Diamond Light Source Ltd

2020/21

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Foreword

It has been a challenging year for all over the past 12 months. The COVID-19 pandemic has led to big changes all over the world, some temporary and some permanent. It is tragic that the pandemic has led to over three million deaths worldwide. Such an event highlights the importance of not only scientific research, but also collaboration; working together and supporting each other to get through a global crisis.

Diamond’s response to the pandemic has been all encompassing, from playing a key part in global research efforts to setting up robust and comprehensive safety measures on-site to supporting the local community by producing 3D printed visors for health workers. Adjustments have been made by all teams to enable remote working and remote use of nearly all microscopes and beamlines. As this review goes to press, the Government’s roadmap to bring the UK out of lockdown is on track and users are expected to return to the facility in limited numbers in the summer.

Research into SARS-CoV-2, the virus that causes COVID-19, became Diamond’s focus at the start of the pandemic. Combining state-of-the-art microscopes and beamlines, and staff and user expertise, Diamond can delve deep inside the inner workings of the virus. Understanding how it operates at the cellular level will open the doors to real possibilities of solutions and therapies. As we look towards the second half of 2021 and beyond, we can hope for a more positive landscape thanks to the many efforts, including Diamond’s, towards creating vaccines to help protect us against COVID-19.

Plans for the Diamond-II Programme, an integrated upgrade of the synchrotron, beamlines and computational facilities, are progressing well and are at the Outline Business Case stage. As social restrictions continue to lift, Diamond hopes to return to a more normal mode of operation and continue to be a world-leading centre for synchrotron science.

Professor Sir Adrian Smith
Chairman of the Board of Directors

CEO Welcome

A year on from the outbreak of the pandemic, a war is raging against the world: a new kind for our generation but a war that science can help win! At Diamond Light Source, we have kept operational throughout 2020 at varying levels, from COVID-19 related research only for the first quarter of the financial year to remote only experiments on all beamlines. It has obviously been challenging to welcome back users, although summer 2020 and early autumn attempts were successful. I was deeply impressed with the commitments of members of our staff mapping the virus at unprecedented scales, looking at targets to find possible roads to the development of therapeutics. I also commend all the people involved in other disciplines who remained focused on getting experiments delivered with users on the other side of a videoconference, together with all staff who worked so hard to keep operations going under very challenging circumstances.

The many COVID-19 related research projects that Diamond is working on are also a great demonstration of the powerful synergy between Diamond and its neighbouring research institutes, the Research Complex at Harwell and the Rosalind Franklin Institute. Diamond is working with its valued users and many partners to look at the fundamental interactions of the virus, from which it is hoped new therapies can be developed. Over 60 projects are enabling the study of how existing drugs, that have already been tested and approved for other diseases, can be repurposed and used to treat patients. The array of specialised tools and instruments at Diamond, along with the scientific and technical expertise of its staff, allow for many different techniques to be used, from looking at the structure of the virus and fitting drugs into it, like a tiny jigsaw puzzle, to taking direct images of the virus without its infectious component, making it possible to see how it interacts with potential drug chemicals.

Diamond also stole the headlines with the first paper on the study of the 3.67 million years old skull of the 'Little Foot' hominid, reaping over 168 pieces of media coverage and amounting to an estimated 10.2 million views of the story and, as you can imagine, driving great traffic to our website and blowing all records on social media!

We closed the year with another big project that is about to be published with our Socio-Economic Impact Study report where Technopolis, who carried out the assessment, estimated that Diamond has so far (2007-2020) had a cumulative, monetised impact of at least £1.8 billion, based on the evidence captured at this relatively early phase of the facility's operations. Bearing in mind that not all activities, outputs and outcomes could be monetised at this stage, this already compares very positively with the £1.2 billion investment in the facility (which includes all capital expenditure and operational costs so far). Of this total, 86% comes from UK taxpayers, with around £1 billion in investment from the Government via UKRI's Science and Technology Facilities Council (STFC), and 14% from the Wellcome Trust.

Diamond has wider societal benefits that it has not been possible to monetise. These include:

- 80,000 visitors reached so far through a programme of engagement at the heart of the facility supporting the UK Skills' agenda in science, technology, engineering and mathematics (STEM).
- Some of the leading scientific questions of the day being investigated by its 14,000-strong user community, with a part to play in 21st century challenges, from new technologies and environmental remediation to health and well-being.
- Widespread awareness of the value and relevance of STEM subjects to our everyday lives through many news articles and outreach activities.

In early 2021, Diamond celebrated its 10,000th publication with lead author Dr Jessica Wade from Imperial College London. The *Nature Communications* paper presented disruptive insights into chiral polymer films, which emit and absorb circularly polarised light, and offers the promise of achieving important technological advances, including high-performance displays, 3D imaging and quantum computing. This could fundamentally change the technology landscape by enabling a new generation of devices and is a great example of the amazing physical sciences being delivered with our instruments.

The Diamond-II Programme, an integrated upgrade of the synchrotron, beamlines and computational facilities, critical to maintaining our world-leading status, has progressed. Led by the Diamond-II Programme Director, Dr Laurent Chapon, and many staff, we have been working hard on the plans for the upgrade, and this is now leading to a formal Outline Business Case (OBC) for submission to the UK Government. We were pleased to have already received, after an independent reviewing process, an early indication of support from the Wellcome Trust subject to UKRI STFC's approval of the Programme. We are under no illusion that the fight for funding from all quarters will be fierce, and that the impact of the pandemic on our economy will be felt for decades to come; but I remain optimistic that the great science we have delivered over the past 14 years of operations sets us and our user community apart as a priority.

In the last financial year, we received 1,675 proposals for experiments on our instruments via peer reviewed access routes, requesting a total of 18,465 shifts. After peer review, 801 proposals were awarded beamtime. This resulted in 7,759 experimental shifts being awarded across 33 beamlines and 10 electron microscopes. We welcomed 488 on-site user visits from academia across all instruments, with an additional 4,473 remote user visits. The machine continues to perform to a high standard with 96.2% uptime and 132 hours mean time between failures (MTBF). Diamond also provides services critical to industry in the UK, with over 180 companies making use of the facility since operations began, normally paying £2.5 to £3 million per annum for proprietary access. We managed to switch all our engagement with the public to online, creating a dedicated site for our coronavirus research, along with many animations explaining how the science takes place and what is being uncovered about this devastating virus. In addition, during the past year Diamond has had approximately 6,161 significant interactions (30+ minutes) with 'virtual' visits from school students and members of the public, and we saw a 57% increase in attendance across our 33 virtual scientific and technical events this year. Likewise, our Student Engagement programme has continued to thrive despite pandemic restrictions, as we welcomed our 2020 Year in Industry and PhD cohorts in September and October respectively, and currently support a total of 116 studentships, at both undergraduate and PhD level, with our 2021 cohorts due to start later this year.

