach. With over 14,000 researchers interested in using our instruments, our position remains very strong given that Diamond has for the period 2007-2022 achieved a cumulative monetised impact of at least £2.6 billion whilst remaining extremely good value for money for the UK taxpayer who each contribute less than the cost of a cup of coffee each year. These tremendous benefits are a credit to our dedicated staff, contractors and agency workers who enable innovation, push the boundaries of what can be measured and offer excellent support and service to the science delivered internally as well as externally.

The financial year 2022-23 also marked our double anniversary – 20 years since the company was started and 15 years of research and innovation together with our user community. In broad terms, the public ultimately pay the taxes that underpin 86% of our funding. We celebrated in part with a large outdoor photo exhibition showcasing some of the beautiful imagery created over the years. We have started again to open our doors to the public, allowing them to see our incredible science and engineering, but more importantly, to experience the range of careers involved with Diamond's operation. We have welcomed over 80,000 visitors since opening in 2007, and it is always astounding how much interest the public show in our work, and humbling to think that many of the young people we are showing around the facility could soon be working here. Diamond is not only a visible landmark in the Oxfordshire landscape but has also become a cornerstone of the Harwell Campus with key investment being brought close to us for synergy.

The Diamond-II upgrade programme is an integrated upgrade of the synchrotron, beamlines and computational facilities, which is critical to maintaining our world-leading status. We further progressed with the first phase of funding allocated by UKRI and Science and Technology Facilities Council (STFC) and Wellcome in June 2022. A major milestone in securing full funding from the UK Government was achieved in November 2021 with approval of the Outline Business Case (OBC) by the then Department for Business, Energy and Industrial Strategy (BEIS) and Her Majesty's Treasury (HMT). This approval built on an early commitment of support from Wellcome for their funding share. This past year saw us deliver the Technical Design Report (TDR) for the machine, alongside Conceptual Design Reports (CDRs) for three flagship beamlines. As we put our finishing touches to the Full Business Case (FBC), which is due for review in June 2023 by the Programme Investment Committee at the newly formed Department for Science Innovation and Technology (DSIT), if approved, will move on to HM Treasury for final approval for release of full funding for the Programme. We are grateful to Dr Richard Walker, who took a lead as Interim Senior Responsible Owner for his leadership of the machine TDR and the FBC. This upgrade will increase electron beam energy from 3.0 to 3.5 GeV will provide up to a factor of 70 increase in brightness and coherence of Diamond's photon beams at the higher energies.

As I lead the organisation towards steps ever closer to its upgrade, I remain determined to see Diamond positioned at the forefront of scientific research in the UK, Europe and on a global stage. Science is ultimately a collaborative endeavour to better our lives, and in Diamond's case, the team remains focused on playing a key role in addressing 21st century global challenges.

Andrea Ward FCMA

CEO & Director of Finance and Corporate Services Diamond Light Source

"As I lead the organisation towards steps ever closer to its upgrade, I remain determined to see Diamond positioned at the forefront of scientific research in the UK, Europe and on a global stage."

Artist's impression.

Governance and Management

Diamond Light Source Ltd was established in 2002 as a joint venture limited company funded by the UK Government via the Science and Technology Facilities Council (STFC), now under UK Research & Innovation (UKRI), and by Wellcome, owning 86% and 14% of the shares respectively. Diamond now employs 786 scientists, engineers, technicians and support staff from 44 countries worldwide. The Chief Executive and Directors are advised by committees representing key stakeholder groups, including the Science Advisory Committee (SAC), Diamond Industrial Science Committee (DISCo) and Diamond User Committee (DUC).

Diamond is free at the point of access for researchers accessing Diamond via peer review, and provided the results are published in the public domain for everyone's benefit. Allocation of beamtime is via a peer review process to select proposals on the basis of scientific merit and technical feasibility. Twelve peer review panels meet twice a year to assess the proposals submitted for each six-month allocation period. Diamond also welcomes industrial researchers through a range of access modes including proprietary research.

SAC: Advises Diamond Management on scientific and technical issues, including facilities and operation.

DUC: Represents the views of users to Diamond Management on matters relating to the operation and strategy of the facility.

DISCo: Advises Diamond Management on all matters relating to industry and industrial users of the facility, including opportunities to engage industry, best practice for industrial engagement and industrial research priorities.

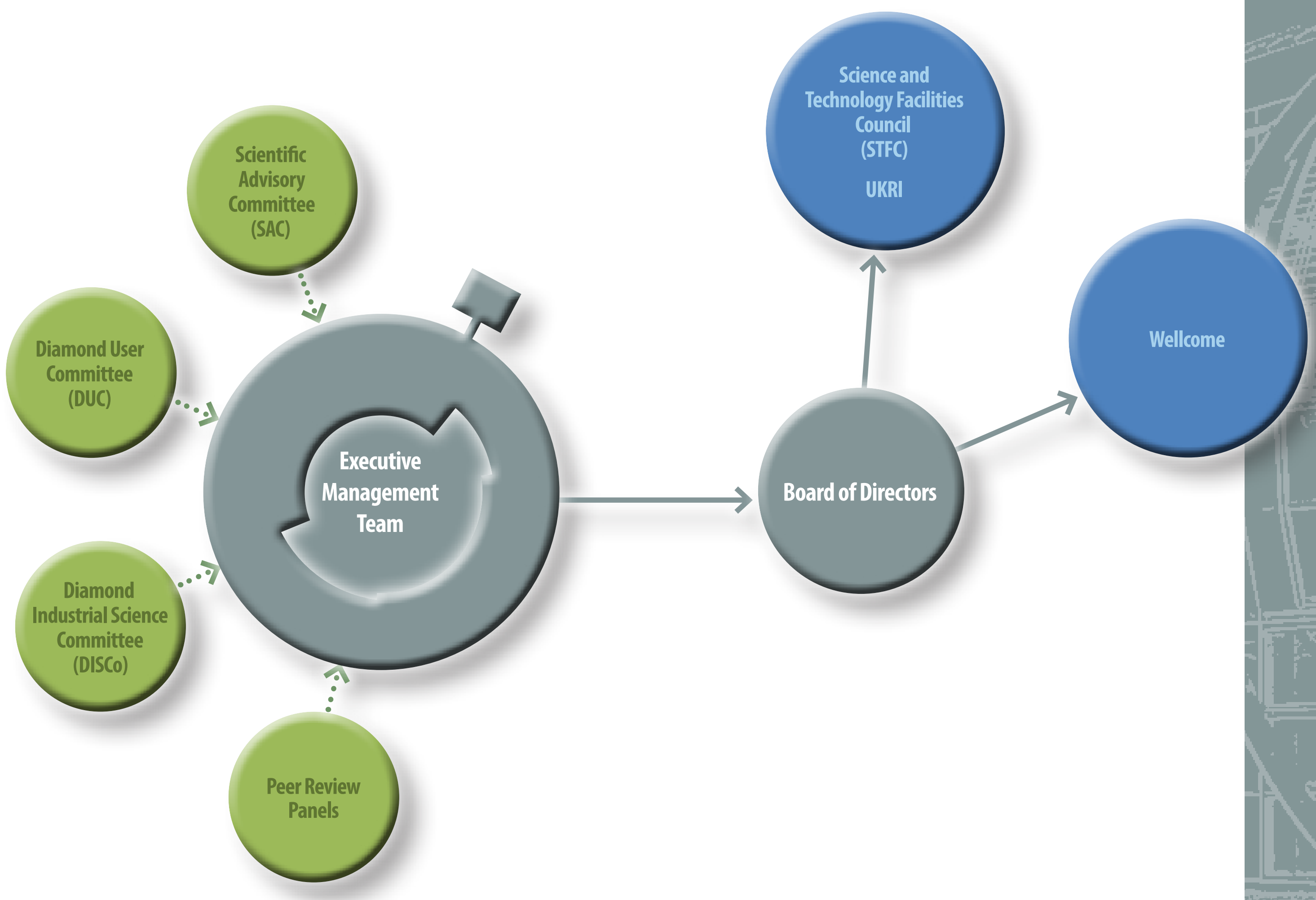
Peer Review Panels: Assess scientific merit of proposals to use the synchrotron and provide recommendations to Diamond Management on the allocation of beamtime to each project.

Executive Management Team: Hears from representatives from around Diamond and provides recommendations on strategy and operation to the Board of Directors.

Board of Directors: Decides on matters relating to Diamond's strategy and operation, and reports to Shareholders.

STFC: Holds 86% of shares as a joint venture partner. Hears from the Board and makes wider strategic decisions.

Wellcome: Holds 14% of shares as a joint venture partner. Hears from the Board and makes wider strategic decisions.



Staffing and Financial Information

Outline Organisational Chart

Chief Executive's Office

- Communications, Engagement & Impact
- Industrial Liaison
- Safety, Health & Environment

Science Division

Science Groups:
- Biological Cryo-Imaging
- Crystallography
- Imaging and Microscopy
- Macromolecular Crystallography
- Magnetic Materials
- Soft Condensed Matter
- Spectroscopy
- Structures and Surfaces

Scientific Software, Controls & Computation Groups:
- Accelerator Control Systems
- Beamline Control Systems
- Data Acquisition
- Scientific Computing
- Scientific Software

- Detector Group
- Experimental Hall Labs Services
- Optics & Metrology
- Planning & Projects Office
- User Office

Technical Division

- Accelerator Physics
- Diagnostics
- Engineering
- Insertion Devices
- Installation & Facility Management
- Operations
- Power Supplies
- Radiofrequency Systems
- Vacuum

Finance and Corporate Services

- Corporate IT
- Commercial Management, Governance & Legal
- Finance
- Human Resources
- Procurement & Goods Handling
- Soft Facilities

Buildings, Infrastructure & Energy Savings

Pete Coll, Head of Installation & Facilities Management Group

Figure 1: Optics Fabrication Building.

Expanding Facility

Since opening in 2007, the Diamond facility has continued to steadily expand. By 2017, I12, I13, I14 (including eBIC/ePSIC) and I21 external buildings had been constructed with the Active Materials Building completed in 2021. Diamond's Installation and Facilities Management (IFM) Group have played a major role in either managing design/construction activities directly or assisting external consultants to deliver these facilities.

A further expansion followed with the completion of the Optics Fabrication Building (OFB) in July 2022 (see Fig. 1). The OFB is a 350m^2 steel framed building with insulated cladding and a mono pitch roof. Foundations were made up of screw piles with cast in-situ concrete ring beams to support a block and beam floor, this work being undertaken during shutdowns to minimise vibrations to the Synchrotron with the rest of the construction work (cladding, screeding, M&E work, flooring and decorations) carried out during operations/shutdowns.

As part of Diamond-II, the Optics Metrology Laboratory (OML) needed to be relocated to allow space to build the CSXID flagship beamline. The new Optics Metrology Laboratory 2 (OML2), located in Zone 4, was recently completed (see Fig. 2). Works will soon commence to relocate equipment from the present OML into the new facility. Demolition of the old laboratory can then begin together with modifications to B16 creating the space required on the Experimental Hall floor for the CSXID beamline.

Figure 2: Optics Metrology Laboratory.

Figure 3: Artist's impression of complete solar panel installation.

Infrastructure Upgrades

As Diamond's facilities grow, there has been a need to expand and upgrade the mechanical and electrical infrastructure to support the expansion. Over the years, there have been significant modifications carried out on the chilled water system including new chillers/adiabatic cooling and introduction of additional cooling water circuits. The high voltage infrastructure has also recently been upgraded to accommodate Diamond's expansion for at least the next ten years.

Due to quality issues in the initial synchrotron roof build resulting in significant deformation, a new roof was needed and has now been installed. Diamond also took the initiative and opportunity of installing solar panels as part of the replacement. The project entailed the removal ~32,000 m^2 of sheeting material, replacing all support fittings, replacing/enhancing the insulation and replacement of the top sheeting before the installation of 2.7 MWp of solar panels (see Fig. 3) which will deliver ~ 2.3 GWh of electricity per annum, being approximately 5% of Diamond's annual electricity consumption.

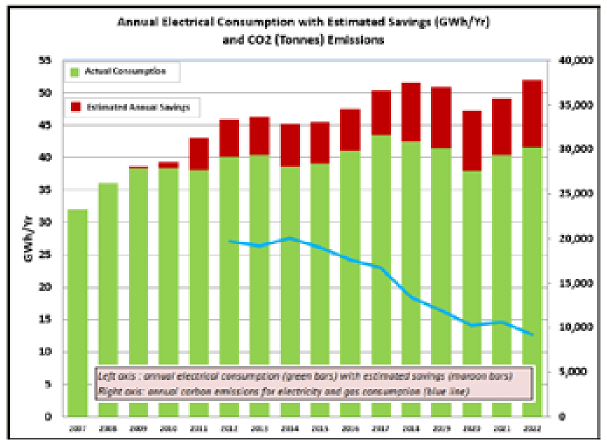


Figure 5: Annual Electricity Consumption with Estimated Savings (kWh/Yr) and Emissions (Tonnes of CO2).

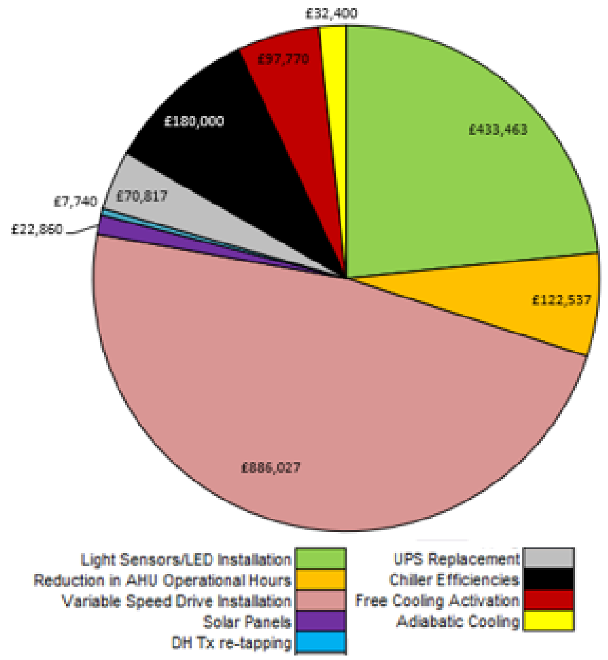


Figure 4: Annual savings by activity for 2022.

Energy Savings

Since 2010, Diamond has matured its energy saving programme culminating in a total estimation of electrical energy savings of £9.3 million to date, with the highest amount of savings being recorded in 2022 at £1.8 million.

The main contributors to electrical energy savings have been the introduction of light sensors, changing fluorescent lights to LEDs and the installation of variable speed drives on numerous fan and pump systems (thus allow 'turn down' in the circulation of unnecessary air/water). The pie chart (Fig. 4) shows annual savings per category for 2022 (excluding the projected savings from the solar panels on the Synchrotron roof).

Savings compared with actual electrical consumption are shown in the left axis in Fig. 5. The right axis shows the reduction of carbon emissions as a result of these energy saving measures in conjunction with the use of 'greener' electricity, the government's target being to drive for full decarbonisation of the National Grid by 2035.

Diamond's Environmental Sustainability Strategy

Diamond SHE Group, in consultation with Diamond employees, has developed an Environmental Sustainability Strategy and action plan, aligning with Diamond's Ten Year Vision, which has sustainability at its core and is geared towards achieving this across its operations. The strategy is guided by the UN's Sustainability Development Goals and Diamond is fully committed to the Paris Climate agreement – 100% carbon neutrality by 2050. At Diamond we are optimistic and proud of our contribution to supporting research and innovation that is developing solutions to better understand and address global environmental sustainability challenges.

Diamond has a strong track-record in enhancing its own environmental performance. Our Safety, Health & Environment Policy states that the effective management of Environmental matters is of prime importance to the organisation. As such, we undertake to provide an environmentally sound workplace. This includes a commitment to continuous improvement in environmental performance and the setting of objectives.

The recently developed strategy sets out bold ambitions and priorities to further enhance operational environmental performance and better support research and innovation that has a positive environmental sustainability impact.

By pursuing extensive sustainability goals, we are not only acting responsibly toward the environment and society – we are also ensuring the long-term sustainability of Diamond as a national facility.

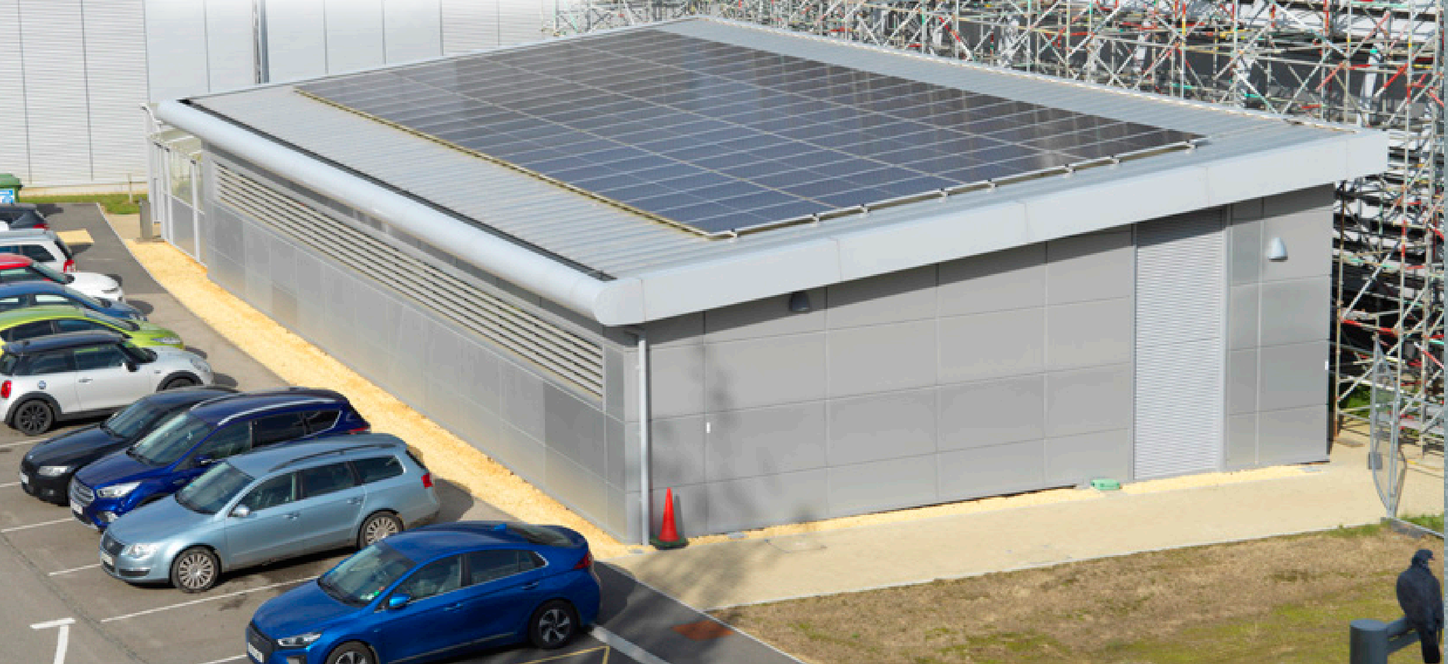
The strategy divides environmental sustainability into three areas; Research, operations and compliance.

Research Impact: These are areas where Diamond is having a positive impact on sustainability through the research and technology development that we facilitate. Our strategy is to maximise the positive impact of these areas. Our Diamond-II infrastructure upgrade programmes has enhancements to these positive impacts at the centre, with the primary commitment of the strategy focusing on directly addressing the Government's Industrial Strategy Grand Challenges of clean growth, mobility and an ageing society.

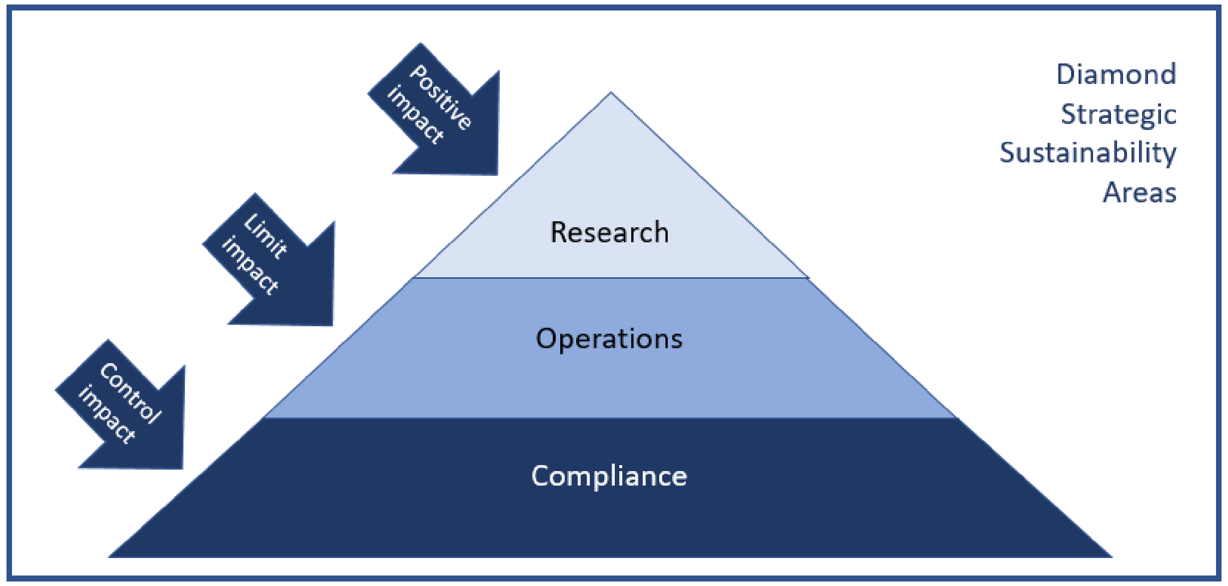
This also includes addressing climate change challenges.

Sustainability research areas at Diamond include:

- **New batteries**: to reduce the carbon footprint linked to the exploitation of batteries and particularly batteries involving rare earth materials, researchers are working on all the elements of a battery: electrolytes, anode, cathode, interface of all the elements. The goal is to limit or even replace the usage of lithium with safer, and more abundant materials (Sodium for example).
- **Hydrogen production:** To reduce the usage of fossil fuel and limit the production of CO_2 or other atmospheric pollution, new ways to produce Hydrogen are being developed by researchers. This will allow the production of H_2 more efficiently, with less cost involved (photocatalysis, or usage of bioreactors with a neutral cost).
- **Photovoltaic development:** The sun is a limitless source of energy for our societies. Nevertheless, researchers are searching new ways to improve the energy production from photovoltaic panels, including new materials (Perovskites or other materials) or increasing the efficiency of existing materials (with an increased absorption window).
- **Plastic depollution:** Plastic pollution has dramatic consequences for the environment. Researchers are working on new enzymes (PETase) to degrade microplastic, reducing plastic pollution and allowing the production of valuable molecules at the same time.
- **Atmospheric pollution:** Research has been conducted at Diamond to understand the ageing and decay of aerosols produced by human activities such as cooking, a source of pollution in large cities.
- **Radioactive pollution:** Different events such as nuclear testing or Reactor meltdown (Fukushima -Daichi, for example) has caused major environmental pollution by radioactive elements. Diamond beamlines are used to understand how the soil is reacting to radioactive pollution and what can be the short- and long-term impact to such pollution.
- **Ecosystem evolution:** Fragile environments such as coral reefs are modified following direct or indirect human activities Synchrotron studies help to understand the evolution of such environments, and how to protect them.
- **Pollution remediation:** Human activities can produce local or global pollution, that can be detrimental for the environment. Researchers are developing new materials to remove toxic elements such as Arsenic or sulphur; or characterising already existing organisms such as algae to understand how they can accumulate toxic elements (Cadmium, for example)
- **Green chemistry:** Scientists are working on new enzymes to enhance the production of valuable molecules with a lower environmental cost. In a comparable manner, enzymes or other materials such as Metal-Organic Framework are modified to process abundant molecules resulting from human activities such as lignin or CO_2 into useful compounds.



The new Active Materials Laboratory with solar panels on the roof



Operational Impact: These are areas related to the operation of Diamond that have impacts on environmental sustainability, such as energy usage. Our strategy is to limit the impact of these areas through a commitment to continual improvement of our performance. Our approach to continuous improvement will be underpinned by adoption of best practice, regular review, and evaluation, monitoring of progress and the identification of areas for development.

Through investment in a wide range of energy saving measures, such as variable speed drives on pumping equipment, motion sensors on lighting and LED light bulbs, Diamond has already achieved ongoing electricity savings of over £1million per annum and continues to identify areas of improvement. The primary focus for energy and resource usage is to work towards 'net-zero' carbon emissions for our directly managed operations by 2040.

Other primary focus areas relating to operational impact include working towards an ambition of zero avoidable waste by 2050; working towards eliminating all avoidable plastic waste by 2042, with earliest possible elimination dates as alternatives and technologies become feasible; developing a procurement culture which prompts staff to consider environmental responsibility and sustainability in their purchasing decisions; and developing sustainable design policies contributing to an environmentally sustainable facility, for the present and future.

The key commitments of our strategy for sustainable operations include the following:

Decision Making & Engagement: We will embed environmental sustainability objectives into Diamond Executive's objectives and business plans.

Energy Resource and Usage: We will perform annual reviews of energy usage metrics, purchasing options and travel related carbon emissions to set reduction targets and select the greenest viable supply sources.

Waste: We will minimise waste, reuse materials as much as we can and manage materials at the end of their life to minimise the impact on the environment.

Sustainable Design: We will optimise the leadership contribution of sustainable design to contribute towards an environmentally sustainable facility, for the present and the future.

Compliance Impact: These are areas where environmental sustainability requirements are mandated by legislation or guidance, for example, environmental permits and authorisations. Our strategy is to continue to control the impact from these areas through our management system and robust procedures and processes.

Related publications:

Wang, X. *et al.* Atomically dispersed pentacoordinated-zirconium catalyst with axial oxygen ligand for oxygen reduction reaction *Angew. Chem. Int. Ed.* **61**, e202209746. (2022) DOI: 10.1002/anie.202209746

Potter, M. *et al*. Combining photocatalysis and optical fiber Technology toward improved microreactor design for hydrogen generation with metallic nanoparticles. *ACS Photonics* **7**, 3 (2020) DOI: 10.1021/acsphotonics.9b01577

Taddei, M. *et al.* Ethylenediamine addition improves performance and suppresses phase instabilities in mixed-halide perovskites. *ACS Energy Lett.* **7**, 12, (2022) DOI: 10.1021/acsenergylett.2c01998.

Erickson, E. *et al.* Sourcing thermotolerant poly(ethylene terephthalate) hydrolase scaffolds from natural diversity. *Nat Commun.* **13**, 7850 (2022). DOI: 10.1038/s41467-022-35237-x

Milsom, A. *et al.* The impact of molecular self-organisation on the atmospheric fate of a cooking aerosol proxy, *Atmos. Chem. Phys.* **22**, 4895–4907, DOI: 10.5194/acp-22-4895-2022, 2022.

Cook, M. *et al.* The nature of Pu-bearing particles from the Maralinga nuclear testing site, Australia. *Sci Rep* **11**, 10698 (2021). DOI: 10.1038/s41598-021-89757-5

Smith, G.L. *et al.* Reversible coordinative binding and separation of sulfur dioxide in a robust metal–organic framework with open copper sites. *Nat. Mater.* **18**, 1358–1365 (2019). DOI: 10.1038/s41563-019-0495-0

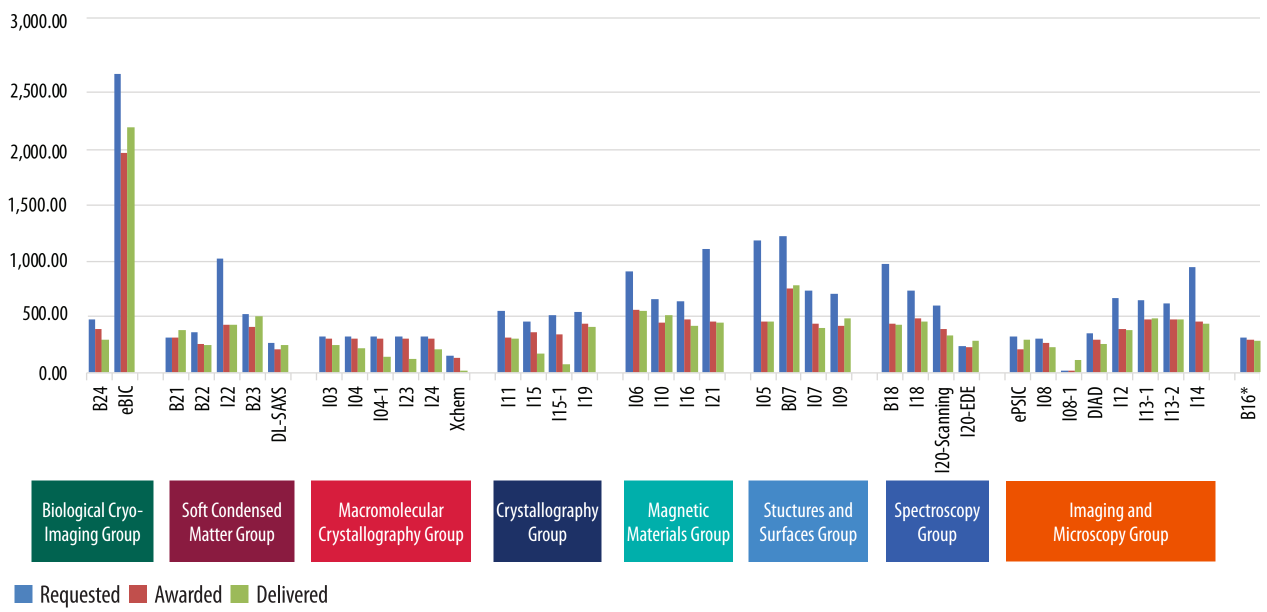
Thorpe, T.W. *et al.* Multifunctional biocatalyst for conjugate reduction and reductive amination. *Nature* **604**, 86–91 (2022). DOI: 10.1038/s41586-022-04458-x

Key Facts and Figures

Facility usage

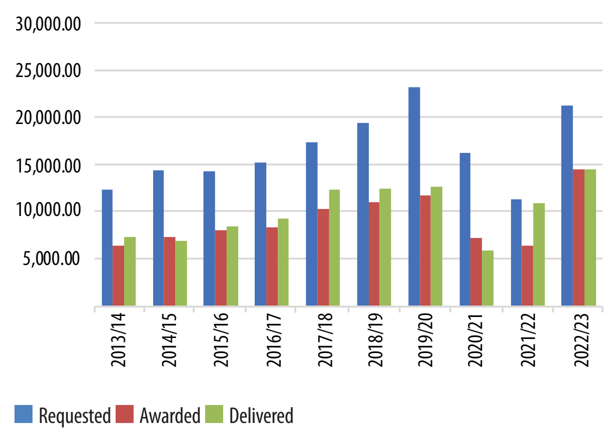
In our sixteenth year of operations (1st April 2022 to 31st March 2023), we received 1,906 proposals for experiments on our instruments via peer reviewed access routes, requesting a total of 24,252 shifts. After peer review, 1,420 proposals were awarded beamtime. This resulted in 16,478 experimental shifts being awarded across 33 beamlines and seven electron microscopes delivering time to academic users. We welcomed 5,279 onsite user visits from academia across all instruments, with an additional 3,914 remote user visits. The machine continues to perform to the highest standard with 97.3% uptime and 112 hours mean time between failures (MTBF).

User shifts requested, awarded and delivered by group, beamline and electron microscope 2021/22



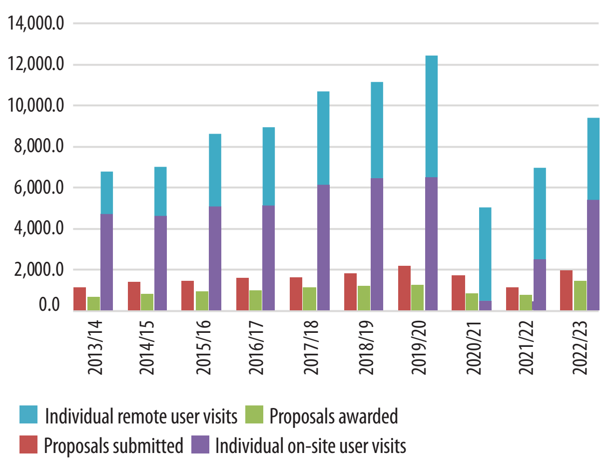
* B16 is the Test beamline, with 50% of beamtime for users. The rest is used for in-house developments for all beamlines.

Total user shifts requested, awarded and delivered



also includes shifts Requested Awarded and Delivered on labs and offline facilities

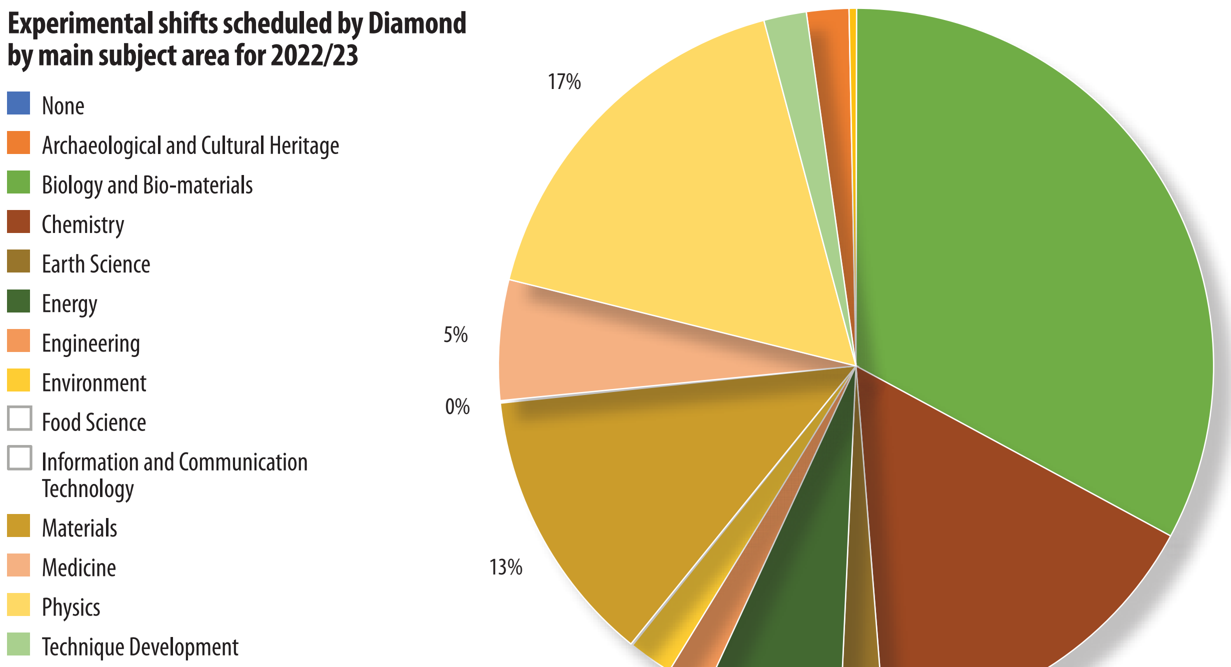
Total numbers of proposals and users per year



** Staff visits are now included for academic access routes, in house research is still excluded*

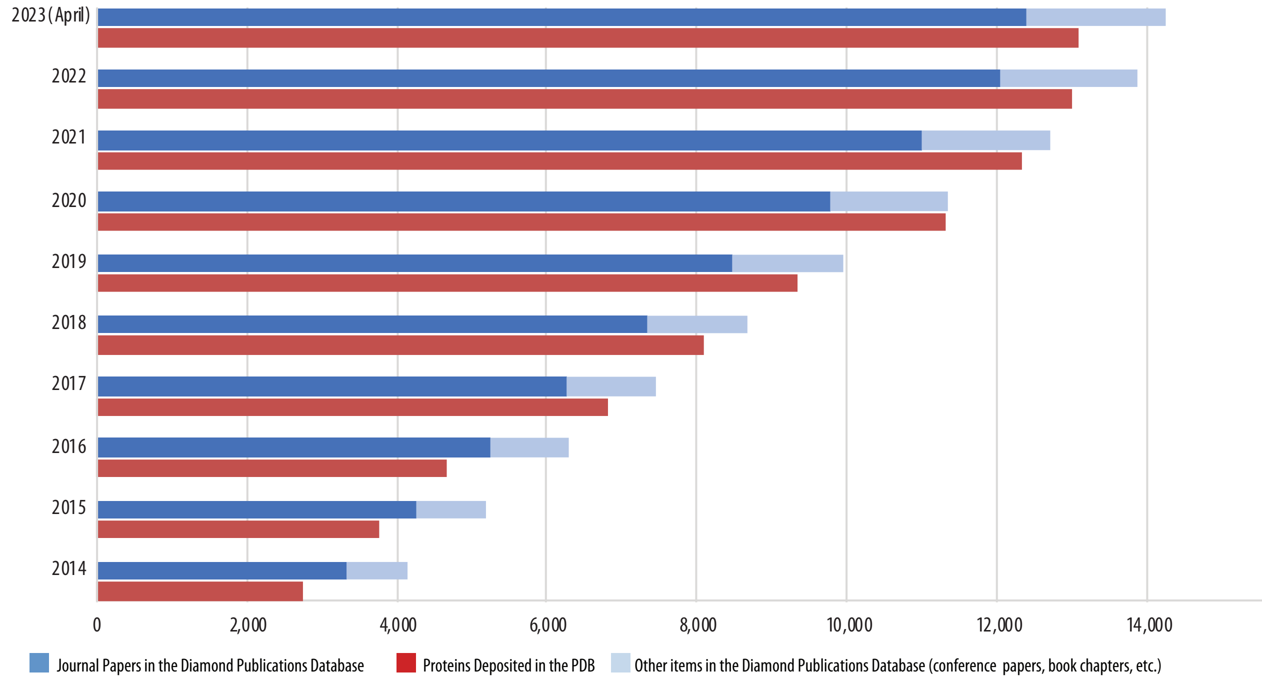
Proposals by discipline and research theme

Experimental shifts scheduled by Diamond by main subject area for 2022/23



** Not all proposals are attached to a science area. This explains the difference in Delivered shifts (+233 have no Science Area in the same access route and instruments)*

Cumulative number of items in Diamond Publications Database by our scientists and users and cumulative number of protein structures solved