The past year also opened our eyes to more flexible working in certain areas, with always at the forefront of our minds, the importance of good internal support that ultimately sets us apart to deliver the best for our user community. I am grateful to all our staff and contractors who worked so hard to keep us going through these unprecedented times. As the financial year closes, we look forward to 2021-22 as we will be laying the foundations for a double anniversary again. In 2022 we will celebrate 20 years since the creation of the company and 15 years of innovation through the research we do and much more!

Professor Andrew Harrison OBE
CEO Diamond Light Source

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 the Wellcome Trust, owning 86% and 14% of the shares respectively. Diamond now employs 775 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.

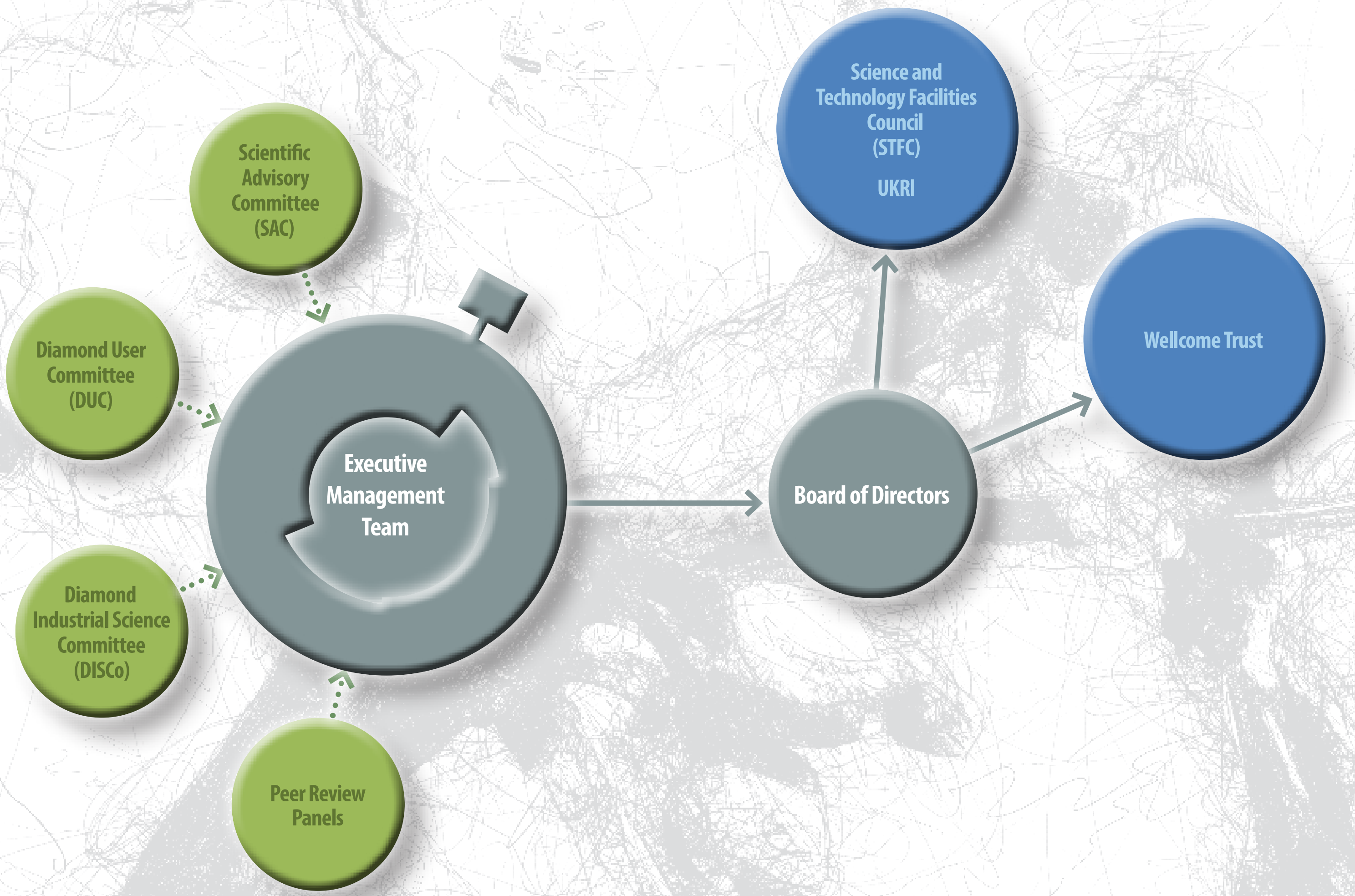
Peer Review Panels: Assess scientific merit of proposals to use the synchrotron and provide recommendations to Diamond Management on the allocation of beamtime to each project.

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.

The Wellcome Trust: 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
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

Summary of Financial Data

	2009/10	2010/11	2011/12	2012/13	2013/14	2014/15	2015/16	2016/17	2017/18	2018/19	2019/20	2020/21
Operating Costs £m	30.5	33.5	36.5	39.9	42.5	44.5	54.6	56.9	62.8	64.5	65.7	69.2
Total Staff (Year End)	401	419	438	481	507	534	582	609	639	680	742	775
Capital Expenditure – Operations £m	5.7	8.6	5.1	8.0	7.5	6.2	8.0	10.5	12.8	17.4	17.8	24.1
Phase II £m	22.0	16.2	9.9	2.8	0.8	0.2	0.0	0.0	0.0	0.0	0.0	0.0
Phase III £m	0.3	3.0	10.3	14.2	17.2	23.7	20.6	11.5	3.7	1.0	0.0	0.0
Other capital projects £m						4.8	5.6	7.3	4.3	5.3	1	2.1

Figures up to and including 2014/15 exclude VAT, thereafter figures include VAT.

Rising to the Challenge of COVID-19

In March 2020 the urgent priorities for researchers were to learn more about SARS-CoV-2, the virus that causes COVID-19. A structural understanding of the virus was critical for developing vaccines and treatments, and Diamond Light Source's facilities would become crucial tools for researchers.