Machine performance

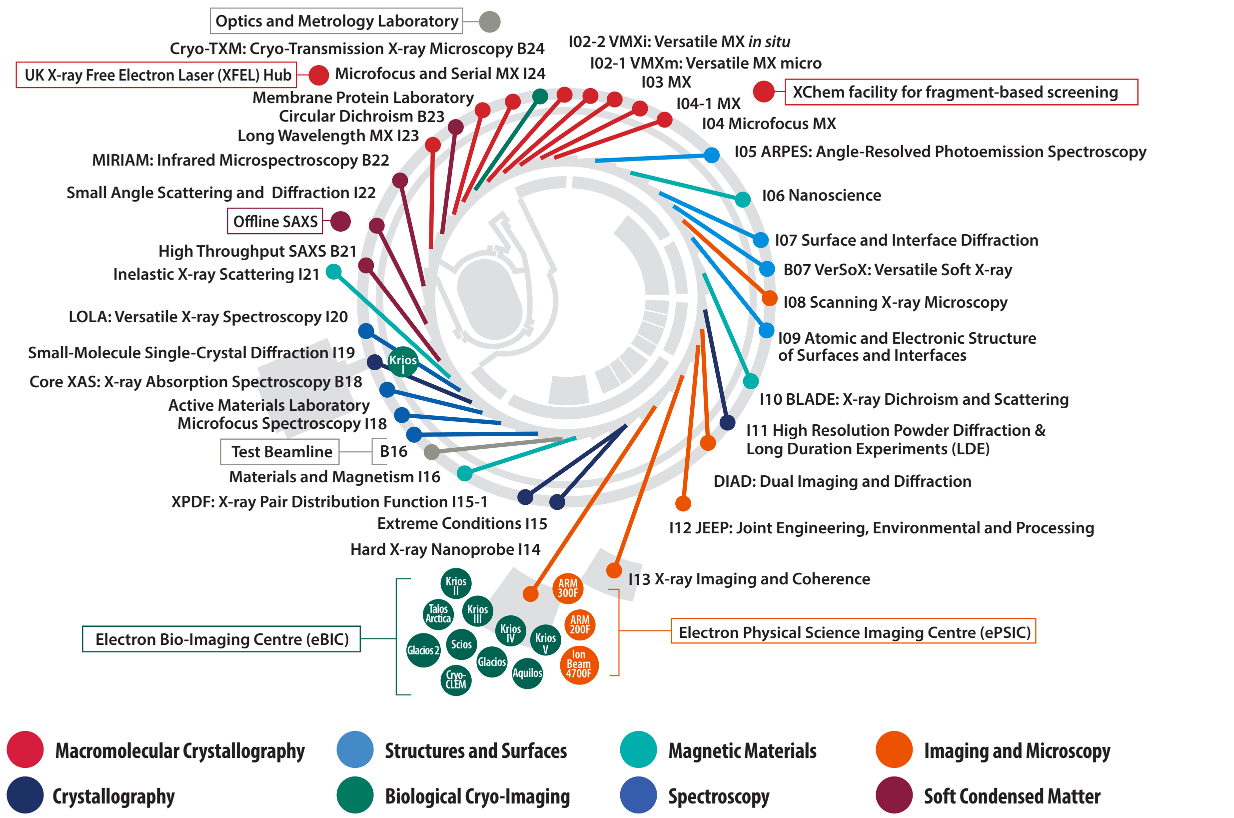
	2010/11	2011/12	2012/13	2013/14	2014/15	2015/16	2016/17	2017/18	2018/19	2019/20	2020/21	2021/22	2022/23
Total no. operational beamlines by end FY	19	20	22	24	25	26	28	31	32	32	33	33	33
Scheduled hours of machine operation	5808	6000	5832	5976	5808	5928	5688	6072	5904	5913	4345*	5396	6009
Scheduled hours of user operation	4728	5064	4872	5088	4944	5040	4584	5160	4992	4992	3445*	4532	5145
Machine uptime %	97.5	97.7	98.3	98.2	97.6	97.6	98.7	98.2	98.4	98.1	96.2	97.4	97.3
Mean time between failures (hours)	28.5	55.4	52.4	60.3	38.6	119.4	103.1	79.9	90.3	104.7	132	110	112

** hours reduced due to COVID*

Beamline Development and Technical Summary

In its sixteenth year of experiments, Diamond is now operating with 33 beamlines and eight electron microscopes dedicated for experiments. A further five instruments are available for experiment support and sample preparation. Six of the instruments specialise in life sciences and make up eBIC (electron Bio-Imaging Centre), with two provided for industry use in partnership with Thermo Fisher Scientific. Two of the electron microscopes are dedicated to advanced materials research and are supplied by Johnson Matthey and the University of Oxford. These, along with a further instrument for sample preparation, form ePSIC (electron Physical Science Imaging Centre) and are operated under strategic collaboration agreements to provide for substantial dedicated peer reviewed user access. Both eBIC and ePSIC are next to the Hard X-ray Nanoprobe beamline (I14). Along with eBIC and ePSIC, the UK X-ray Free Electron Laser (XFEL) Hub, the Membrane Protein Laboratory (MPL), the XChem fragment screening facility and the Offline SAXS facility make up the complementary integrated facilities available at Diamond. For academic research, Diamond instruments (beamlines and microscopes) are free at the point of access through peer review. For proprietary research, access can be secured through Diamond's industry team.

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



Electron Microscopes

Microscope	Main Capabilities	Accelerating Voltages	Operational Status
Titan Krios I	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV	Operational since 2015
Titan Krios II	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV	Operational since 2016
Titan Krios III	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV	Operational since 2017
Titan Krios IV	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV	Operational since 2017
Titan Krios V (Industrial)	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV	Operational since 2018
Glacios (Industrial)	Cryo-EM, Cryo-ET	200 kV	Operational since 2019
Aquilos 2	Cryo-SEM, Cryo-FIB	3 to 30 kV	Operational since 2020
Leica cryo-CLEM	Cryo-CLEM	N/A	Optimisation
JEOL ARM200F	Atomic scale STEM imaging, EELS, EDX, electron diffraction	80, 200 kV	Operational since 2017
JEOL ARM300F	Atomic scale TEM and STEM imaging, electron diffraction, 4D-STEM, EDX	30, 60, 80, 160, 200, 300 kV	Operational since 2017
JEOL Ion Beam 4700F	SEM, FIB	1 to 30 kV	Operational since 2020

Diamond's beamlines: current operational status April 2022

Beamline Name and Number	Main Techniques	Energy / Wavelength Range	Status
I02-1 - Versatile MX micro (VMXm)	Micro- and nano-focus in vacuum cryo-macromolecular crystallography (VMXm)	7 - 28 keV	Optimisation
I02-2 - Versatile MX *in situ* (VMXi)	*In situ* microfocus macromolecular crystallography, Serial Synchrotron Crystallography	10 - 25 keV	Optimisation
I03 - MX	Macromolecular crystallography (MX), Multiwavelength Anomalous Diffraction (MAD)	5 - 25 keV	Operational
I04 - Microfocus MX	MX, MAD, variable and microfocus MX	6 - 18 keV	Operational
I04-1 - Monochromatic MX	MX, XChem fragment screening	13.53 keV (fixed wavelength)	Operational
I05 - ARPES	Angle-Resolved PhotoEmission Spectroscopy (ARPES) and nano-ARPES	18 - 240 eV; 500 eV	Operational
I06 - Nanoscience	X-ray Absorption Spectroscopy (XAS), X-ray photoemission microscopy and X-ray magnetic circular and linear dichroism	80eV - 2200eV	Operational
I07 - Surface and Interface Diffraction	Surface X-ray diffraction, Grazing Incidence X-ray Diffraction (GIXD), Grazing Incidence Small Angle X-ray Scattering (GISAXS), X-ray Reflectivity (XRR)	6 - 30 keV	Operational
B07 - VerSoX: Versatile Soft X-ray	Branch C: Ambient Pressure XPS and NEXAFS	110 - 2800 eV	Operational
	Branch B: NEXAFS and High-Throughput XPS	45 - 2200 eV	Operational
I08 - Scanning X-ray Microscopy	Scanning X-ray microscopy, NEXAFS/ XANES, X-ray fluorescence	I08 branch: 250 eV - 4.4 keV	Operational
		I08-1 - Soft and Tender X-ray Ptychography branch: 250 - 2000 eV	Operational
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+ keV Soft X-rays: 0.1 - 2.1 keV (currently 0.1 - 1.9 keV)	Operational
I10 - BLADE: Beamline for Advanced Dichroism Experiments	Soft X-ray resonant scattering, XAS and X-ray magnetic circular and linear dichroism	Circular: 400-1600eV; Linear Horizontal: 250-1600eV; Linear Vertical: 480-1600eV	Operational
I11 - High Resolution Powder Diffraction	X-ray powder diffraction	7 - 25keV (1.7 - 0.5 - 2.1 Å)	Operational
DIAD: Dual Imaging and Diffraction	Simultaneous time-resolved X-ray imaging and X-ray powder diffraction	8 - 38 keV	Operational
I12 - JEEP: Joint Engineering, Environmental and Processing	Time-resolved imaging and tomography; 2D detector for time-resolved powder diffraction, single crystal diffraction and diffuse scattering; energy dispersive X-ray diffraction (EDXD); high-energy small angle X-ray scattering (limited capability)	53 keV - 150 keV monochromatic or continuous white beam	Operational
I13 - X-ray Imaging and Coherence	Phase contrast imaging, tomography, full-field microscopy (under commissioning), coherent diffraction and imaging (CXRD,CDI), ptychography and photocorrelation spectroscopy (XPCS) (under commissioning), innovative microscopy and imaging	Imaging branch: 8 - 30keV Coherence branch: 7 - 20keV	Operational
I14 - Hard X-ray Nanoprobe	Nanofocus X-ray fluorescence (XRF), X-ray absorption spectroscopy (XAS), and transmission diffraction (XRD) mapping., differential phase contrast (DPC) imaging,), ptychography and tomography	5 - 23 keV	Operational
I15 - Extreme Conditions	Powder diffraction, single crystal diffraction	Monochromatic and focused 20 - 80 keV White beam	Operational
I15-1 - XPDF	X-ray Pair Distribution Function (XPDF)	40, 65, and 76 keV	Operational
I16 - Materials and Magnetism	Resonant and magnetic single crystal diffraction, fundamental X-ray physics	2.5 - 15 keV	Operational
B16 - Test beamline	Diffraction, imaging and tomography, topography, reflectometry	4 - 20 keV monochromatic focused 4 - 45 keV monochromatic unfocused White beam	Operational
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	Operational
B18 - Core XAS	X-ray Absorption Spectroscopy (XAS)	2.05 - 35 keV	Operational
I19 - Small-Molecule Single-Crystal Diffraction	Small-molecule single-crystal diffraction	5 to 25 keV / 0.5 to 2.5 Å	Operational
I20 - LOLA: Versatile X-ray Spectroscopy	X-ray Absorption Spectroscopy (XAS), X-ray Emission Spectroscopy (XES) and Energy Dispersive EXAFS (EDE)	Dispersive branch: 6 - 26 keV	Operational
		Scanning branch: 4.5 - 20 keV	Operational
I21 - Inelastic X-ray Scattering	Resonant Inelastic X-ray Scattering (RIXS), X-ray Absorption Spectroscopy (XAS)	Currently 250 - 1500 eV (to be upgraded to 250 - 3000 eV)	Operational
B21 - High Throughput SAXS	BioSAXS, solution state small angle X-ray scattering	8 - 15 keV (set to 13.1 keV by default)	Operational
I22 - Small Angle Scattering and Diffraction	Small angle X-ray scattering and diffraction: SAXS, WAXS, USAXS, GISAXS. Micro-focus SAXS Tensor Tomography.	7 - 20 keV	Operational
DL-SAXS (Offline SAXS instrument)	SAXS/WAXS, GiSAXS/GiWAXS	9.2keV	Operational
B22 - MIRIAM: Multimode InfraRed Imaging And Mircrospectroscopy	FTIR microscopy & FPA imaging FTIR and THz spectroscopy NEW FTIR nanospectroscopy s-SNOM and AFM IR	microFTIR: 5,000-500cm^{1}(2-20µm) FTIR/THz:10,000-10cm^{1}(1-1000µm) nanoFTIR: 14000-800cm^{1}(2.5-12.5µm)	Operational Commissioning
I23 - Long Wavelength MX	Long wavelength macromolecular crystallography	2.1 - 11 keV (1.1 - 5.9 Å)	Operational
B23 - Circular Dichroism	Circular Dichroism (CD)	Module A: 125-500nm for CD Imaging at 50 µm spatial resolution, and 96-cell HTCD. Module B: 180-650nm for MMP Imaging at 50 µm spatial resolution.	Operational
I24 - Microfocus and Serial MX	MX, MAD, Serial Crystallography, high energy MX	7 - 30.0 keV	Operational
B24 - Cryo Transmission X-ray Microscopy (TXM)	Full field X-ray imaging	200eV - 2600eV	Operational

Macromolecular Crystallography Group

Macromolecular crystallography (MX) exploits the hard energy, high flux X-rays created at Diamond Light Source to enable our 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.

Diamond provides access to a suite of seven MX beamlines (I03, I04, I04-1, I23, I24, VMXi and VMXm) to a large international academic and industrial user community. 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, (time resolved) serial synchrotron crystallography (SSX), a fragment-based screening platform (XChem) and the Membrane Protein Laboratory.

Important research studies conducted this year included new insights into the role of inositol in gut bacteria, the development of new therapeutic nucleic acids and a new software developed at Diamond to solve structure base on multi crystals analysis.

Understanding the biochemistry of gut bacteria

Lipids are vital components of all cells, forming the main component of cell membranes. Many different lipids are found in membranes, with a wide range of functions. Inositol is a carbocyclic sugar that is a key player in eukaryotic cells and forms the polar head group of inositol lipids. Inositol lipids are not major components of eukaryotic cell membranes, but they play important roles in cell division and signalling between cells. While inositol lipids are widely distributed across eukaryotes, little is known of their role and structure in bacteria.

An international team of researchers investigated how the dominant gut microbe *Bacteroides thetaiotaomicron* makes inositol lipids. *B. thetaiotaomicron* is an important member of the human gut microbiome and can use a wide range of dietary carbohydrates as carbon sources.

After identifying the genes responsible for *B. thetaiotaomicron* inositol lipid synthesis, the researchers deleted each of these from the genome to see their effect on the production of the inositol lipids.

B. thetaiotaomicron bacteria with genomic deletions in the inositol lipid synthesis genes are less able to survive in their host.

Changes in the composition of the gut microbiome can affect host health. By developing an understanding of the biochemistry of bacteria in the gut, we can gain knowledge of the roles they play in various diseases, such as inflammatory bowel diseases.

Heaver, SL, *et al.* DOI: 10.1038/s41564-022-01152-6

Structural studies of the enhanced binding affinity of therapeutic nucleic acids to proteins

Introducing phosphorothioate (PS) linkages to the backbone of therapeutic nucleic acids significantly increases their stability and potency. The phosphorothioate backbone is the most widely used modification in therapeutic nucleic acids, including antisense oligonucleotides (ASOs). This modification involves a replacement of one of the two oxygen atoms in the repeating phosphate groups of the DNA with sulphur. PS-modified nucleic acids show improved properties, such as metabolic stability from nuclease-mediated degradation.

The molecular mechanisms of interactions between PS nucleic acids and proteins have not been fully established. To better understand how PS ASOs interact with cellular proteins, researchers used the I23 beamline to solve two crystal structures of PS ASO bound to annexin A2 (AnxA2), a calcium-binding protein previously implicated in the release of PS ASOs from endo-lysosomal compartments.

Their results unambiguously confirmed, for the first time, that van der Waals contacts between the sulphur atom and hydrophobic parts of arginine and lysine side chains are the driving force for enhanced interaction of PS ASO with proteins.

Overall, their results provide valuable insights into the general mechanism of the enhanced binding of PS ASOs to cellular proteins and indicate that the interaction between PS linkages and lysine and arginine residues is a general phenomenon that is observed not only for nucleic acid-binding proteins but may also account for the association of ASO with proteins that are not known to bind DNA. This work provides information that will be instrumental in the rational design of improved nucleic acid-based drugs.

Hyjek-Składanowska M. *et al*. DOI: 10.1093/nar/ gkac774

xia2.multiplex - a new pipeline for multi-crystal data analysis

A team of scientists at Diamond has developed a new program, xia2.multiplex, to facilitate and help to optimise the scaling and merging of multiple data sets.

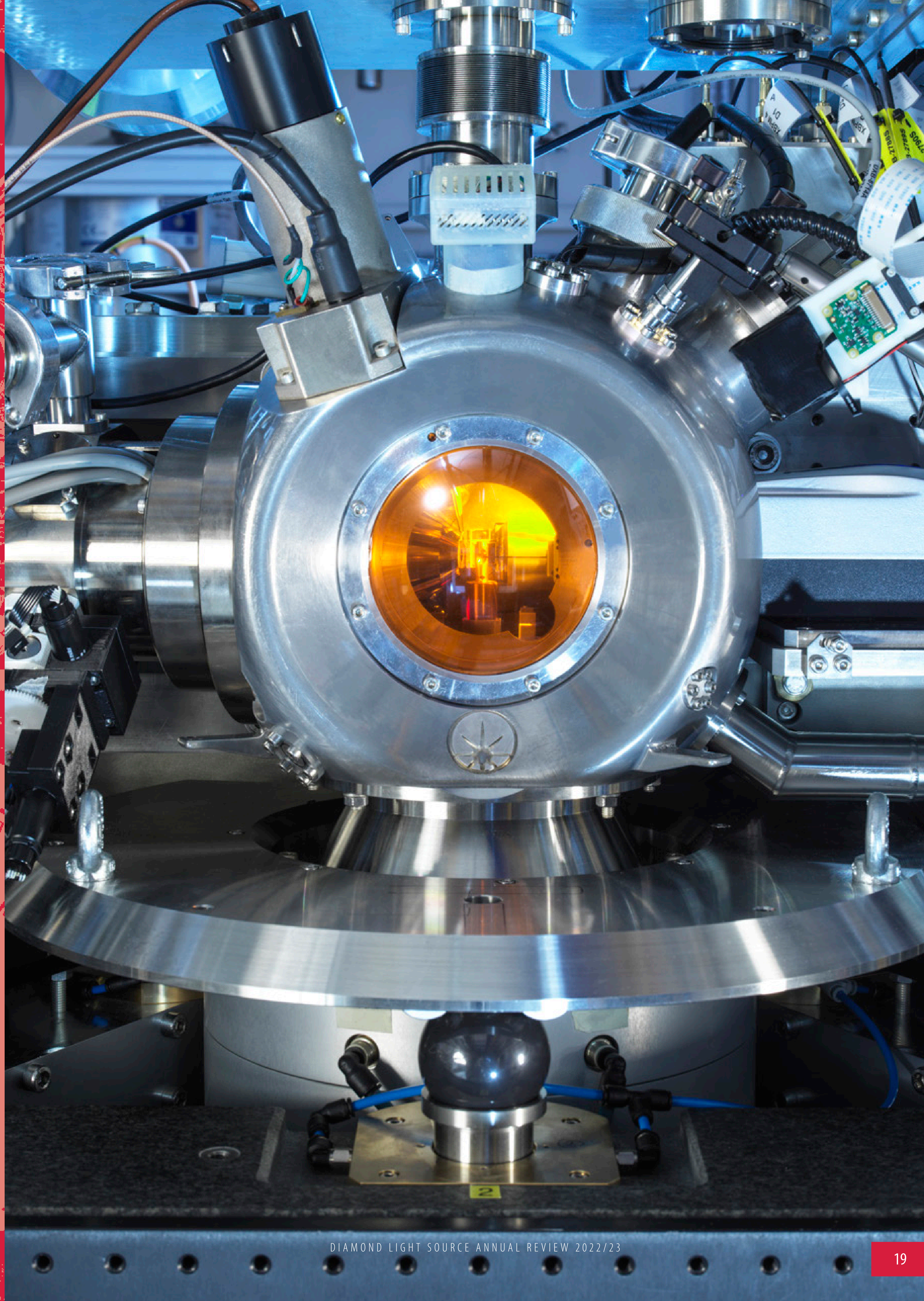
At the very beginning of macromolecular crystallography, structures were obtained using room temperature data collection, and it was common to merge together data from multiple crystals to obtain a complete data set. With the increasing availability of synchrotron sources with ever more intense beams in the 1990s, radiation damage was becoming a limiting problem, leading to the popularisation of "cryogenic" data collection. Such flash-cooling of crystals to around 100 K significantly extends the crystal lifetime in the X-ray beam.