Over the past few years, Diamond has been developing technology and software for highly-automated, high-throughput beamlines. This allows more experiments to be run remotely, with users sending samples to Diamond rather than visiting. This became Diamond's standard way of working during the pandemic, with beamtime reserved for research related to COVID-19. Diamond allocated beamtime via a new COVID-19 specific rapid access route, and more than 60 projects have benefited from expedited access in the last year.

The many COVID-19 related research projects are a great demonstration of the powerful synergy between Diamond and its neighbouring research institutes. The COVID-19 research taking place at Diamond can be loosely grouped into five major strands.

Understanding the virus structure and function

By August 2020, an international team of researchers had discovered a new site on the SARS-CoV-2 virus that could be neutralised by a specific antibody. Using the Electron Bio-Imaging Centre (eBIC) at Diamond, and working with a group at a hospital in Taiwan, the team identified antibodies from a convalescent patient with potential for a drug target.

In November 2020, a research group led by Peijun Zhang, Director of eBIC, published the results of their investigation of the virus replication and showed the profound cell changes caused by infection. This enabled modelling of genome replication, virus assembly and egress pathways, which was critically important to help combat COVID-19. Diamond then created a detailed scientific animation showing how the virus infection mechanism works at the cellular level. This was the first time the virus had been depicted in this way, showing in detail how the virus infection mechanism operates.

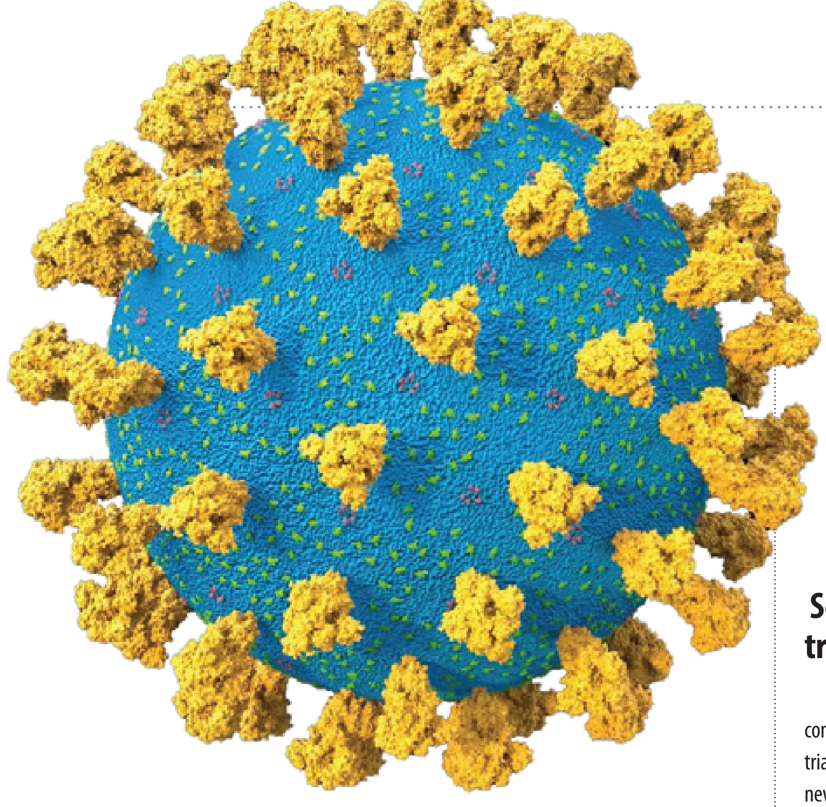
In March 2021, a study reported results from a large cohort of COVID-19 patients. X-ray crystallography and cryogenic electron microscopy (cryo-EM) at Diamond allowed an international research team to visualise how antibodies interact with and neutralise the virus. The study provided a basis for understanding the effect on antibody neutralisation of mutations in several of the variant viruses which are now a cause for concern around the world.

Vaccine design

In April 2021, eBIC published the first images of cells exposed to the Oxford-AstraZeneca vaccine and supported the use of modified adenovirus in the vaccine as a leading platform to combat COVID-19. The challenge now is to stay ahead of the mutations, and the race is on to understand the consequences of these changes and to develop new vaccine constructs tailored to the variants. Ongoing studies are providing valuable new information on how previously infected or vaccinated individuals respond to new variants and antibodies.

New drug development

To defeat the virus, a combination of vaccines and treatments will be needed for people who become infected. An attractive drug target is the so-called main protease of SARS-CoV-2. This protein is essential for viral replication. Work initiated in the Walsh Group at Diamond in January 2020, in collaboration with the von Delft Group, inspired a novel crowd sourcing initiative led by PostEra Inc – the COVID Moonshot, established to develop an effective antiviral more rapidly than ever before. The project crowdsourced designs of new inhibitors from chemists around the world who were using the Diamond 'fragment' data, which had been released in real-time to enable worldwide collaboration and rapid progress. Promising compounds were synthesised and tested for antiviral activity and toxicity. This is ongoing drug discovery work.



By the end of March 2020, a massive fragment screening effort to develop an antiviral targeting the SARS-CoV-2 main protease had identified potential ways to rapidly design improved and more potent compounds in the fight against COVID-19. The team combined mass spectrometry with Diamond's XChem facility to rapidly identify lead compounds for drug development to treat the disease.

Six SARS-CoV-2 proteins have now been subjected to fragment screening at Diamond. One of these protein drug targets forms part of another SARS-CoV-2 protein essential for viral replication, and was targeted by a collaboration of researchers. They focused on a specific protein domain, known as the macrodomain, that is an attractive target for drug discovery. Previous research has shown that without a functioning macrodomain, coronaviruses are unable to replicate in human cells. This work is thus foundational for preparing for future pandemics.

Developing new therapies

Critically ill patients with COVID-19 given a transfusion of serum from convalesced individuals, who have antibodies against the virus, greatly improves their chances of survival. However, a lab-based product that can be made on demand would have considerable advantages and could be used earlier in the disease where it is likely to be more effective.

In July 2020, researchers showed that antibodies derived from llamas could neutralise the SARS-CoV-2 virus in lab tests. Using advanced imaging at Diamond and Oxford, the team also showed that the antibodies bind to the spike protein in a new and different way to other antibodies already discovered. These antibodies – known as nanobodies due to their small size – could eventually be developed as a treatment for patients with severe COVID-19.