In recent years, there has been an increasing awareness that cryocooling can "hide" biologically significant structural features. So there has been interest in collecting data under more physiologically relevant room temperature conditions.

In addition, many scientifically important targets, such as membrane proteins and viruses, frequently yield small, weakly diffracting microcrystals. Improvements in beamline, detector technology and experimental techniques have made collecting data from such crystals more tractable. However, data processing remained challenging compared to the user experience for more routine experiments and multiple crystals are often required even at 100 K.

The research team has demonstrated that xia2.multiplex can be used to combine multi-crystal datasets. Its implementation within the wider MX data analysis pipelines makes it readily available to MX users at Diamond, providing them with timely feedback on multi-crystal experiments. xia2.multiplex can be applied to a wide variety of multi-crystal datasets, from multi-crystal phasing experiments on I23 to room temperature *in situ* data collections on I24 and VMXi.

Gildea, RJ. *et al* DOI 10.1107/S2059798322004399



Biological Cryo-Imaging Group

The Biological Cryo-Imaging Group brings together dedicated facilities for X-ray, light, and electron microscopy at Diamond Light Source. The electron Bio-Imaging Centre (eBIC) is the national centre for Cryo-Electron Microscopy (cryo-EM) in the UK and provides a range of capabilities and supporting facilities for cryo-EM and Correlative Light and Electron Microscopy (CLEM). 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 cryo-EM. 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 (Cryo-SXT) and Cryo Structured Illumination Microscopy (Cryo-SIM) with user friendly protocols.

Recent studies on B24 and eBIC this year include those to understand modifications in cells infected by the Herpes virus, insights into filaments of Parkinson's disease and determining the structure of key proteins involved in many cellular process relevant to cancer

Herpes simplex virus can rearrange the contents of human cells

Herpes simplex virus (HSV)-1 is a highly prevalent human pathogen that usually manifest as cold sores or genital herpes. However, HSV-1 infection can cause life-threatening disease, and people with weakened immune systems such as neonates, the elderly and patients on certain immunosuppressive drugs tend to be more at risk. HSV-1 has also been developed as a potential therapeutic; it is already in use as an anti-cancer agent (T-VEC) and is under development as a delivery vector for gene therapy.

Researchers from the University of Cambridge sought to image infected cells that are as close as possible to how they would look in the cellular context.

They used the facilities on Diamond's B24 beamline to flash-freeze infected cells in liquid ethane, cryogenically preserving them in a 'near-native' state, and to perform cryo-soft-X-ray tomography (cryo-SXT). The cryo-SXT analysis allowed them to reconstruct 3D images of infected cells at very high resolution.

Combining this analysis with a special fluorescent 'timestamp' strain of HSV-1, constructed in Cambridge, allowed them to work out the stage of infection each cell was in when it was frozen.

They were able to identify individual virus particles within the infected cells and to see how virus infection progressively changes the shape and distribution of celullar components and organelles.

This study demonstrates the power of cryo-SXT for monitoring virus infection and highlights which organelles to focus on as we study the molecular characteristics of herpes virus infection.

Nahas, KL. *et al.* DOI: 10.1371/journal. ppat.1010629

The atomic structure of alpha-synuclein filaments of Parkinson's disease

Parkinson's disease is a neurodegenerative disorder that affects millions of people around the world. Although Parkinson's disease is most commonly diagnosed in older adults, it can also affect younger people.

In many neurodegenerative diseases, one or a few different proteins form aggregates, i.e. amyloid filaments, in the brain. In Parkinson's disease, the amyloid filaments are made of the protein alpha-synuclein. However, the structures of the filaments from Parkinson's disease remained unknown. One of the difficulties was that many of them do not twist, which leads to technical problems in the structure determination process. An international team of researchers solved the structure of alpha-synuclein filaments. They collected many electron microscope images at eBIC and sifted through them all to find the minority of the filaments that did twist.

Knowledge of the structure of the alpha-synuclein filaments can be used to develop new molecules that could be useful in the clinic. For example, it may now be possible to use structure-based design to develop small molecules as new ligands for positron emission tomography (PET). Such ligands allow the presymptomatic detection of α-synuclein assemblies in brain tissues, which is crucial to early intervention. The results can also be used to develop better model systems of disease and will help to develop methods for producing α-synuclein filaments with structures identical to those in human brains. In the long term, this work could lead to the development of new therapies for Parkinson's disease.

Yang, Y. *et al.* DOI: 10.1038/s41586-022- 05319-3

Understanding a protein that fuels bowel cancer

Tankyrase is an important protein that regulates a wide range of processes relevant to cancer and other conditions, such as diabetes, neurodegeneration and fibrosis. It supports 'Wnt signalling', essential for cell division and development and maintaining stem cells. Therefore, tankyrase has received substantial attention as a potential drug target.

The protein remains poorly understood, with scientists unsure of how the protein is switched on, how it functions and how to block it without causing unwanted side effects.

It self-assembles to form filamentous polymers, but how polymerisation contributes to its function and catalytic activity was unknown.

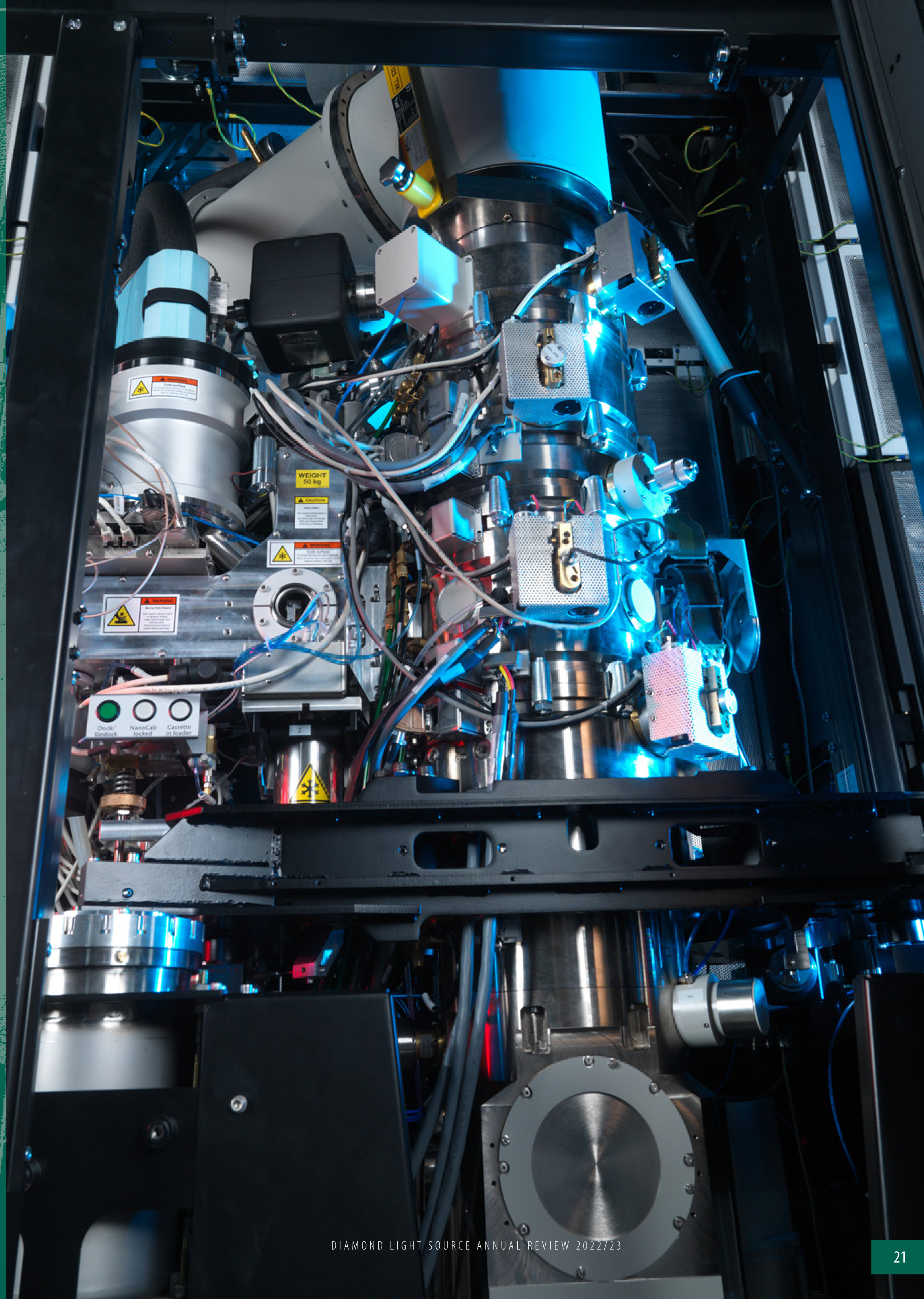
Scientists at The Institute of Cancer Research used cryo-EM at eBIC to investigate the architecture of filaments. In particular, they were keen to identify any potential contacts made by the catalytic domains, as these interactions may control the effect of polymerisation on tankyrase's activity.

They revealed the architecture of a tankyrase filament to be a double helix. Their results revealed extensive interactions between different domains of tankyrase, including those involving the catalytic domain. Based on subsequent biophysical, biochemical and cell-based studies, the researchers proposed that a polymerisation induced allosteric switch regulates tankyrase's catalytic functions.

The scientists suggest tankyrase works by being recruited to a specific site and 'self-assembling', activating itself by clustering and changing its 3D structure.

This work provides novel insights into fundamental biological mechanisms but should also enable the development of novel tankyrase inhibitors and overcome the limitations of currently available molecules.

Pillay, N. *et al.* DOI: 10.1038/s41586-022- 05449-8



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 (Atomic and Electronic Structure of Surfaces and Interfaces). 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. The group continue to benefit from many key developments during remote working restrictions, such as enhanced automation, but recognise that many of the more complex studies rely on the expertise of the user groups, especially for sample preparation and experiment planning.

This year's studies include investigating the electronic properties in a stack of crystals, a new NEXAFS end-station at B07 and study of disorderly crystals.

The electronic properties in a stack of crystals

Traditional solid-state physics focuses on crystals with a well-defined periodicity. However, in recent years it has become increasingly clear that stacks of thin crystals with non-compatible periodicities can bring about new properties that are different from those of the constituent parent crystals. Researchers from Aarhus University in Denmark wanted to develop a better understanding of this phenomenon.

The research team chose to investigate a so-called misfit compound. A misfit compound is a naturally occurring infinite stack of two-dimensional materials with incompatible. Their chosen misfit compound was a stack of square and hexagonal layers with no common periodicity.

Using Diamond's I05 nanoARPES branch allowed them to study the surface with a very high spatial resolution. This is necessary because the misfit crystal is a stack of two types of layers. It can have two terminations at the surface with either one or the other layer.

Their results showed that the properties of each layer strongly resemble those expected for a free-standing version of that layer, without the influence of the other layer. However, there were some new properties arising in the form of one-dimensional electronic states.

The findings provide a new way to create one-dimensional electronic states. Such states have interesting fundamental properties that could potentially be used for next-generation electronic devices in the future.

Chikina, A. *et al.* DOI: 10.1103/ PhysRevMaterials.6.L092001

New NEXAFS beamline rapidly characterises bonds in noncrystalline materials

Drugs are commonly manufactured in the form of tablets that contain other materials. The role of these additional ingredients is to ensure that drug release in the body is controlled, with just the right dose over a defined amount of time. There is a lot of interest in the idea of manufacturing the drug itself by crystallisation with a second ingredient, giving access to drug release profiles that cannot be achieved through tablet formulation.

The products of crystallisation with a second component are typically held together by electrostatic bonds associated with the sharing of hydrogen atoms between the two components. Such bonds are called hydrogen bonds. Often, the hydrogen nucleus separates from its electron and forms an ionic bond, and the resulting product is called a salt. Clarity about which type of bonding occurs is essential for predictive modelling of properties as well as for regulatory approval and patenting of the resulting medicine.

Diamond and the University of Leeds partnered to develop the new high throughput Near-Edge X-ray Absorption Fine-Structure (NEXAFS) spectroscopy end station at the B07 beamline. The team then used it to characterise three 2-component systems to examine whether the sensitivity of NEXAFS to the hydrogen position is sufficient to identify the nature of the intermolecular bond.

The high-throughput NEXAFS capability of the new B07 beamline facilitates the characterisation of local bonding in organic crystal structures on timescales of minutes. The capability to identify these interactions quickly and correctly will be an invaluable aid in the development of new technologies and products.

Edwards, PT. *et al.* DOI: 10.1021/acs.jpca.2c00439

Taming disorderly oxides

Gallium oxide (Ga_2O_3) is an interesting electronic material with potential applications in, for example, power electronics, solar-blind UV photodetectors, gas-sensing devices, and solar cells. It exists in a number of different crystal structures (polymorphs), known as alpha, beta, gamma, delta and epsilon.

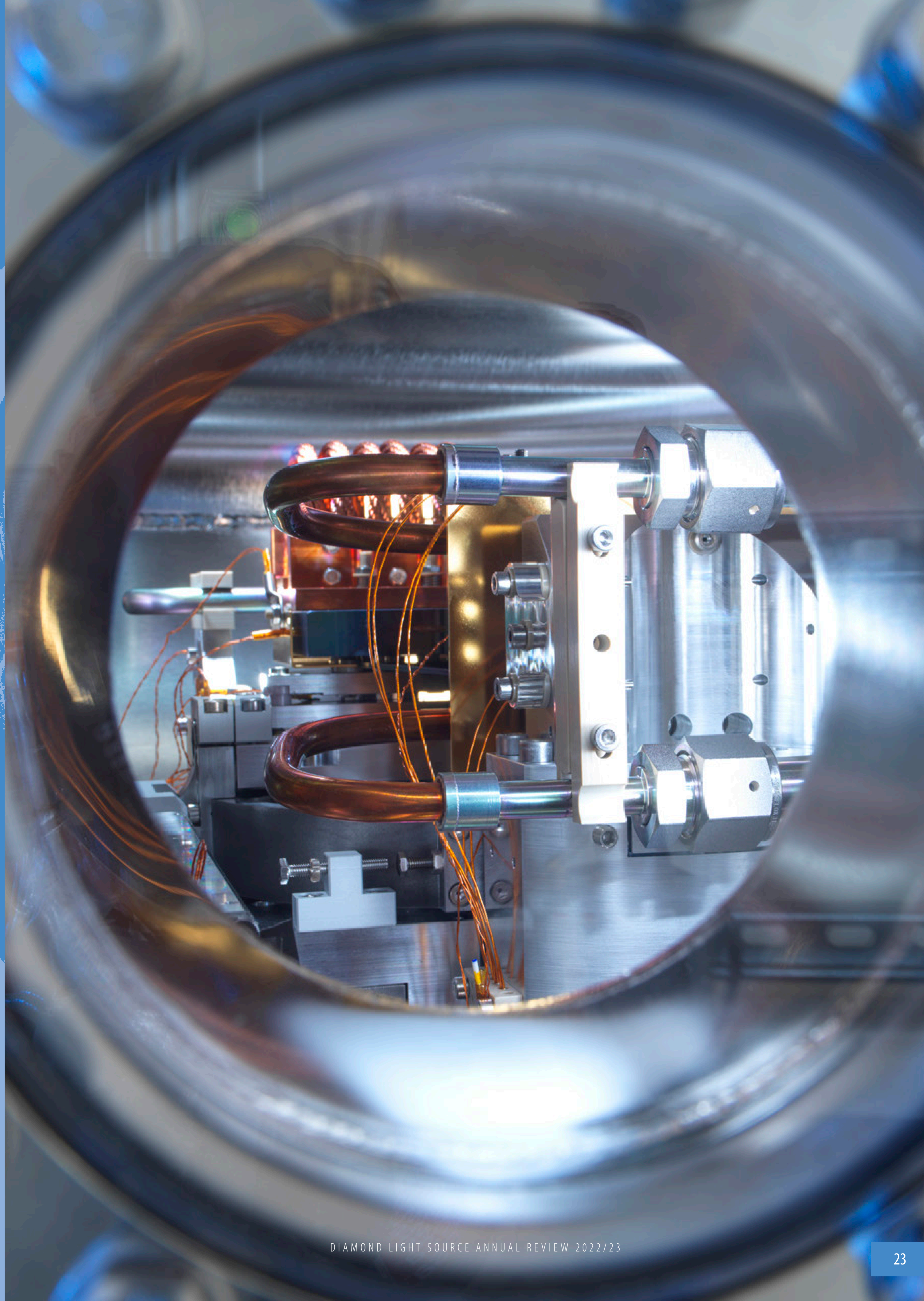
An international team of researchers wanted to understand how structure influences the electronic structure of one particular phase, γ-Ga_2O_3, which is highly disordered and, therefore, incredibly challenging for experiment and theory.

They used both soft and hard X-ray Photoelectron Spectroscopy as well as X-ray Absorption Spectroscopy at beamline I09 at Diamond to investigate the electronic properties of γ-Ga_2O_3 and how this relates to its crystal structure.

Using the theoretical approach, they were able to identify a small number of possible structures γ-Ga_2O_3 could realistically have. They then validated this by directly comparing theory with the photoelectron spectroscopy results. By using this combined approach, they could identify good descriptions of both structure and electronic structure of this complex material.

Disordered systems are increasingly interesting for electronic and optical applications. Unlocking their full potential will involve engineering their structure through targeted synthesis in a way that enables finetuning of their electronic and optical behaviour and performance in a device. This is only possible if we have the fundamental knowledge about the relationships between these aspects and the tools to describe and probe them.

Ratcliff, L, E. *et al.* DOI: 10.1002/adma.202204217



Magnetic Materials Group

The Magnetic Materials Group develops and uses a range of polarised X-ray probes, including Resonant Inelastic X-ray Scattering (RIXS), Resonant Elastic X-ray scattering (REXS), X-ray Absorption Spectroscopy (XAS) and PhotoEmission Electron Microscopy (PEEM) on beamlines I06, I10, I16, and I21 to tackle a variety of challenges and opportunities in exploiting the changes in magnetic properties of on materials. Areas covered include topological states of matter, superconductivity, spintronics (the study of electron spinning and associated magnetism in solid state devices), two-dimensional systems, skyrmions (particles that may provide new forms of data storage) and multiferroics. Over the last year, our research community has used these probes to gain fundamental insights into new materials and how to tune materials to discover exotic new properties.