Screening existing drugs as potential COVID-19 treatments

Developing new drugs is a long and costly process. However, more than 15,000 compounds have been approved and extensively tested for human safety in clinical trials or regulatory pre-clinical safe studies. In March 2020, Diamond launched a new initiative with Exscientia and Scripps Research to accelerate the path to clinical trials for potential COVID-19 antiviral treatments and applied biosensor platforms to screen a number of clinical drug molecules against several viral drug targets of SARS-CoV-2.

Beyond the science

Diamond is a world-class science facility, but is also a community. In March 2020, Diamond's staff joined an initiative to create stocks of 3D printed visors for local health workers. A team used 20 3D printers to make over 1,000 visors a week. Visor parts were brought to Diamond for sterilisation and packing before distribution. By June, the effort had produced more than 10,000 visors, filling the gap until commercial production could meet demand.

Diamond started offering PCR tests for staff working on-site to quickly identify any infected individuals and trace their contacts, preventing COVID-19 from spreading. This and other protective measures gave staff the confidence that working at Diamond was as safe as possible. Lateral flow tests were also provided for visitors.

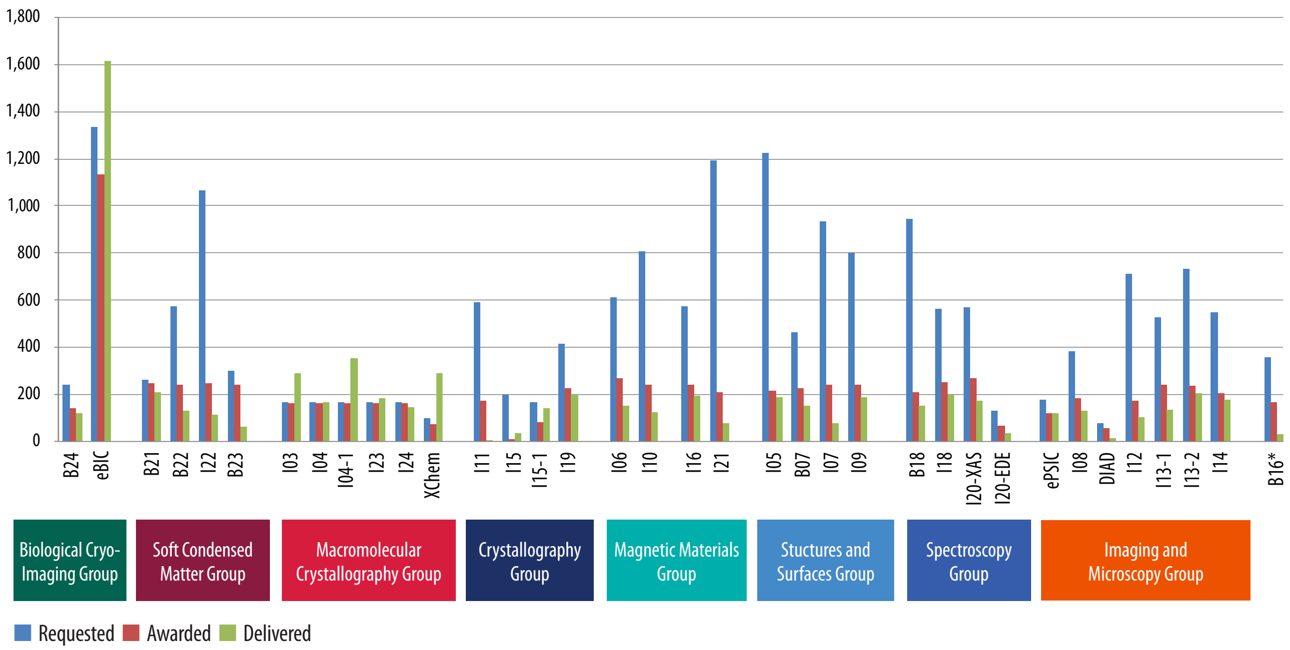
Diamond was able to run for four or five days each week during the first year of the pandemic, although not all of the beamlines were operational. Moving our programme of public events online has allowed us to continue engaging with the public, in a year in which the contribution of science to humanity's future has never been more prominent.

Key Facts and Figures

Facility usage

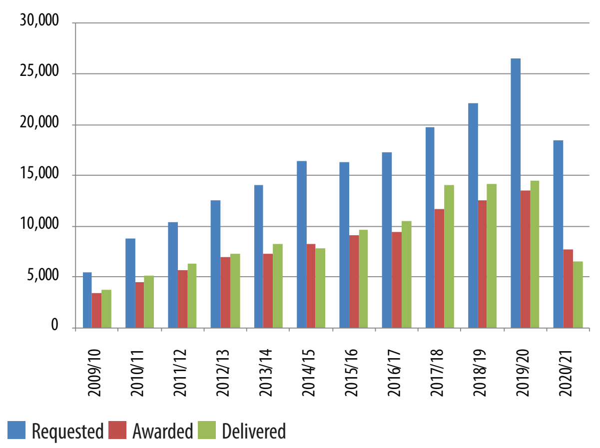
Our fourteenth year of operations (1st April 2020 to 31st March 2021) was affected by the COVID-19 pandemic. With weekly operating hours reduced to four days, there was less experimental time available and the user programme was adjusted as a result. There was a limited call for proposals (for three months and for the physical sciences only) in that period, which had an impact on the number of submitted and awarded proposals, as well as the number of awarded shifts. We received 1,675 proposals for experiments on our instruments via peer reviewed access routes, requesting a total of 18,465 shifts. After peer review, 801 proposals were awarded beamtime. This resulted in 7,759 experimental shifts being awarded across 33 beamlines and 10 electron microscopes. We welcomed 488 on-site user visits from academia across all instruments, with an additional 4,473 remote user visits. Since March 2020, Diamond Light Source has been offering priority rapid access for groups who require instrument time for projects directly related to SARS-CoV-2 viral proteins. The machine continues to perform to a high standard with 96.2% uptime and 132 hours mean time between failures (MTBF).