Research from this group this year has included investigating ferroelectric superlattices, developing new methods of fast and energy efficient computing storage and discovering new superconductors that operate at closer to room temperature.

REXS reveals chiral structures of polar vortices in ferroelectric superlattices

Recent research discovered polar vortex domains consisting of polar dipole vectors in ferroelectric superlattices. Because of their high potential as next-generation memory devices or functional devices, it is important to understand in detail the structure of polar vortices because it affects their properties and how they can be utilised in devices. Resonant Elastic X-ray Scattering (REXS) offers a non-destructive method to understand the complete 3D structure of the vortex.

An international team of researchers used Diamond's I10 REXS to determine the distribution of the three-dimensional polar vectors formed in a $PbTiO_3/SrTiO_3$ superlattice.

The research team observed that the sign of X-ray Circular Dichroism varies depending on the incident angle of the X-rays. Using a newly developed quantitative calculation, they revealed that this result meant a three-dimensional vortex array structure, not a simple one-dimensional helix.

This research on the polar structure of ferroelectrics corresponds to the counterpart of X-ray resonant magnetic scattering for the magnetic structure, which has already been extensively studied. These similarities naturally trigger X-ray resonant scattering studies on multiferroics that exhibit both properties at the same time. There is still no way to simultaneously measure two properties of the same atom or system, and X-ray resonant scattering is likely to be the answer.

Kim, KT. *et al.* DOI: 10.1038/s41467-022-29359-5

Ferroelectric topological structures

Although ferromagnetism and ferroelectricity are similar effects, they were thought to be fundamentally different. However, theoreticians suggested that we might see that the two phenomena are surprisingly similar if we could get a close enough look. In ferromagnetism, the Dzyaloshinskii–Moriya interaction (DMi) gives rise to effects such as skyrmions, which are potentially very useful for next-generation electronic devices (spintronics). If an analogous mechanism were present in ferroelectric materials, it would offer intriguing possibilities for future applications.

A team of researchers used Diamond's I16 beamline to perform high-resolution X-ray diffraction. The high resolution and high flux coupled with area detectors enabled them to study periodicities in reciprocal space with necessarily high resolution.

The X-ray data showed periodicities in two orthogonal directions that are aligned with the orthorhombic crystal symmetries. The X-ray data are in complete agreement with the more myopic cross-sectional Transmission Electron Microscopy (TEM) and show that the observed topology indeed extends throughout the crystal.

In the studied sample, the topologies arise from small tilts of the atomic positions within the crystal, which induce both a small electrical polarisation and strain. The observed ferroic topologies arise as the system attempts to minimise the internal energy. The observation of an electrical equivalent of the DMi shows that complex topologies of the polarisation are now possible. By changing the material properties, this interaction strength can be tweaked, driving new, ever more complex structures that can be stabilised. The plethora of technologies based on ferromagnetic spin textures shows what may be possible in these electrical equivalents.

Rusu, D. *et al.* DOI 10.1038/s41586-021-04260-1

Charge-ordered phase in layered nickelates

Unconventional high-temperature superconductors are at the core of quantum materials and advanced technological applications. Recently a new family of superconductors with layered nickelate-oxide structure was successfully obtained. The latest resonant X-ray spectroscopic studies reveal them to be very close cousins to copper-oxide superconductors (cuprates)

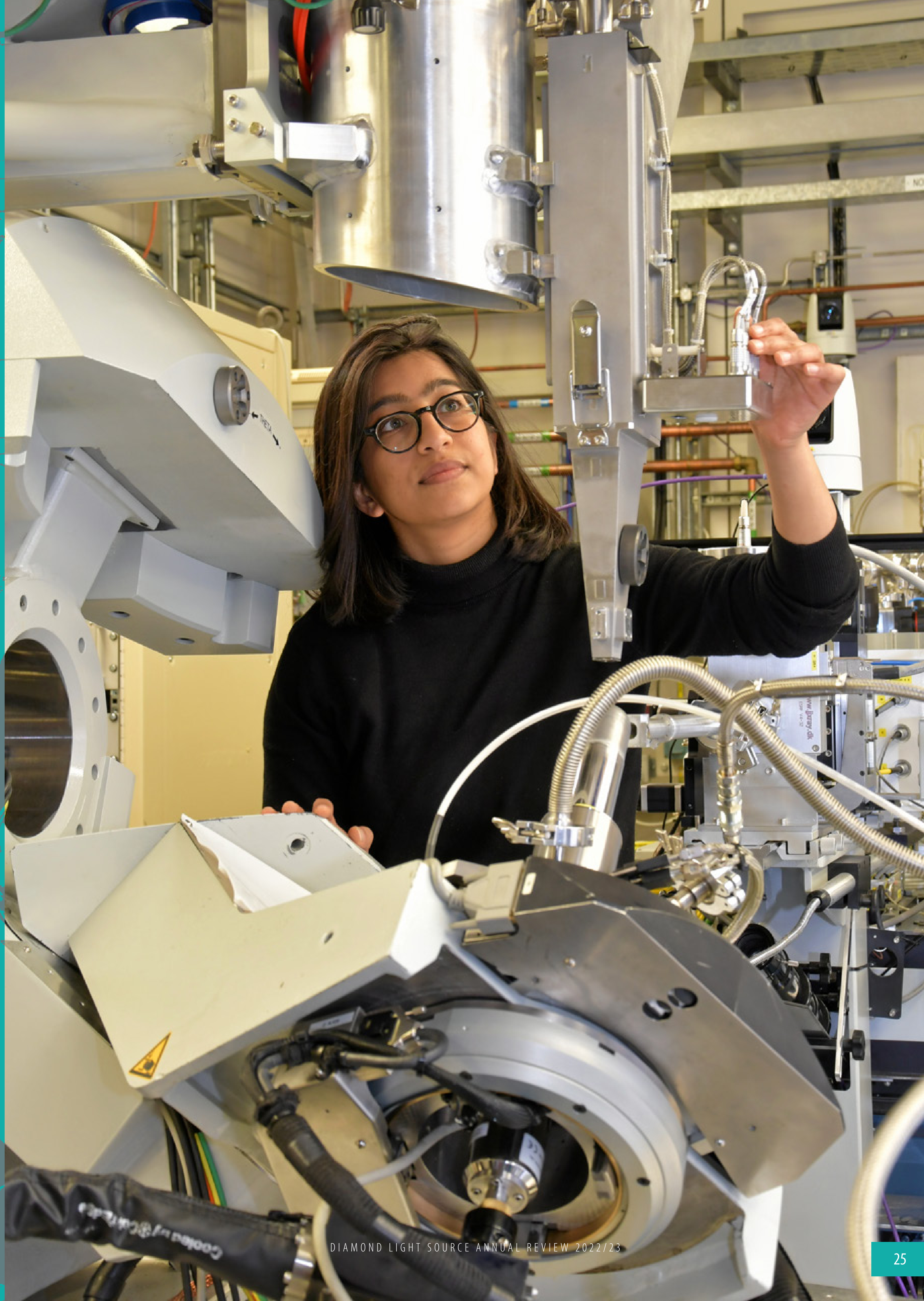
An international team of researchers used Diamond's I21-RIXS beamline. Resonant Inelastic X-ray Scattering (RIXS) is one of the few techniques capable of probing the charge-ordered state. In particular, owing to the sub-100 nm probing depth, RIXS is particularly suited for the nm-thick nickelate films. Moreover, as I21 is equipped with high energy resolution and high photon flux, it is an ideal facility for this type of study.

The research team found the charge-ordered states exist in the parent layered nickelate NdNiO2. They show strong resonance at both Ni 3d and Nd 5d states, illustrating the coupled electronic structure between the two. The charge-ordered state also shows clear temperature dependence, a hallmark of an ordered state with an electronic origin. Using the continuous tunability of the RIXS spectrometer, they found the charge-ordered state has non-negligible L-dependence, hinting it's a three-dimensional object.

Despite the differences to cuprates, the existence of the charge-ordered state demonstrates that the layered nickelates are remarkably similar to cuprate superconductors.

Many materials in condensed matter physics exhibit remarkable properties such as zero-resistivity, colossal magneto-resistance and the magneto-optical Kerr effect. These novel properties lie in the competition of electronic and magnetic interactions under the angstrom and nanometre scale. A spectroscopy technique such as RIXS is imperative to understand and eventually make newer materials with richer functionality, due to its remarkable sensitivity.

Tam, CC. *et al.* DOI: 10.1038/s41563-022-01330-1



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 Imagine 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 extract image sample properties in minute detail lends itself to a wide range of scientific areas, from chemistry and catalysis to environmental science, materials science, biology, medicine, and cultural heritage.

Studies from the group this year include the search of life on Mars, tomography to help study back pain, and perovskite material for new solar materials.

Searching for life and for our origins are two sides of the same coin

In 1996, researchers at NASA Johnson Space Center released a paper in Science entitled "Possible relic biogenic activity in Mars meteorite ALH84001". This caused intense scientific examination of this meteorite, ultimately leading to the formation of the field of Astrobiology and renewed interest in sending missions to Mars. After several years, the scientific consensus was that there was no evidence of Martian life in the meteorite, but the question of organic material remained ambiguous. So the question remained for many years: if ALH84001 does not contain signs of martian life, what is the nature of organic material in this meteorite, and what is its origin?

A team of researchers undertook a series of investigations to spatially resolve the presence, nature and possible synthesis mechanisms for the organic material in ALH84001.

At Diamond's I08 beamline, they carried out high spatial resolution STXM analysis across the C and N edges to look at the presence and bonding environment of the carbon present.

From these analyses, the team were able to show that the organic carbon was synthesised *in situ* on Mars in two processes: serpentinisation and carbonation. These two organic synthesis mechanisms had not been seen on Mars before and are indicative of water-rock reactions 3.6 billion years ago. Water-rock interactions are relevant to planetary habitability, influencing mineralogical diversity and the production of organic molecules.

Steele, A. *et al.* DOI: 10.1126/ science.abg7905

Detailed measurement of spinal disc mechanics provides insight into common back pain

The leading cause of years lived with disability is from people suffering with lower back pain. It severely affects the quality of life of all global populations. The spine intervertebral discs (IVD) are the soft tissue in the spinal column. When injured or degenerated, they are responsible for the majority of these lower back pain cases. Currently, only symptomatic treatment or spinal surgery is available; therefore, understanding the mechanical pathogenesis of degeneration is crucial to developing non-invasive therapies.

Researchers used synchrotron Computed Tomography (sCT) on Diamond's I13-2 beamline to investigate collagen fibre bundles in 3D throughout an intact native rat lumbar IVD under increasing compressive load.

By directly examining the functional response of intact spinal discs, in high enough detail to observe the critical collagen fibres, this study contributed to the understanding of disc degradation and failure. Portions of the disc that fail most frequently (posterior-lateral) have an inherently different fibre architecture from regions less prone to failure (anterior) and have a lower capacity to respond to compressive loading. The level of detail in these observations, with tens of thousands of individual fibres visualised and measured within each region, is essential to a full understanding of disc mechanics.

The authors also provide a roadmap for attempts to restore spinal tissues to a more functional state. Being able to perform detailed characterisation of numerous individual collagen fibres from *in situ* imaging of intact tissues and structures will enhance our understanding of tissue biomechanics.

Disney, CM. *et al*. DOI: 10.1016/j.actbio.2021.10.012

Nanoscale impurities seed degradation in novel solar materials

Perovskite materials offer a cheaper alternative to silicon for producing solar cells and also show great potential for other optoelectronic applications, including energy-efficient LEDs and X-ray detectors.

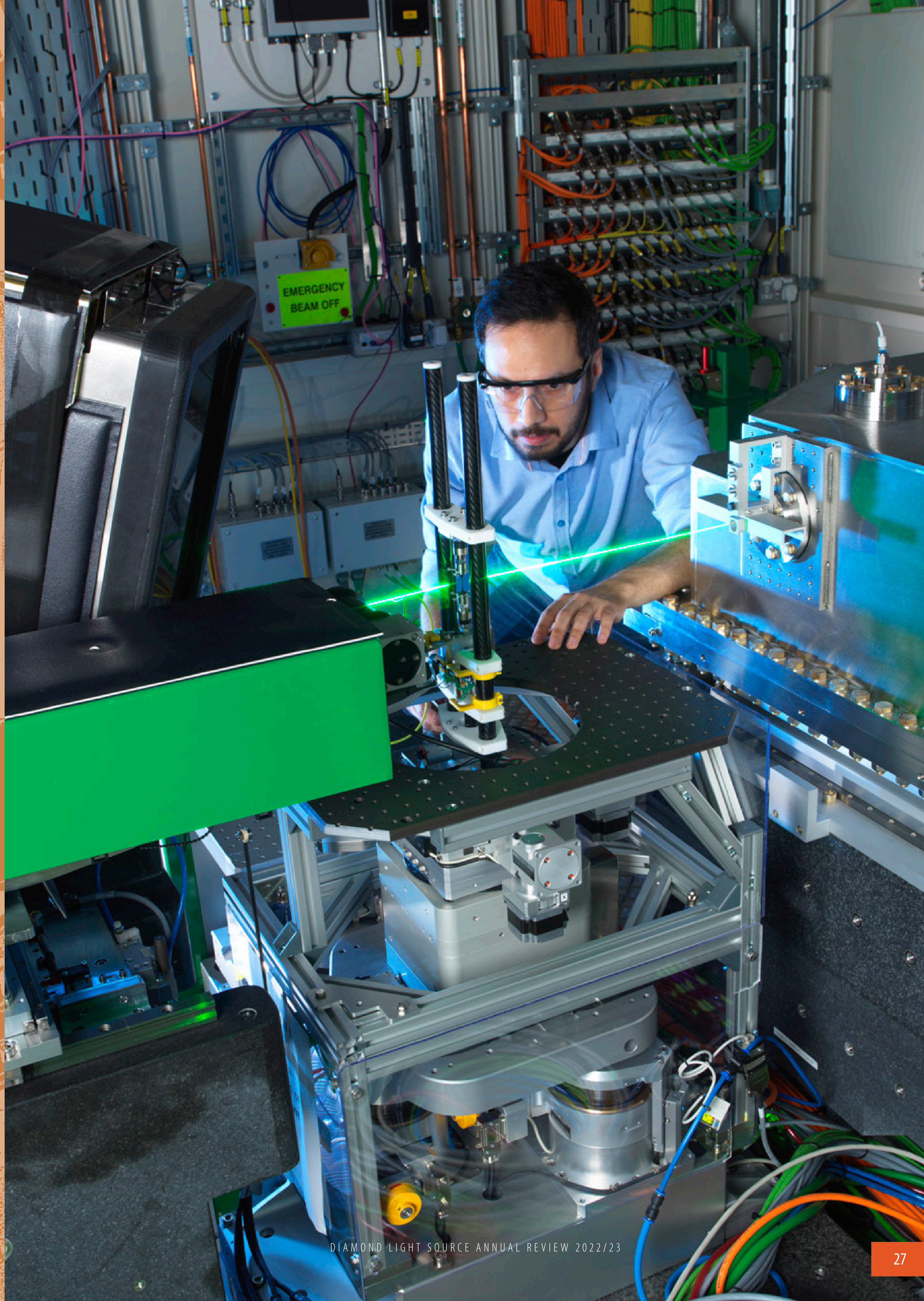
Metal halide salts - abundant and much cheaper to process than crystalline silicon - can be prepared in a liquid ink used to print a thin film of the material.

In the past decade, improvements in the design and fabrication of metal halide perovskite (MHP) based solar cells have seen their efficiencies rise to compete with incumbent technologies and have laid the pathway to commercialisation. However, MHP stability, and thus the longevity of these light-harvesting devices, remains deficient. A multidisciplinary team of researchers used Diamond's Hard X-ray Nanoprobe beamline (I14) and the electron Physical Science Imaging Centre (ePSIC) to gain new insight into the perovskite materials that hold so much potential in the field of optoelectronics.

Their findings suggest that the localised presence of phase impurities are direct indicators of failure points in the absorber layer. The detection of such species through nanoscopic screening (e.g. high resolution electron microscopy) offers a means of predicting sites of instability during film optimisation and manufacturing for application in solar cells. New approaches should be developed to realise scalable, uniformly tilted and, thus, photo-stable MHP films on the manufacturing line.

This research could significantly accelerate the development of long lasting, commercially available perovskite photovoltaics.

Macpherson, S. *et al*. DOI: 10.1038/s41586- 022-04872-1



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 its teams to provide the basis for future development and pioneering experiments. The Group's beamlines use various 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 and Materials, and Life Sciences.

Studies in the past year have included structural changes in MOF under pressure, understanding the movements of electrons in complex molecules and Lithium-ion batteries.

Porous framework materials compress like a spring under high mechanical pressure.

Metal-organic frameworks (MOFs) are modular porous materials possessing a wide range of functions. Some MOFs reversibly switch between two different states, an open pore state with voids accessible for guest molecules and a closed pore state, where the voids of the framework are inaccessible for guest molecules. Usually, this transition is discontinuous, and only two different states/structures are accessible.

Researchers wanted to generate a MOF system featuring a continuum of available states/structures between the open and the closed states. They used Diamond's I15 beamline to investigate the high-pressure structural behaviour of a series of MOFs of the ZIF-62 family, which feature the same framework structure but possess various fractions of small- and large-sized organic linker molecules.

At I15, they could use a dedicated hydraulic high-pressure cell for the experiments.

The required pressure for pore closure increases with increasing fraction of the large-sized linker included in ZIF-62. For very large fractions of the larger linker, ZIF-62 continuously transforms from the open pore to the closed pore form with increasing pressure. Structure refinement and detailed analyses revealed that the pore size of the continuously transforming ZIF-62 derivative also gets continuously narrower and narrower with increasing pressure.

The pressure driven open-pore to closed-pore transition of ZIF-62 could lead to applications of these materials as shock absorbers or nano-dampers. The material can be fine-tuned for a specific molecular separation task by applying a pressure that sets an appropriate pore size cut-off.

Song J. *et al.* DOI: 10.1002/anie.202117565

Electron movement between components of mechanically interlocked molecules

Controlling photoinduced charge transfer within molecules is a significant challenge. An international team of researchers previously demonstrated that a macrocycle (wheel-shaped molecule) could reversibly lose an electron. They wanted to see if threading an electron-accepting molecule through this macrocycle could make a mechanically interlocked system, known as a rotaxane, where the electron could be stimulated to hop from the wheel to the thread.

They obtained the single crystal structure of the most complex compound, a hetero[4]rotaxane, using data from Diamond's I19 beamline. A [4]rotaxane is a molecular thread passing through three wheel-shaped molecules. Crystal structures of such intricate molecular systems are incredibly rare, so it was valuable for this work to obtain this structure that showed the position and arrangement of all the interlocked pieces.

In this study, combining the data from the synchrotron X-ray source with electron diffraction studies allowed the complete determination of the structure of this fascinating molecule.

The movement of the electron can be stimulated with photons (laser light), which causes an electron to rapidly hop from the wheel to the thread. This event occurs at different rates in the different systems, which led the research team to conclude that a distinct wheel molecule was supplying the electron in each system.

Understanding how to control the movement of electrons in complex molecular systems is useful in the construction of organic electronic devices, such as OLEDs and solar cells.

Pearce, N. *et al.* DOI: 10.1038/s41467-022-28022-3

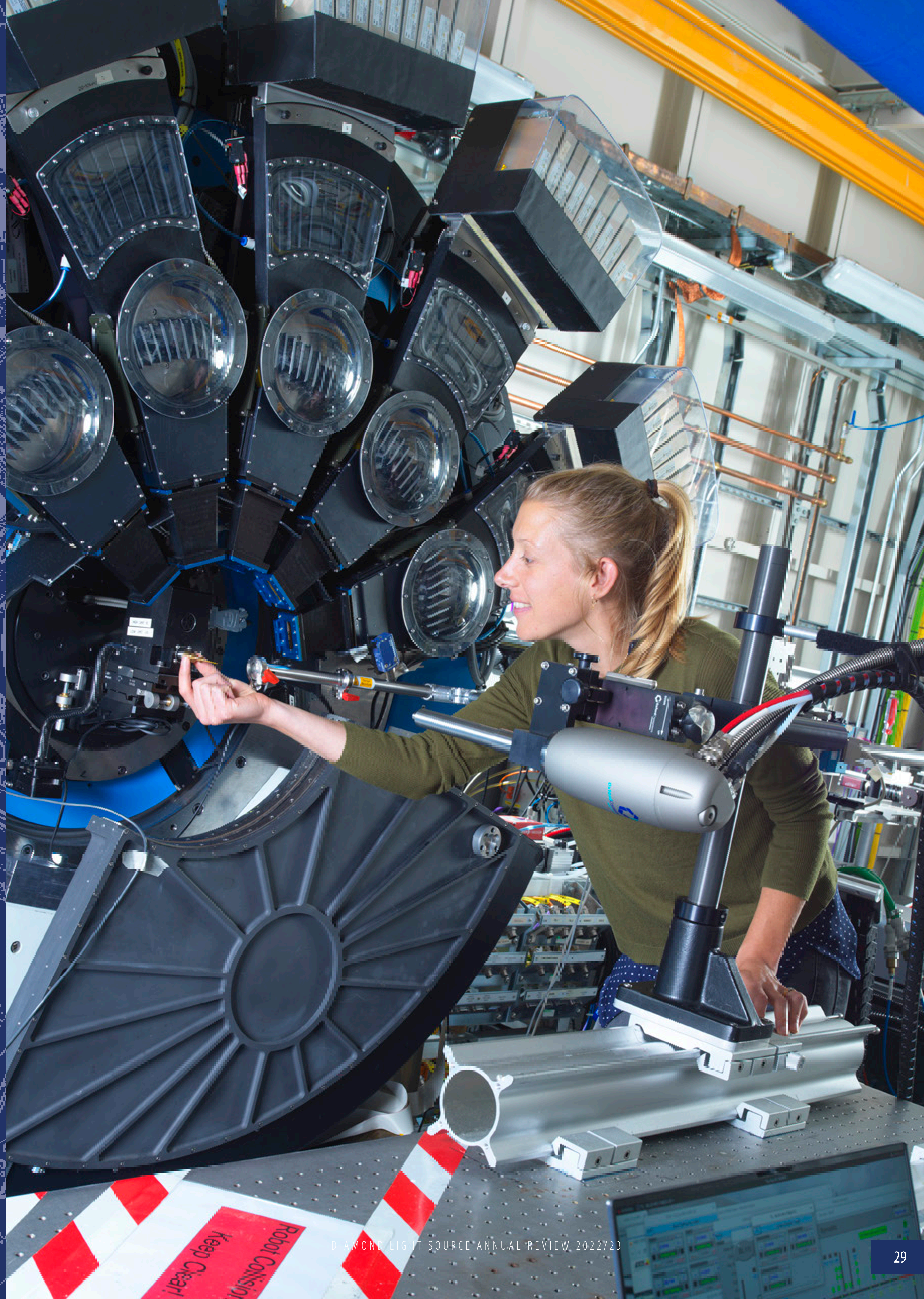
Local cation ordering in 'disordered' Li-ion cathodes

The modern world relies on high-performance lithium-ion (Li-ion) batteries for numerous applications. Demand for these batteries is increasing, but current cathode materials limit the energy density and dominate the cost. In recent years, there has been a surge of interest in lithium rich cathodes with a cation Disordered Rock Salt (DRS) structure. DRS cathodes are relatively low cost, and their high first charge capacities offer tantalising promise for high-energy-density Li-ion batteries. However, they suffer from a large irreversible capacity loss on the first charge-discharge cycle.

The origin of the capacity loss in DRS is not well understood. Researchers used *operando* techniques to investigate the evolution of the average structure, short-range ordering and charge during the cycling of a DRS, using both spectroscopic and structural probes. To understand the structural evolution of nanostructured DRS cathodes *operando*, they acquired pair distribution function (PDF) data at Diamond's I15-1 beamline.

This work provides insight into the design of better DRS cathodes and highlights the importance of local structures in the cyclability of battery materials. Furthermore, successful control of the coexistence of layered and DRS sublattices offers a novel route to electrode design, opening a new path to developing high-performance cathode materials. This research is an example of how multimodal, *operando* experiments across complementary techniques including HERFD-XANES, XES (Kβ main line, V2C), and X-ray Total Scattering (Bragg, XPDF), can aid the complete understanding of complex electrochemical processes in new battery materials.

Diaz-Lopez, M. *et al.* DOI: 10.1039/D2TA04262B



Spectroscopy Group

The Diamond Spectroscopy Group consists of four beamlines: the Microfocus Spectroscopy beamline (I18), the Core EXAFS beamline (B18), and the two independently operating branches of the Versatile X-ray Absorption Spectroscopy beamline, I20-Scanning and I20-EDE. These spectrometers are highly complementary, most notably in the energy ranges they cover, the size of their focussed beam spots, and the time resolutions they can 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, and cultural heritage. The fast-scanning capabilities of the I20-EDE beamline will be covered by the new spectroscopy beamline that will be built as part of the Diamond-II upgrade programme. The new beamline, called SWIFT (Spectroscopy WithIn Fast Timescales) will be a wiggler-based, quick-scanning EXAFS beamline dedicated to *operando* studies, also at micrometric scale. This year's studies included investigating catalyst for green chemistry, understanding superconductors damage under irradiation, and optimising sodium-ion batteries.

Control of zeolite microenvironment for biomass conversion

Pentadienes serve as key building blocks for the chemical and polymer industries and are widely used as monomers in the production of adhesives, plastics, and resins. However, state-of-the art processes to produce pentadienes rely on fossil fuels. Therefore, the sustainable production of pentadienes from renewable resources is a vitally important and urgent task.

Methyltetrahydrofuran (2-MTHF) can be produced readily from lignocellulose-derived furfural and has been identified as a sustainable resource for making pentadienes. Leading catalysts for this reaction include amorphous SiO_2/Al_2O_3, and Al or B- zeolites.

MCM-41 is a mesoporous silica-based material used as a catalyst or catalyst support for a wide range of reactions; emerging niobium-based catalysts have shown exceptional performance for the hydrodeoxygenation of biomass under mild conditions.

The research team aimed to determine the full molecular details of the catalytic mechanism through the use of *operando* X-ray Absorption Spectroscopy (XAS), combined with Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) and *in situ* high-field solid-state Nuclear Magnetic Resonance spectroscopy on Diamond I20-EDE beamline.

This work reported the synthesis of a series of new (Al,Nb)-bimetallic mesoporous silica materials for the first time. AlNb-MCM-41(35/1/0.9) shows excellent catalytic performance for converting biomass-derived 2-MTHF to pentadienes.

The direct transformation of biomass derivatives to C5 dienes under mild conditions described in this study will have a significant impact on the development of future sustainable chemical processes.

Fan, M. *et al.* DOI: 10.1002/anie.202212164

Investigating the damage tolerance of superconductors for fusion power plants

High-temperature superconductors are an essential component of compact tokamak fusion reactors, which promise to provide a commercial route towards fusion power plants by the mid-2030s.

Researchers sought to discover what kinds of defects are generated by irradiation with energetic particles in the high-temperature superconducting tapes used to make demonstrator fusion magnets by companies such as Tokamak Energy and Commonwealth Fusion Systems.

Superconductivity in high-temperature superconductors is strongly suppressed by structural disorder. When neutrons or other energetic particles collide with atoms in the superconductor, some get knocked out of position, creating defects in the crystal that reduce superconductivity.

Using high energy resolution X-ray Spectroscopy, the I20-Scanning beamline allowed the team to probe changes in the local chemical bonding environment around the copper atoms that occur when oxygen atoms move to different sites in the structure.

The researchers identified specific crystal defects that may be responsible for the loss of superconductivity. Their results gave conclusive evidence for the first time that irradiation produces considerable changes to the environment surrounding the copper atoms that reside in the superconducting planes of the crystal.

Comparing the nature of the defects created in high-temperature superconductors under irradiation by different kinds of energetic species, and at different temperatures, is a key part of being able to predict how these materials will behave in operation in a real fusion device.

The fundamental understanding gained from these experiments will lead to more robust interpretation of a range of irradiation data. Ultimately, the hope is that it will provide magnet designers with more reliable information.

Nicholls, RJ. *et al.* DOI: 10.1038/s43246- 022-00272-0

Developing a deeper understanding of electrode materials for sodium-ion batteries

Various materials can be used as electrodes in sodium-ion batteries (SIBs). Researchers from Germany used X-ray Absorption Spectroscopy (XAS) on Diamond's B18 beamline as part of a rigorous study of the sodium storage properties of ultra-small Fe_3S_4 nanoparticles. This material exhibits excellent electrochemical performance as an anode material for SIBs.

Previous research had shown different structural phase transformations during the discharge and charge of the anode material. For a more detailed understanding, the researchers needed to analyse the local structure around the elements Fe and S and their oxidation states, in the pristine nanocrystalline material and during charging and discharging. Such element-specific information, combined with other techniques (*e.g.*, to determine the crystallographic structure), can yield important insights into the reaction mechanism of a battery material during operation and allow optimisation of battery cells, *e.g.*, by tailoring materials properties or by adjusting cut-off potentials.

Their results showed that the Na storage mechanism of this anode material can be attributed to cationic redox chemistry involving Fe. The experiments revealed the oxidation states of both elements at specific discharge/charge voltages. Using this information, the researchers were able to explain the long-term cycle stabilities of Na/Fe_3S_4 cells during cycling to different lower cut-off potentials.

Such studies can be used to find root causes for cell failure, precisely adjust battery cell limits and find optimal cycling conditions to improve the electrochemical performances and battery lifetime.

Hartmann, F. *et al.* DOI:10.1039/D1NR06950K

Soft Condensed Matter Group

The Soft Condensed Matter (SCM) Group is comprised of four beamlines at Diamond: High Throughput Small Angle X-ray Scattering (SAXS) (B21), Multimode Infrared Imaging and Microspectroscopy (MIRIAM) (B22), SAXS and Diffraction (I22) and Circular Dichroism Microspectroscopy (B23). This unique portfolio of instruments enables studies of non-crystalline materials at nano- to meso-scale resolutions that include two-dimensional thin-films (photovoltaics, OLEDs), living mammalian cells, three-dimensional matrices (metalorganic frameworks, gels, and waxes) and nanoparticles in non-crystalline states. SCM science is "the science that underpins continued improvements to quality of life".

The SCM user community is international, with nearly 70% of our peer reviewed allocated beamtime to UK users with the remaining time shared between other international users.

Studies this year focused on nanomaterials development as new treatments.

Functionalised cubic phase nanoparticles

Focused delivery of chemotherapy drugs at tumour sites can increase the effectiveness of the treatments while reducing potential side effects. This long-standing challenge is being addressed using next-generation nanostructured liquid crystalline nanoparticles (NPs) called cubosomes. Cubosomes have high loading capacity, biocompatibility and thermostability, and have been shown to effectively deliver therapeutics to tumour sites in the patient's body.

Researchers evaluated an active tumour targeting cubosome system directed towards rhabdomyosarcoma (RMS) cells. They employed a top-down synthesis approach to produce blank cubic phase NPs, which were subsequently functionalised with hyaluronic acid (HA), anti-CD221 half-sized antibodies (ha-Abs) and superparamagnetic iron oxide nanoparticles (SPIONs).

They used Small-Angle X-ray Scattering (SAXS) measurements on Diamond's B21 beamline to investigate the lipid lattice patterns and verified the formation of cubic phases. Both SAXS and cryo-Electron Microscopy (cryo-EM) performed at the Electron Bio-Imaging Centre (eBIC) played an important role in optimising the cubosome synthesis method and validating the structures throughout the investigation.

The cubosome-based drug delivery platform constructed in this study can encapsulate large quantities of hydrophilic, lipophilic, or amphiphilic therapeutics and confine the chemotherapy to tumour tissues in an active manner. In addition, the cubosome synthesis and functionalisation procedures the team has established may also be useful in structural biology, vaccine, transfection, cosmetics, or biomedical imaging.

Mun, H. *et al.* DOI:10.1007/s12274-022-5037-4

Directing lipid nanoparticles for anticancer therapy

Nanomedicine is a rapidly growing field that uses nanoparticles to diagnose and treat diseases. The advantages of using nanoparticles include targeting treatments to specific cells or tissues, which can improve the effectiveness of treatment and reduce the risk of side effects. Lipid nanoparticles (LNPs) have attracted enormous interest as drug delivery vehicles. LNPs with an internal cubic symmetry, termed cubosomes, are an emerging class of nanoparticles that offer several advantages, such as high encapsulation of cargo and biocompatibility. To date, however, cubosomes have mainly been used for passive targeting, which often leads to off-target toxicity.

Researchers attached a synthetic antibody, known as an Affimer, to the surface of engineered cubosomes that were loaded with a model chemotherapeutic drug to actively target colorectal cancer cells.

The team used Diamond's I22 beamline and the Diamond-Leeds offline SAXS instrument (DL-SAXS) to characterise the internal nanostructure adopted by the LNPs upon surface functionalisation and drug encapsulation.

The results showed that surface functionalisation and drug encapsulation didn't alter the internal nanostructure symmetry of the LNPs. The cubosomes exhibited preferential accumulation in cancer cells compared to normal cells both *in vitro* and *in vivo*, whilst showing low non-specific absorption and toxicity in other vital organs. Mice subjected to targeted drug-loaded cubosomes experienced: increased drug accumulation in the tumour tissue compared to other vital organs, a decrease in tumour growth, and increased survival rates compared to control groups, demonstrating the exciting potential for Affimer-tagged cubosomes in therapeutic applications.

Pramanik, A. *et al.* DOI: 10.1021/acsami.1c21655

Fine-tuning poly-L-lysine-based antiviral nanomaterials

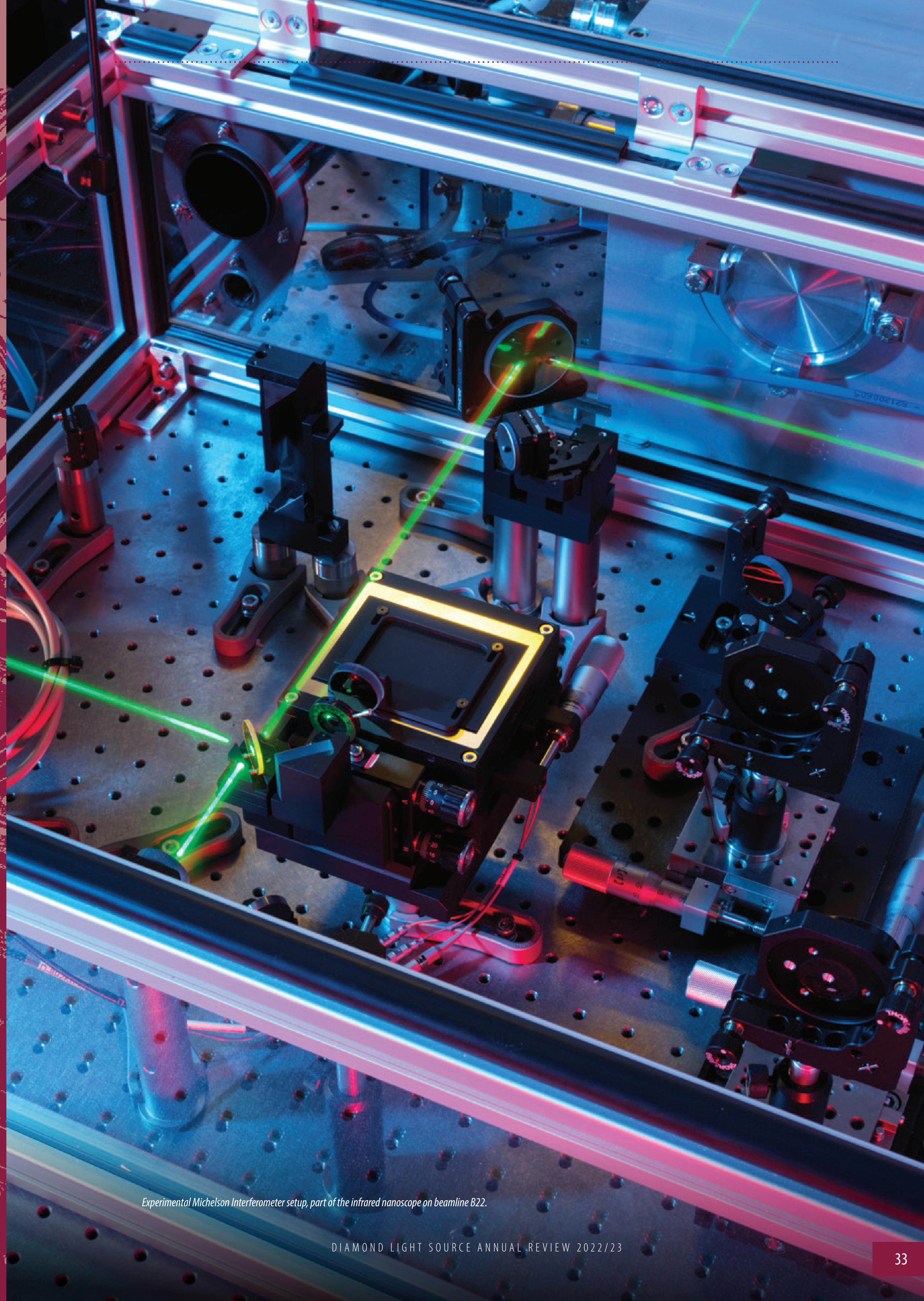
The appearance of new and lethal viruses requires innovative antiviral systems. Nanomaterials can represent alternative resources to fight viruses at different stages of infection by selective action or in a broad spectrum. A fundamental requirement is non-toxicity. However, biocompatible nanomaterials often have little or no antiviral activity, preventing their practical use. Carbon-based nanomaterials have displayed encouraging results and can present the required mix of biocompatibility and antiviral properties. Researchers recently synthesised a polymeric nanomaterial, derived from the amino acid L-lysine, with an antiviral activity against SARS-CoV-2 and a good safety profile *in vitro*.

The research group is developing a new generation of lysine-based nanostructures by modifying the lysine branched structure with other amino acids, such as arginine and glycine, whose structure is not yet understood. They used Synchrotron Radiation Circular Dichroism (SRCD) on Diamond's B23 beamline to understand the supramolecular structure of this peculiar class of biomaterials.