User shifts requested, awarded and delivered by group, beamline and electron microscope 2020/21

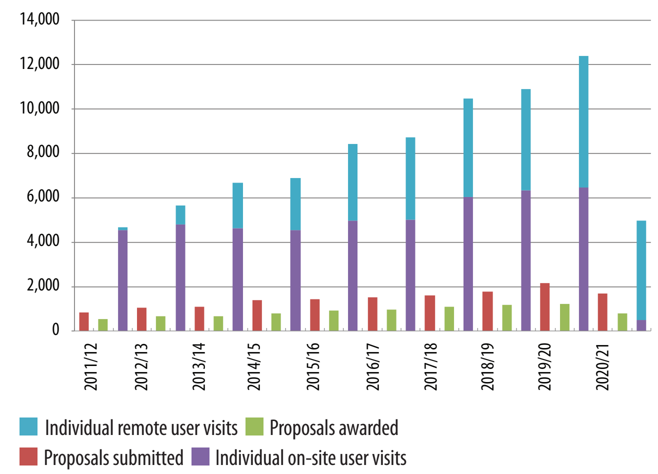


* B16 is the Test beamline, with 50% of beamtime for users. The rest is used for in-house developments for all beamlines.

Total user shifts requested, awarded and delivered



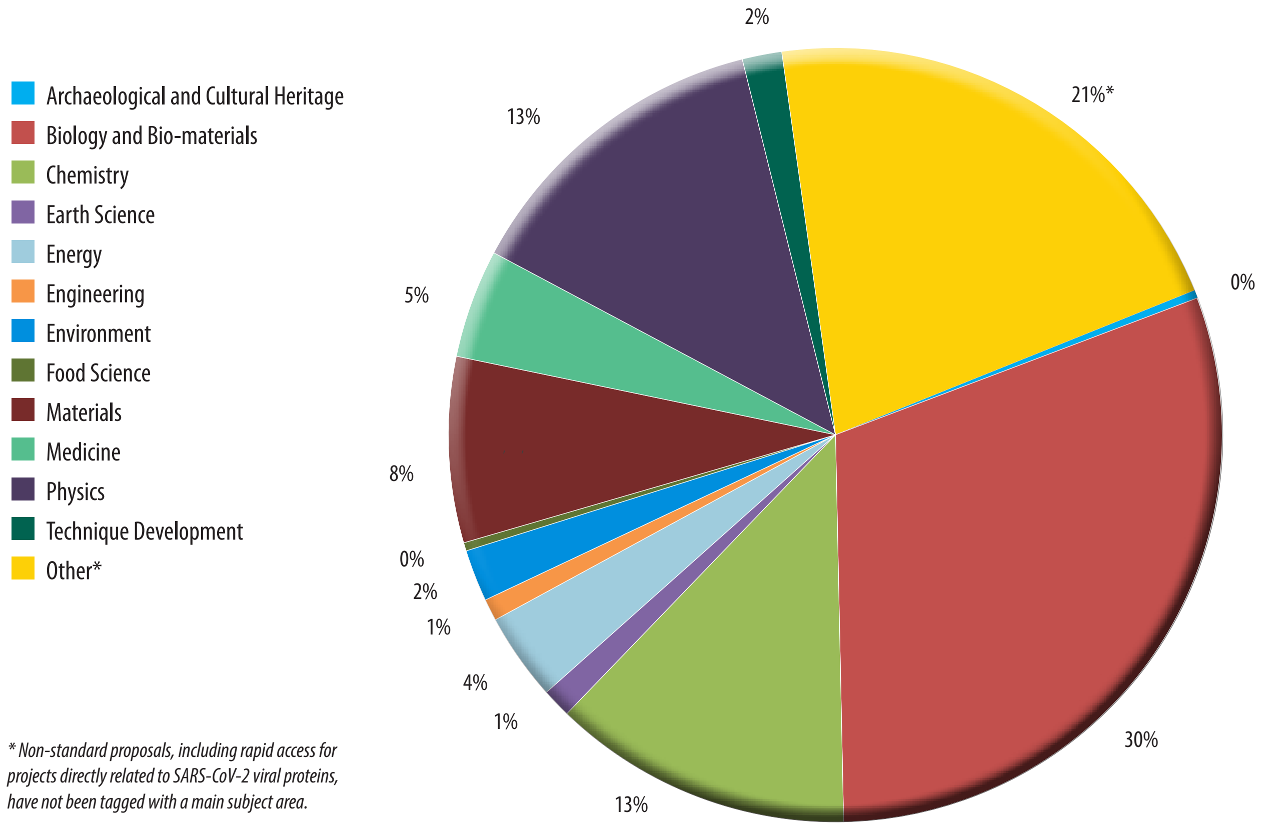
Total numbers of proposals and users per year



Members of staff visiting as part of peer reviewed access routes are included in the count for user visits. In-house research is excluded from this report.

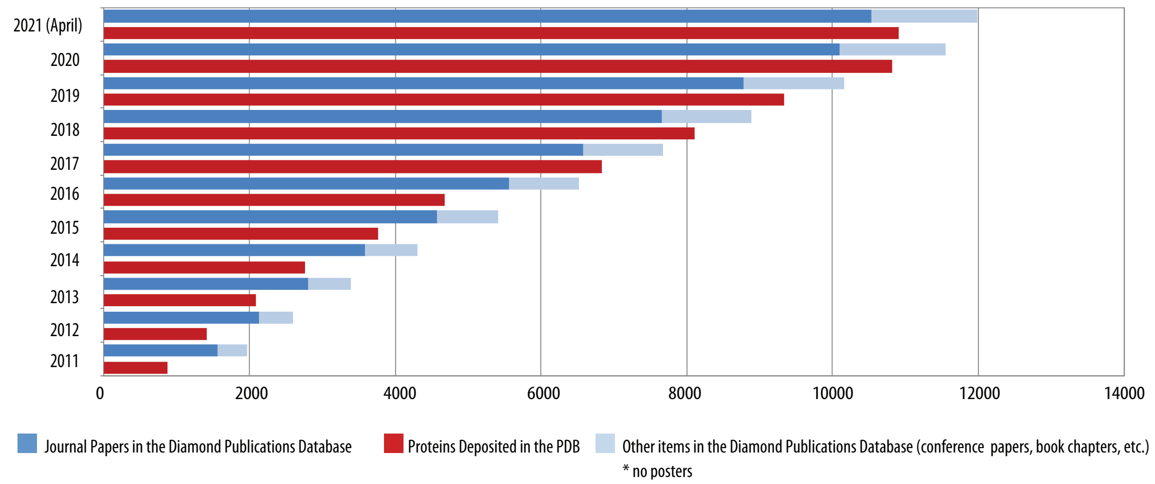
Proposals by discipline and research theme