The structural analysis of the poly-L-lysine (PLL) obtained after a hydrothermal treatment (HT) at 200 °C of L-lysine showed significant differences in the homopeptide architecture as a function of pH.

It is, therefore, possible to tune the synthesis process to obtain cross-linked or linear lysine polymers by modulating the pH of the starting solution. The knowledge acquired in this study has enabled the design of very specific L-lysine-based nanosystems that can inhibit the replication of different types of viruses with potential broad-spectrum responses.

Stagi, L. *et al.* DOI: 10.1038/s41598-022-24109-5



Experimental Michelson Interferometer setup, part of the infrared nanoscope on beamline B22.

Integrated Facilities and Collaborations

As a world-leading centre for synchrotron science and a cornerstone of a world-class site for scientific discovery and innovation at Harwell, Diamond Light Source has powerful synergies with its neighbouring research institutes and beyond the campus, through collaborations and shared visions. The integrated facilities at Diamond present academic and industrial users with a one-stop-shop for research opportunities, enabling them to combine cutting-edge techniques and capabilities to advance their studies. During the period 2022/23, Diamond was active on over 75 grant funded projects (20 of which were Diamond led). Our grant portfolio involves projects with over 65 national and international collaborators, where Diamond has contributed to projects worth over £316m.

The Membrane Protein Lab

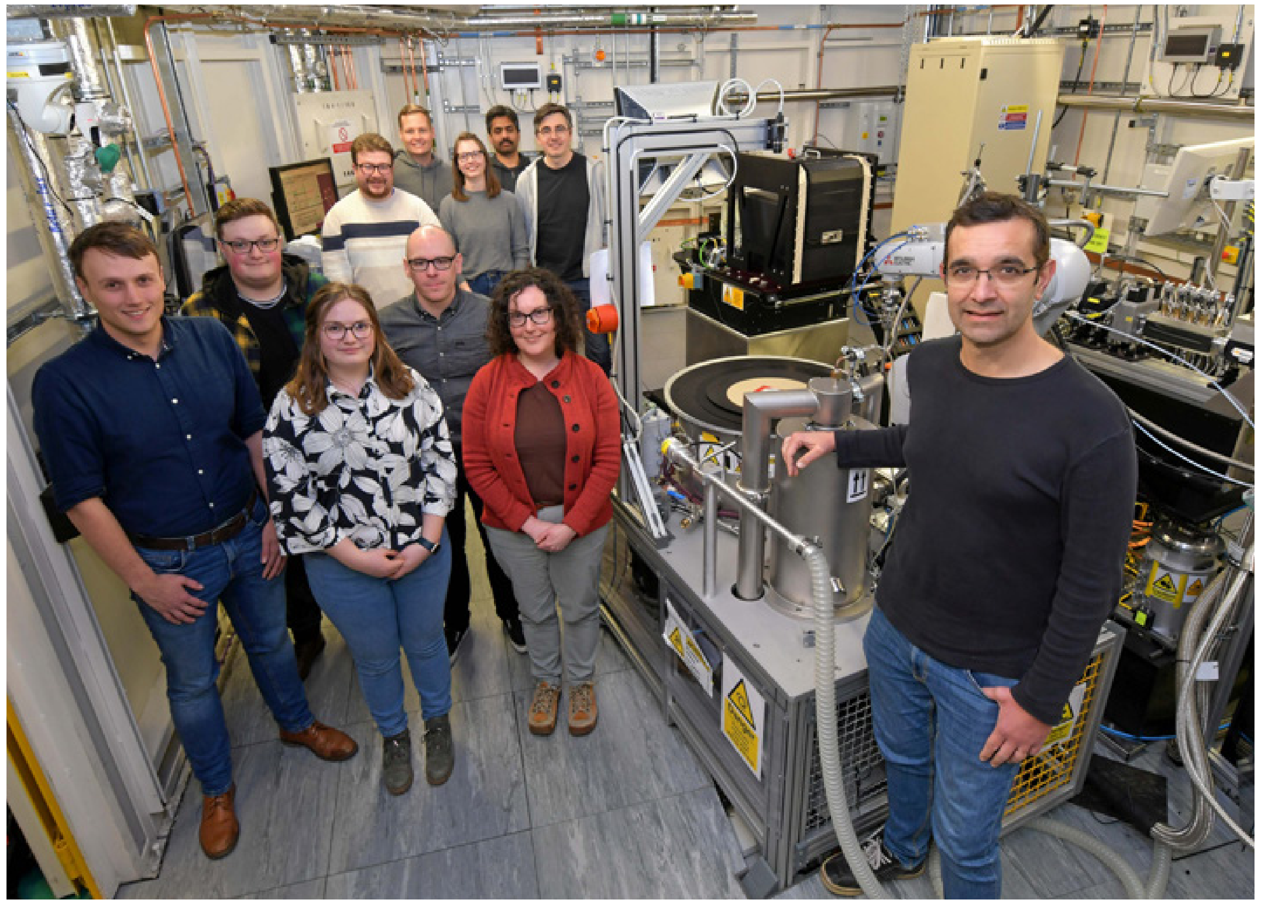
The Membrane Protein Laboratory (MPL), at Diamond is a Wellcome funded resource that supports integrated membrane protein structural biology. Located within the Research Complex at Harwell the MPL enables membrane protein research through the delivery of high-quality samples to Diamond's beamlines and microscopes as well as providing a platform to support membrane protein biochemistry. Membrane proteins are found at the junctions between the outside world and the inner workings of the cell. Multicellular organisms such as humans use membrane proteins for communication, to acquire nutrients and detect threats. Membrane proteins are important targets for biomedicine with over half of all medicines altering membrane protein function. Understanding the structure and function of these proteins in isolation as well as within the wider cellular context will helps us to develop new therapeutics to tackle disease.

Visiting scientists to the MPL can spend anywhere between a day and year in our labs supported by state-of -the art equipment and our experienced support scientists. Working with researchers from Brazil, MPL and eBIC scientists have solved two new single-particle cryo-EM structures from yeast; Ach1p (PDB: 8DH7) and cytochrome C oxidase (complex IV) (PDB: 8DH8) were deposited in the protein databank.

In collaboration with the Rosalind Franklin Institute MPL scientists contributed to a publication in the journal *Science* which looked at new nuclear magnetic resonance (NMR) based methods to quantify interactions between host glycan-proteins and pathogens[1]. Specifically, the authors revealed a distinctive sugar-binding mode mediated by the unusual N-terminal domain from B-origin-lineage SARS-CoV-2 spike protein which is lost in later variants.

In other work MPL and eBIC scientists have published a review of cryo-EM structures of membrane proteins smaller than 100kDa and provided an analysis of the sample preparation routes, data collection methods and processing approaches that were taken[1] in an effort to highlight successful approaches to understanding these difficult proteins.

1. Buchanan CJ, *et al.* Pathogen-sugar interactions revealed by universal saturation transfer analysis. *Science* **377**(6604): eabm3125. (2022) DOI: 10.1126/science.abm3125.



Expanded XChem/I04-1 team.

The XFEL Hub and collaborators in Pohang South Korea in December 2022 at PAL-XFEL for experiments. Left to right: Dr Pierre Aller, Dr Matin Maly, Mr Jack Stubbs, Ms Charlotte Cordery, Dr Ivo Tews, Allen M. Orville, Dr Anastasya Shilova, Dr Sam Horrell, Dr Philip Hincliffe, Dr Jos Kamps.

2. Harrison PJ, *et al.* A review of the approaches used to solve sub-100 kDa membrane proteins by cryo-electron microscopy. *J Struct Biol.* **215**, 107959. (2023) DOI: 10.1016/j.jsb.2023.107959.

XChem

Installation of the new insertion device on I04-1 has increased working flux by 10x. Alongside the EIGER2 X 9 M detector installed previously, this allows us to collect high-quality data collection in 7.2 seconds exposure time. This has had the most impact on the industrial XChem programme who were previously collecting 60 seconds collections, saving up to 53 seconds per dataset.

The XChem platform has also expanded the sample preparation facility to accommodate increased activity driven by user demand (from both academia and industry), grant funded projects and delivery on new collaborations (EUbOpen and Infratec). Investment in the facility, coupled with growth of the XChem team, enabled a 50% increase in the number of samples produced in Q1 2023 with almost 13,000 crystals mounted for academic user experiments and grant-funded research alone.

Alongside capital investment in the platform, work is ongoing in collaboration with Scientific Software at Diamond to improve the robustness and reliability of the XChem software pipeline ahead of future redevelopment of the software stack to meet the demands of Diamond-II. As part of this work a new deep learning model (Crystal Hits in My Plate (CHiMP)) and user interface (EchoLocator) has been developed to automate crystal identification and selection of coordinates for dispensing compounds.

Following the success of the COVID Moonshot's development of a pre-clinical candidate for the SARS-CoV-2 Main protease, the XChem team and collaborators at Diamond have contributed to two successful National Institute of Health (NIH) grants funding the establishment of Antiviral Drug Discovery (AViDD) Centers for Pathogens of Pandemic Concern: the AI-driven Structure-enabled Antiviral Platform (ASAP) and the Rapidly Emerging Antiviral Drug Development Initiative (READDI). The XChem fragment screening platform is central to both Centers' pipeline for identifying chemical starting points for drug discovery projects. Furthermore, ASAP will also leverage the platform's approach to high-throughput structural biology to enable the rapid development from hit to lead-like molecules. Both centres are also committed to open-science and sharing their data to further enable drug discovery projects and methodology development elsewhere.

Key publications:

Skaist Mehlman T, *et al.* Room-temperature crystallography reveals altered binding of small-molecule fragments to PTP1B *eLife* **12**, e84632 (2023) DOI: 10.7554/eLife.84632

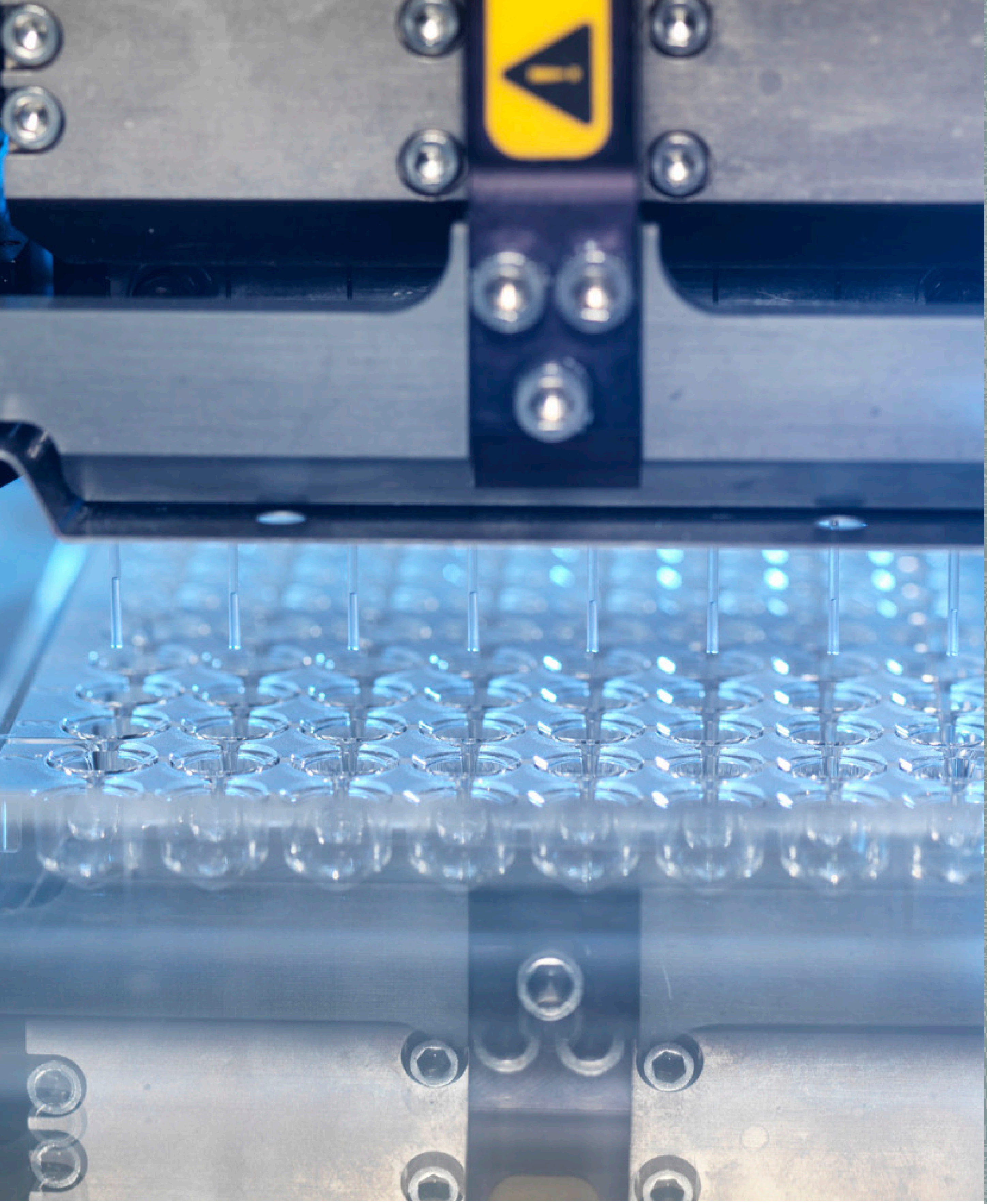
Saar K L, *et al.* Turning high-throughput structural biology into predictive inhibitor design *PNAS* **120**, (11) e2214168120 (2023) DOI: 10.1073/pnas.2214168120

Zaho Y, *et al.* Structural analysis and development of notum fragment screening hits *ACS Chem. Neurosci.* **2022**, 13 (2022) DOI: 10.1021/acschemneuro.2c00325

XFEL-Hub

The XFEL Hub at Diamond continues to provide expertise and support to the UK community engaged in serial crystallography and XFEL-related life science research. This ranges from experimental conception to beamtime proposals, through sample preparations and testing, to XFEL data collection, analysis, and publication. Our Diamond-based activities continue to include organizing and running the block allocation group "Dynamic Structural Biology at Diamond and XFELs" for serial crystallography and time-resolved studies at various MX beamlines at Diamond. This fiscal year, members of the Hub participated in 9 XFEL experiments at the LCLS in the USA, SACLA in Japan, PAL-XFEL in Korea, or the European XFEL in Germany, as well as a site visit to SwissFEL in Switzerland.

Highlighting the synergistic overlap and technology transfer between XFEL and synchrotron facilities, the XFEL Hub spearheads two major projects at Diamond, funded roughly 50:50 by Dr Orville's Wellcome grant and the STFC/UKRI, that will establish methods for time-resolved serial crystallography studies using on-demand sample delivery and reaction initiation strategies that can be correlated with time-resolved X-ray emission spectroscopy (tr-XES) too. Commissioning activities for these two projects are progressing at Diamond beamline VMXi and is a world's first installation at a synchrotron. Our plans also include a collaboration with SwissFEL, which along with the Hub plans to host the Diamond sample delivery capabilities and XES capabilities. The Hub has been testing prototypes for sample delivery and XES data collection with von



Hamos geometry at Diamond. We have analyser crystals to enable XES from copper- and/or iron-dependent metalloenzymes, and an order out for a set of analyser crystals suitable for Ni-containing enzymes.

Dr Orville continues to serve as the life science lead for the UK XFEL project. He delivered a talk at the Royal Society in London on 30 January 2023 as part of the launch event for the Conceptual Design and Options Analysis phase of the project. Comments from the community are always welcome throughout this process.

Active Materials Laboratory

In 2019 Diamond was awarded a grant by the EPSRC to build an Active Materials Laboratory at the synchrotron as part of the National Nuclear User Facilities II scheme to provide more research facilities for nuclear researchers in the UK. The principal aim of this laboratory is to enable Diamond's users to handle active materials on site, either in the short term or performing longer term experiments. All beamline samples will be contained before studying them on one of Diamond beamlines. Before the laboratory was built nearly

Sofia Diaz-Moreno, Fred Mosselmans, Robin Ibbotson, Chief Technology Officer of Sellafield Ltd, and Adrian Mancuso, Diamond Physical Sciences director.

all radioactive samples had to be brought to site in the containment in which they were going to be measured on the beamlines. This, in particular, made doing experiments in which the sample was heated or exposed to gases on a beamline very hard as the whole cell had to be transported intact. The areas of research that will benefit from the laboratory include materials for new nuclear fission, long-term storage of nuclear materials, a geological disposal facility for medium and high activity waste, how radionuclides behave in the environment and materials for nuclear fusion.

The building was constructed over the period October 2020 – July 2021, before a fit out that was extended due to various Covid-related supply issues. The lab is now complete. It consists of two working labs, one nominally a wet laboratory and the other a dry one. They house two glove boxes, a high temperature furnace, an anaerobic Coy chamber, microscopes, centrifuges and other standard lab equipment. Furthermore, there is a counting room with a Gamma spectrometer and liquid scintillation counter. The Laboratory building also houses a storage room for storing active materials in a safe and secure manner.

In 2022 the lab welcomed its first users, the group of Susannah Speller from Oxford. They are studying the effects of irradiation on high temperature superconductors, that may be used in fusion reactors. Several other groups have used the lab since then and Robin Ibbotson, Chief Technology Officer of Sellafield Ltd formally opened the laboratory in November 2022.

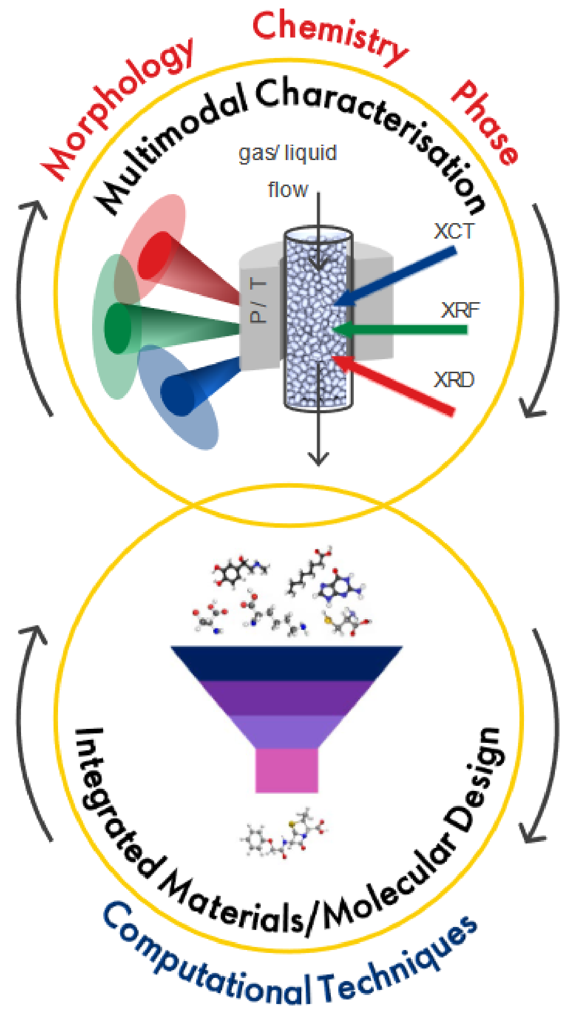
InFUSE: INterface with the Future – Underpinning Science to support the Energy transition

The InFUSE collaboration is a large-scale Prosperity Partnership funded by the EPSRC and SHELL. There are three partners; Imperial College London, SHELL and Diamond Light Source with multiple departments involved across many sites. The aim is to understand and overcome some of the fundamental problems that are hampering the efforts to achieve Net-Zero. Addressing Climate Change on the timescales required needs a rapid translation of technology through close partnership between academia and industry, with a shared vision and commitment.

In this project, the team have identified how important the processes occurring at solid-fluid interfaces are in determining the properties of the system. The influence reveals itself in many relevant science areas such as carbon capture, utilisation and storage (CCUS), electrochemistry (for example at interfaces in battery materials), catalysis and lubricants amongst many others. It is clear that the interface morphology, phase and chemistry all play a role as to how the interface influences the properties.

A complete picture can only be formulated by studying the problem on many fronts, adapting a correlative multi-technique approach, as shown in the Figure. Diamond Light Source contributes to this effort in a number of ways; three of the science groups from the physical science division are actively involved – structures and surfaces, spectroscopy and imaging. Three post-doctoral researchers based at Diamond complement those based in the research groups at Imperial College London. They aim to develop new sample environments that can move between beamlines to simplify such correlative studies, especially in ensuring that *operando* environments expose the sample to the same conditions on the different instruments. Such combined experiments also open up studies at different length scales or processes occurring at differing timescales. Importantly, the InFUSE team is also concentrating on developing modelling and analysis tools, such that interpreting the data from the different techniques will identify the important correlative behaviour.

The sample environments and analysis methodology developed as part of InFUSE will be made available to all Diamond users; at present this includes small cells for catalysis studies at relevant pressures together with improved electrochemistry cells. The InFUSE team is committed to using the techniques at Diamond to optimise the interfaces to deliver improved performance. If you would like further details of the project please contact any of the relevant science group leaders at Diamond, Chris Nicklin, Paul Quinn or Sofia Diaz-Moreno.



The InFUSE methodology combines multimodal characterisation with computational modelling for materials design.

Industrial Liaison

Industrial Liaison Office

Following on from the upheaval of the pandemic years, 2022 felt like a return to the stability of former times. As the world settles into the new normal way of working, our years of preparation in developing remote access, mail in data collection and a range of services for our clients enable us to react quickly to our clients' changing needs. The industrial programme at Diamond continues to thrive with fully operational life and physical science programmes. Building on last year's successes, we are again celebrating our busiest year to date.

The increase in industrial engagement has also naturally led to expansion of the team and this year we welcome Isabel Barker to the industrial XChem team as a Research Technician. Izzy recently achieved her first class MSci (Hons) degree in Biochemistry at the University of Sussex and is bringing her skills in protein preparation and macromolecular crystallography to complement the XChem team and support delivery of industrial XChem campaigns.

With travel becoming possible once again, our clients returned to Diamond to perform a wide range of experiments and our team were able to travel and attended conferences and events, meeting clients and friends both old and new. Highlights include members of the life sciences team attending Protein Structure Determination in Industry (PSDI) in Eindhoven and the Novalix conference in Munich along with the Fragments and MiBio conferences both taking place in Cambridge. Representing the physical science team, Anna Kroner gave an invited talk at the XAFS 2022 conference in Sydney, Australia. Rachel Freeman represented Diamond at the Big Science Business Forum in Granada, working with counterparts at other European research infrastructures to engage with industry. We are now looking forward to meeting our valued clients at wide range of events over the coming year.

Diamond continues to support our industrial clients across a wide range of techniques and facilities with experiments ranging from routine analysis to complex bespoke solutions. Please do not hesitate to contact us on industry@diamond.ac.uk to discuss your analytical needs, we'd be happy to help.

Alex Dias and Ailsa Powell preparing pucks for XChem experiments.

Engaging with Diamond Light Source

Communications and Engagement Team

Over the past year the impact of COVID pandemic restrictions on Diamond's engagement activities has lessened and in person activities have resumed to pre-pandemic levels. The knowledge and experience we acquired in developing and delivering remote activities have not been abandoned, as virtual activities have been integrated into many of our existing programmes from events to school engagement, maintaining the increased accessibility this format allows.

During the 2022-23 period, Diamond has had approximately 8098 significant interactions[i] with visitors, an increase from the previous year (7323 interactions). These include 2890 for scientific and technical events, 452 undergraduate and postgraduate interactions, 4364 school students and members of the public, and 392 VIPs and Stakeholders. In 2022, the majority of these interactions were virtual, however in 2023 we have seen a move back towards in person events, with the majority happening in person onsite (3594) or in person offsite (1249). While most interactions have happened in person, we are proud to have maintained a high level of interaction with visitors online (3255), increasing the accessibility of Diamond to a wide range of audiences.

[i] Significant Interaction is defined as a talk/tour/meeting of 30+ minutes, typically longer.

In 2023, we have worked hard to transition from an almost exclusively remote program of activities put in place to continue to engage audiences during the pandemic, back to in person activities once again. We successfully reinstated our core program of in-person Public Engagement activities, but expanded this to include successful virtual activities that reached underserved audiences during the pandemic. For example, we have continued to run bespoke virtual school visits, whereby individual schools can request a virtual visit to Diamond to fit around their school timetable. This continues to give access to Diamond to all schools, regardless of their situation. We have continued to work with our existing partners such as STFC, at RAL and Daresbury, and Canterbury Christ Church University, to reach both new and larger audiences.

> *We loved the experience and found it absolutely fascinating. Thank you to the whole team for making us welcome, showing us around and, in particular, inspiring the next generation .*

Public Inside Diamond open day attendee, March 2023.

In July 2022 we were delighted to be able to run a fully in person Schools/College Work Experience week for students in years 10-13. We welcomed 48 students across 24 projects, a record-breaking number of both students and projects for Diamond's Work Experience Academy program. Projects spanned all divisions of Diamond, from mechanical engineering to electron structure. On the student's final day at Diamond we welcomed MP David Johnston to help celebrate the success of the programme.

> *It was so exciting to work at the facility and see the synchrotron in real life and to learn about the multitude of research projects being undertaken! It was a real privilege to work on the nanoimaging of Li-ion batteries project with Dorota as my supervisor and the placement has further sparked my interest in Materials Science and Engineering.*

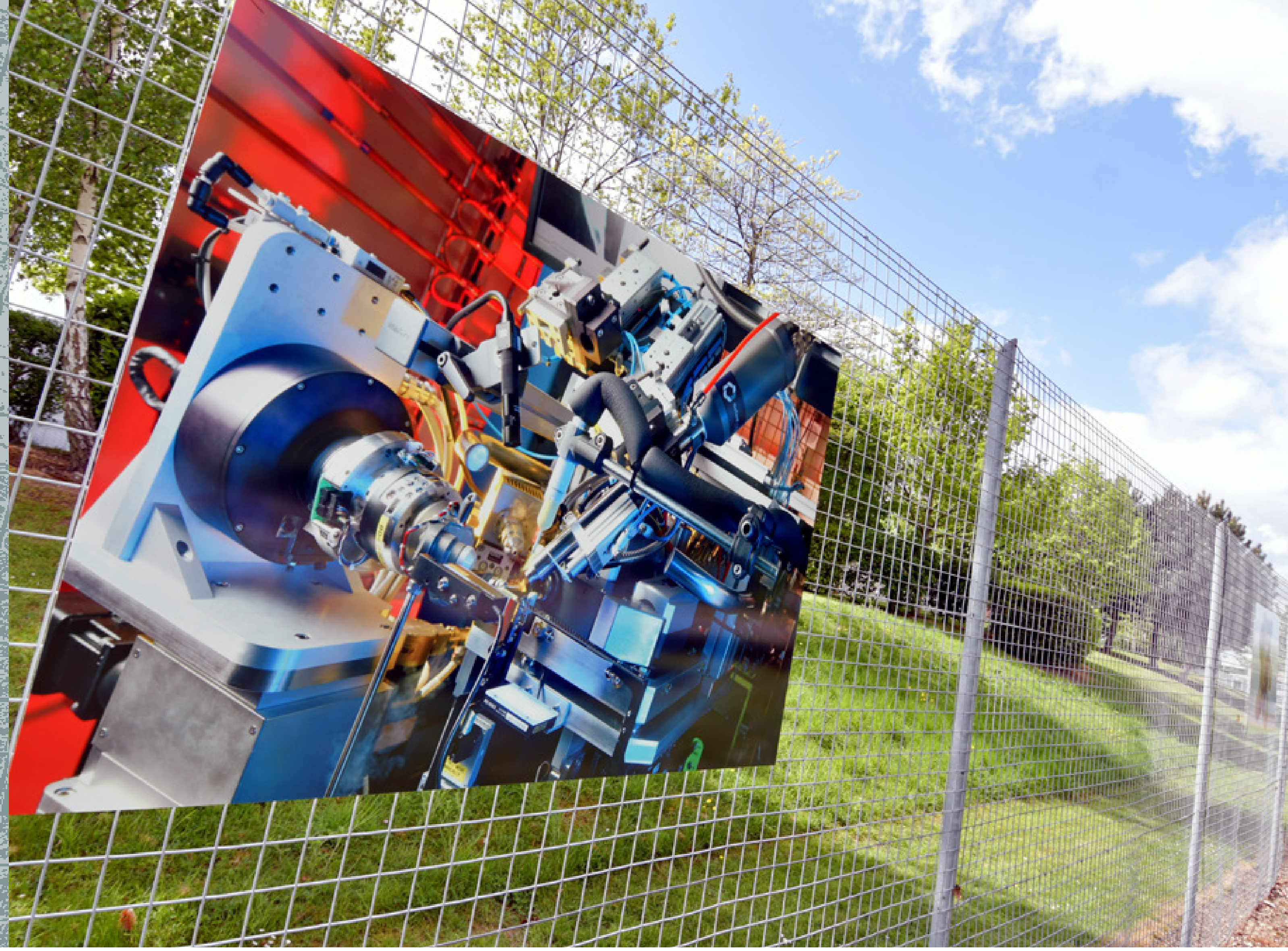
Work Experience student 2022.

In addition to the annual Schools/College Work Experience week, we also ran a special one-off project with a small group of students trailing the functionality and capabilities of Diamond's Visible Synchrotron Radiation (ViSR) beamline, a resource developed to allow visitors to interact with visible synchrotron light and carry out simple experiments. The students joined us for 3 days and worked together to ensure ViSR is fully functional and ready to be used for future engagement activities.

> *The project opened my eyes to how science as a whole is conducted. It was fascinating to learn exactly what happens in and around Diamond.*

> *It was a good way to visualise areas we learn in school and it is nice to see theory applied in the real world.*

Students taking part in the ViSR Project.



Diamond has continued its commitment to widening participation and dedicated more efforts towards community engagement, working with groups such as the Amos Bursary, Science Oxford, Science Together, the Careers Transition Partnership and the Social Mobility Foundation, delivering/supporting outreach activities in a variety of formats to audiences with lower science engagement.

In 2022 Diamond celebrated its 20th anniversary and 15 years of research and innovation, and to help commemorate the occasion we presented to the public a special exhibition of selected photographs from throughout Diamond in an outdoor photographic exhibition. The images circumnavigated the "ring" of the synchrotron along the perimeter fence and gave a behind-the-scenes insight into that goes in inside our iconic building. The exhibition formed part of the wider Oxfordshire Artweeks festival, highlighting our work to the community in an accessible format.

Higher Education Engagement

Our work with students at both undergraduate and postgraduate level continues to play a vital role in Diamond's wider mission to be a world-leading centre for synchrotron science and to keep the UK at the forefront of scientific research. Our student-dedicated programmes aim to welcome and harness the talent, curiosity and development of students both at undergraduate and postgraduate level and provide them with exciting opportunities to encourage and nurture a career in STEM, ultimately contributing to the wider skills agenda in the UK.

In 2022, 23 joint-PhD students joined Diamond as part of our 2022 PhD cohort. These doctoral projects are linked with 16 universities and other world leading facilities, and we have been able to welcome the majority of them on an individual basis here at Diamond. This brings the total number of active Diamond PhD Studentships to 109. We received 62 submissions for our 2023 Diamond Doctoral Studentship call for proposals, which were linked with 32 different universities and institutions. Following the internal review process, we will be welcoming 26 students in October 2023.

This year, we held a PhD Development Days Event, open to all our jointly funded students. It was a 2-day event with a networking dinner on the first day. Day 1 was career focused with talks from a range of different areas from those still in the scientific field through to publishing, patents and government. We were thrilled to have three Diamond PhD alumni talk as part of the careers panel. Day 2 focused on personal resilience development for the PhD students, aiming to engage students to step back, train their personal resilience and start a process of identifying their professional purpose. We had 31 PhD students attending the event overall.

A student commented:

> *I very much enjoyed the Development Days, not only was it useful to hear talks from people from different careers, it was also valuable to be able to network and chat with other students in the evenings.*

The 2021 Year in Industry cohort finished their placements in September, and we were able to have their final poster session and presentations in person, giving wider Diamond staff the opportunity to gain insight into their research, any challenges and results during their 12-month placement.

> **Doing a year in industry at Diamond Light Source provides a life-changing opportunity for any undergraduate student, and a massive stepping stone onto the career ladder. This paired with an amazingly supportive student engagement team, and a strong community between the year in industry students makes the 12 months that you'll spend here fly by!**

We were pleased to welcome 12 new Year in Industry students as part of the 2022 cohort intake in September and to have them in-person and on-site at Diamond. Since starting the 2022 cohort have been busy progressing their projects, completing various training including Scientific Communications, Peer Reviewing and Presentation Skills as well as getting involved with wider outreach activities.

In June 2022, we welcomed our 12 Summer Placement students. As restrictions had been fully lifted, we were delighted to have the cohort working fully in-person and on-site at Diamond. The projects spanned life and physical sciences, engineering and software computing. After a summer of work experience, training and networking, the students presented their results to staff via a poster event in the Atrium and end of project presentations.

Due to the lifting of COVID restrictions, Diamond was once again able to welcome undergraduate and postgraduate students in person to Diamond, where we offered a range of talks and training. We welcomed 452 students for this type of visit, which is comparable to pre-pandemic levels.

Scientific workshops and conferences

Diamond organises a broad portfolio of scientific and technical workshops, training courses and conferences tailored towards the needs of our staff and user communities. In 2022, we hosted 38 events and engaged with 2,890 scientists and engineers from all over the globe.

In August 2022, Diamond hosted the 12th International Conference on Inelastic X-ray Scattering (IXS2022). The conference was held at the SAID Business School in the city of Oxford. Taking place over five days, we welcomed international experimentalists and theorists interested in the use and development of both Resonant and Non-resonant Inelastic X-ray Scattering to address a broad range of materials science challenges.

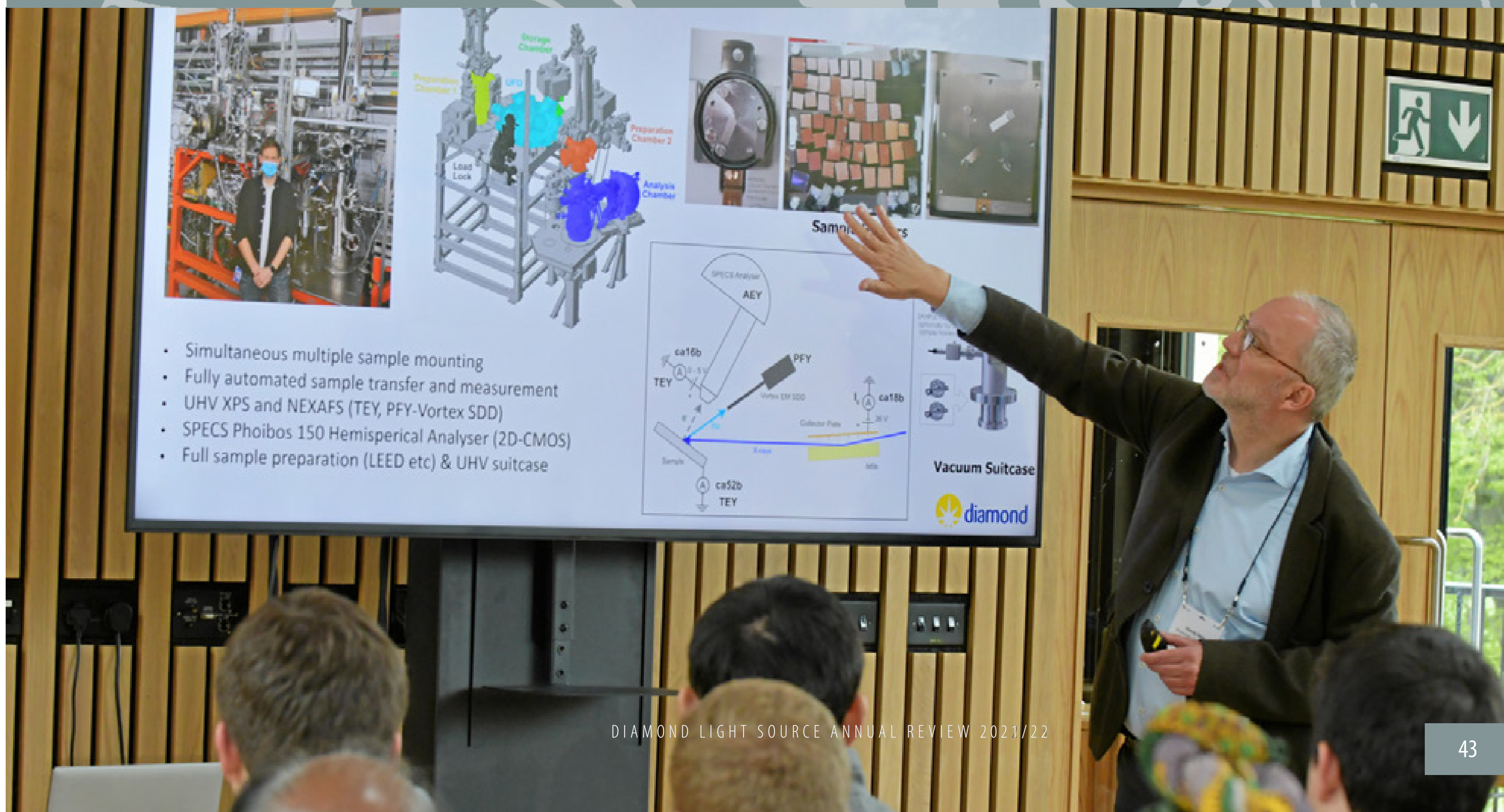
In the autumn, we hosted the 6th edition of our Early Career Scientists Symposium. This annual event featured talks from eminent speakers such as Nobel Prize winning biochemist Prof. Jennifer Doudna and theoretical physicist, author and broadcaster Prof. Jim Al-Khalili. The symposium was by far the most popular event of the last 12 months and brought together over 800 junior scientists looking for inspirations to shape their future careers.

Amongst many workshops and user training opportunities, we moved into 2023 with events focused on boosting national and international collaborations. These included the annual Lightsources.org event, which focussed on the capabilities and career opportunities at 4th generation light sources, and the CONEXS Conference, which highlighted x-ray spectroscopy to achieve new levels of understanding, especially for the interpretation of experimental data.

With an eye on the future and the prospect of the Diamond-II upgrade on the horizon, we also ran a series of scientific workshops to directly engage with our academic and industrial user communities to explore how Diamond-II can best support research and innovation.

Our 2022 Year in Industry Cohort after completing their two-day Presentation Skills Workshop, held at Cosener's House in Abingdon, March 2023.

CONEXS 2023



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