Experimental shifts scheduled by Diamond by main subject area for 2020/21



** Non-standard proposals, including rapid access for projects directly related to SARS-CoV-2 viral proteins, have not been tagged with a main subject area.*

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



Machine performance

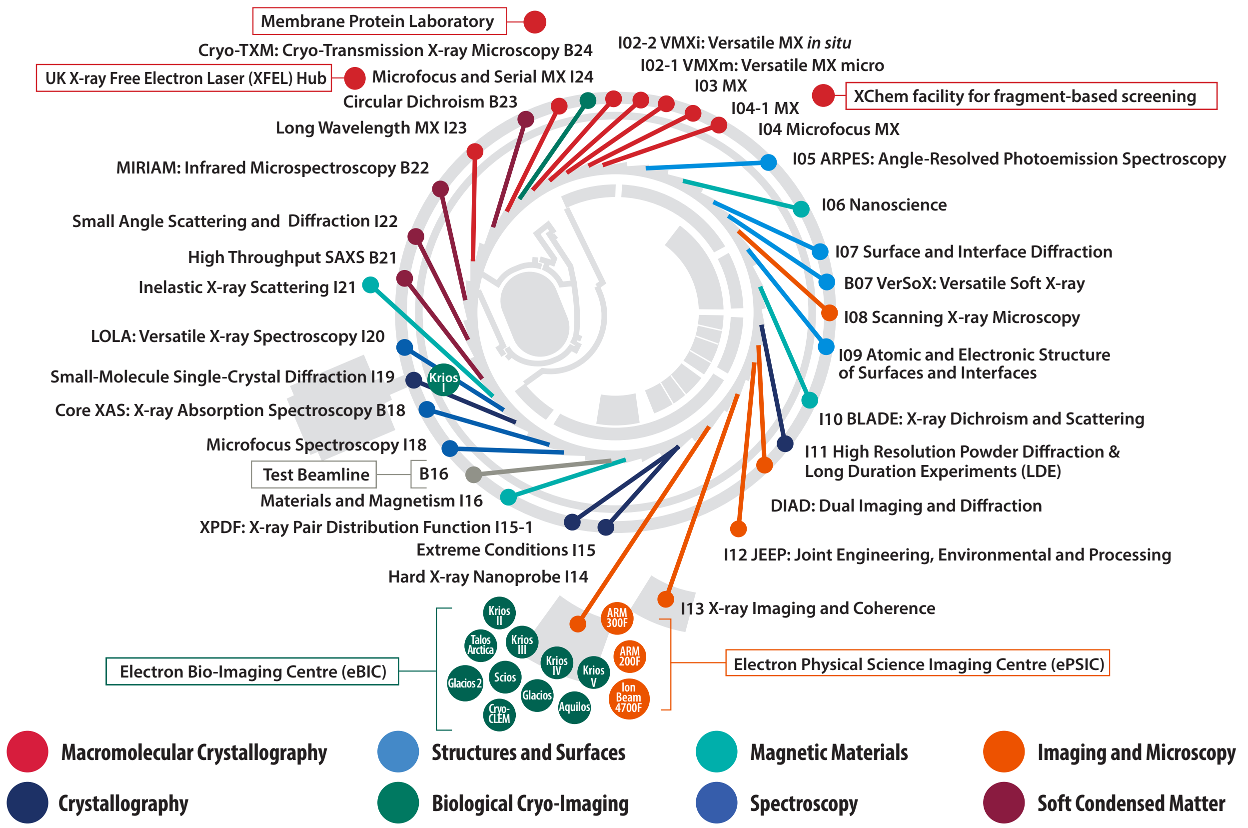
	2009/10	2010/11	2011/12	2012/13	2013/14	2014/15	2015/16	2016/17	2017/18	2018/19	2019/20	2020/21
Total no. operational beamlines by end FY	17	19	20	22	24	25	26	28	31	32	32	33
Scheduled hours of machine operation	5712	5808	6000	5832	5976	5808	5928	5688	6072	5904	5913	6120*
Scheduled hours of user operation	4728	4728	5064	4872	5088	4944	5040	4584	5160	4992	4992	5088*
Machine uptime %	97.0	97.5	97.7	98.3	98.2	97.6	97.6	98.7	98.2	98.4	98.1	96.2
Mean time between failures (hours)	26.2	28.5	55.4	52.4	60.3	38.6	119.4	103.1	79.9	90.3	104.7	132

** The number of machine and user operation hours delivered was reduced to 4345 and 3445 respectively, as a result of the pandemic.*

Beamline Development and Technical Summary

In its fourteenth year of experiments, Diamond Light Source is now operating with 33 beamlines and 14 electron microscopes. This year saw the DIAD beamline welcome first users, with experiments carried out remotely in February 2021 due to COVID-19 restrictions at Diamond. Of the electron microscopes, 11 are cryo-electron microscopes specialising in life sciences and make up eBIC (Electron Bio-Imaging Centre), with two provided for industry use in partnership with Thermo Fisher Scientific. The three remaining microscopes dedicated to advanced materials research are supplied by Johnson Matthey and the University of Oxford. These microscopes 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) and the XChem fragment screening 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 Industrial Liaison Office.

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	Cryo-EM, Cryo-ET	80, 120, 200, 300 kV	Operational since 2018
Talos Arctica	Cryo-EM, Cryo-ET	200 kV	Operational since 2016
Glacios	Cryo-EM, Cryo-ET	200 kV	Operational since 2019
Glacios 2	Cryo-EM, Cryo-ET, MicroED	200 kV	Operational since 2021
Scios	Cryo-SEM, Cryo-FIB	3 to 30 kV	Operational since 2017
Aquilos 2	Cryo-SEM, Cryo-FIB	3 to 30 kV	Operational since 2019, updated to Aquilos 2 in 2020
Leica cryo-CLEM	Cryo-CLEM	n/a	Operational since 2021
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 2021

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	Commissioning
I02-2 - Versatile MX *in situ* (VMXi)	*In situ* microfocus macromolecular crystallography, Serial Synchrotron Crystallography	10 - 25 keV	Commissioning
I03 - MX	Macromolecular crystallography (MX), Multiwavelength Anomalous Diffraction (MAD) , Containment Level 3 (CL3) capable	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	250 - 2800 eV	Operational
	Branch B: NEXAFS and High-Throughput XPS	50 - 2200 eV	Commissioning
I08 - Scanning X-ray Microscopy	Scanning X-ray microscopy, NEXAFS/ XANES, X-ray fluorescence	I08 branch: 250 eV - 4.4 keV	Operational
		J08 - Soft and Tender X-ray Ptychography branch: 250 - 2000 eV	Optimisation
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	6 - 25keV (0.5 - 2.1 Å)	Operational
DIAD: Dual Imaging and Diffraction	Simultaneous imaging and diffraction	8 - 38 keV	Optimisation
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 (under development)	53 keV - 150 keV monochromatic or continuous white beam	Operational
I13 - X-ray Imaging and Coherence	Phase contrast imaging, tomography, full-field microscopy, grating interferometry, (Diamond-Manchester Imaging branchline); ptychography combined with fluorescence and tomography, Bragg-coherent diffraction and imaging, innovative microscopy and imaging (Coherence branchline)	Imaging branch: 8 - 30keV Coherence branch: 7 - 20keV	Operational
I14 - Hard X-ray Nanoprobe	Nanofocus X-ray fluorescence (XRF), X-ray absorption spectroscopy (XAS), differential phase contrast (DPC), transmission diffraction (XRD), and ptychography for 2D and 3D imaging	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 - 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.	7 - 20 keV	Operational
B22 - MIRIAM: Multimode InfraRed Imaging And Mircrospectroscopy	Fourier Transform IR (FTIR) microscopy & Focal Plane Array (FPA) imaging FTIR and THz spectroscopy NEW: Nanospectroscopy FTIR via Atomic Force Microscopy (AFM) IR and scattering Scanning Nearfield Optical Microscopy (s-SNOM) (commissioning)	microFTIR: 5,000-500cm^{1}(2-20μm) FTIR/THz: 10,000-10cm^{1}(1-1000μm) nanoFTIR: 10,000-650cm^{1}(1-15μm)	Operational
I23 - Long Wavelength MX	Long wavelength macromolecular crystallography	2.1 - 11 keV (1.1 - 5.9 Å)	Operational
B23 - Circular Dichroism	Mueller Matrix Polarimetry (MMP) Circular Dichroism (CD) High-Throughput CD (HTCD))	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	6.5 - 30.0 keV	Operational
B24 - Correlative Cryo-Imaging; Soft X-ray Tomography and Fluorescence Imaging	Full field X-ray and laser light fluorescence imaging	Visible spectrum, 200-2600eV	Operational

DIAMOND LIGHT SOURCE ANNUAL REVIEW 2020/21

Macromolecular Crystallography Group

Biological interactions underpin and can undermine the processes of life, as exemplified this year by the SARS-CoV-2 pandemic. The technique of Macromolecular Crystallography (MX) uses X-rays to reveal the details of biological molecules at atomic and temporal scales and is an enabler in our understanding of the processes and interactions of life. Seven beamlines (I03, I04, I04-1, I23, I24, VMXi and VMXm), alongside the XChem fragment screening facility, the UK X-ray Free Electron Laser (XFEL) Hub and the Membrane Protein Laboratory (MPL) at Diamond Light Source are dedicated to exploiting the technique of MX for the benefit of the worldwide structural biology community.

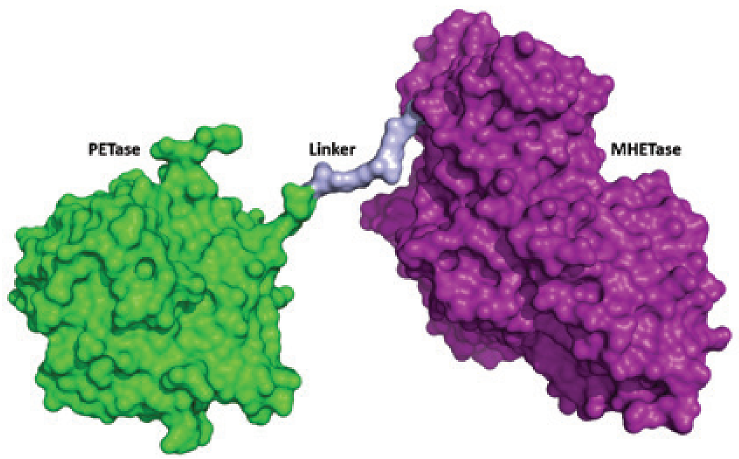
Some of the exciting studies taking place in the MX Group this year have included new insights into key enzymes that can degrade plastics, improved understanding of an anti-tuberculosis therapy, and discoveries in our gut bacteria which could lead to valuable new diagnostic tests for various diseases.

Engineering enzymes to recycle plastics

An international team is continuing its pioneering work on discovery and engineering of enzymes that can help break down plastics for recycling. Previous studies at Diamond Light Source focused on characterising the structure and function of the enzyme PETase, which is able to break down one of the most commonly-polluting plastics, polyethylene terephthalate (PET), that is used for bottles and textiles. The enzyme was isolated from the bacterium *Ideonella sakaiensis*, originally discovered 'feeding' on plastic waste in a Japanese recycling centre. This new study, carried out on beamline I03, studied a partner enzyme called MHETase which is secreted from the same bacterium.

The structures collected from the beamline are at the highest resolution available and provide a detailed insight into the MHETase enzyme. Combined with detailed bioinformatics, biochemistry and molecular simulations, they show a highly synergistic relationship between the PETase and MHETase enzymes. The team investigated if tethering the proteins together could improve the breakdown and demonstrated that this was significantly faster than PETase alone or a PETase-MHETase cocktail. This ongoing research effort adds significantly to the global focus on finding low-energy methods to recycle plastics and to reduce our requirements for fossil resources.

Knott B. C. *et al.* DOI: 10.1073/pnas.2006753117



Developing new anti-tuberculosis drugs

An international group of Chinese, Australian and UK researchers used beamline I04-1 at Diamond Light Source to determine the detailed crystal structure of a mycobacterial complex that provides fresh understanding of the biochemical function of proteins associated with tuberculosis (TB).

The TB bacterium *Mycobacterium tuberculosis* is able to build a complex cell wall to protect and support itself. This cell wall has been a key target for anti-TB drugs. For example, the front-line anti-TB drug ethambutol inhibits synthesis of the bacterial cell wall by targeting certain key proteins. Although this drug has been in use for 50 years, its precise mode of action remains unclear.

The team focused on the action of the EmbC protein which plays a key role in synthesis of the bacterial cell wall. They discovered compelling new information on its binding capacity, showing that ethambutol functions by competing with the substrates for binding to EmbC. These results provide a structural basis for understanding the biochemical function and inhibition of EmbC and for the exciting development of new anti-TB agents.

Zhang L. *et al.* DOI: 10.1126/science.aba9102

Developing diagnostic tests from gut bacteria

New studies on gut flora may have important implications for human health and disease including greater understanding of certain cancers and diabetes.

The microorganisms that live in the human gut have a profound impact on our health. The microbes living in intestinal mucus, a complex network of proteins and attached sugars, act as 'gatekeepers' by maintaining gut barrier function. However, the mechanisms by which they interact with the host remain largely unknown. Researchers investigated *Ruminococcus gnavus*, a common resident of the human gut that has a role in health and disease. They investigated its potential to process the sugar fucose using enzymes called fucosidases. They also explored the pool of fucosidases produced by different *R. gnavus* strains.

Using the Versatile Macromolecular Crystallography *in situ* (VMXi) beamline at Diamond Light Source allowed the team to track their crystallisation experiments in real-time. They were also able to test crystal diffraction quickly and easily, rapidly optimising crystallisation conditions to produce consistent, high-quality protein crystals for X-ray diffraction experiments on MX beamlines I03 and I04.

This new understanding of fucosidases may allow scientists to design new diagnostic assays for diabetes and a number of cancers.

Wu H. *et al.* DOI: 10.1007/s00018-020-03514-x

Biological Cryo-Imaging Group

This 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. The group provides a unique platform for correlative light and X-ray microscopy, as well as cryo-EM.

Studies undertaken this year include new understanding of the structure and function of cytotoxic proteins which protect the body from cancers and infections, pioneering design on new antibiotic therapies, and structure-based design of drugs with reduced side effect profiles.

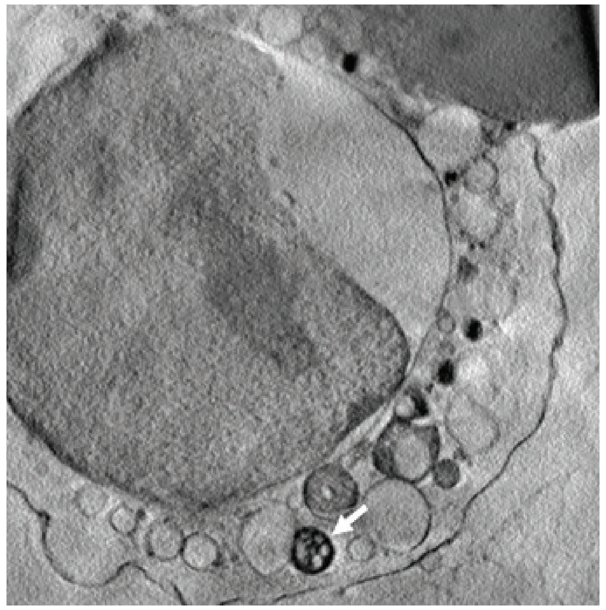


Image from a tomogram of a white blood cell interacting with an electron microscopy grid and highlighting a multicore granule (arrow).

New insights on our immune system

The white blood cells called cytotoxic T lymphocytes (CTL) and Natural Killer (NK) cells are components of the immune system that help cure viral infections and prevent the progression of cancers. CTL and NK cells kill infected cells by secreting cytotoxic proteins (so-called 'protein bombs') onto their surface. An international team of researchers interested in new biological therapies for cancer set out to examine how these proteins avoid dilution and enter target cells.

The team used Diamond Light Source's beamline B24 with low-energy (soft) X-rays to generate 3D maps of organic material in cells and small particles released from cells. Soft X-rays allow imaging of entire T cells, although the resolution is lower than when using high-energy X-rays. The results allowed the team to confirm that the 'protein bombs' are packaged in supramolecular attack particles (SMAPs) which contain more than 280 kinds of protein. They also demonstrated detailed structures and identified potential storage sites for the 'protein bombs' in the T cells. This synchrotron technology shows great promise in the study of cellular structures and how T cells protect the body and can be used to further improve cancer therapies.

Balint S. *et al.* DOI: 10.1126/science.aay9207

Designing new therapies

Bacteria use a wide range of trans-membrane secretion systems to transfer proteins into target cells. These 'bacterial effector proteins' interfere with host cell functions and could have important applications in designing new antibiotics. An international team of researchers worked to understand the mechanism by which *Legionella pneumophila* (which causes Legionnaires' disease) uses a secretion system to infect human cells.

They were able to determine the atomic resolution structure of the system using single-particle cryo-EM with data collected at eBIC at Diamond Light Source. This showed a five-protein core complex which combines with others to form a large nanomachine, containing a channel in the membrane, that protein effector molecules can pass through. Analysis of multiple cryo-EM maps, further modelling and mutagenesis provided working hypotheses for the mechanism of binding and delivery of two classes of *Legionella* effectors.

Gaining a better understanding of how secretion systems work and resolving the high-resolution structure of the *Legionella* secretion system provides essential information to help design antibiotics that block the system and could also provide the basis for engineering secretion systems capable of injecting therapeutic drugs into human cells.

Meir A. *et al.* DOI: 10.1038/s41467-020-16681-z

Designing drugs with reduced side effects

The human body relies on an extensive network of signalling molecules (agonists) such as hormones to coordinate bodily functions. Receptors on the surface of cells bind these hormones and activate a signalling cascade to alter the cell's biochemistry. G protein-coupled receptors (GPCRs) are the largest and most diverse family of these receptors and therefore many therapeutic drugs have been designed to target them.

GPCRs have two signalling pathways (the G protein-coupled pathway and the arrestin-mediated pathway) and, in many cases, one is the therapeutic pathway while the other may produce side effects. If a drug could be developed that could signal only down the therapeutic pathway (a 'biased agonist'), then side effects could be significantly reduced.

To investigate this, an international research team used cryo-EM at eBIC at Diamond Light Source to determine the structure of a GPCR coupled to arrestin and compare its structure to the G protein-coupled state, with the same agonist bound to both receptors. They identified two regions of the GPCR that could be used in the development of 'biased' agonists and the study provides valuable data for structure-based drug design.

Lee Y. *et al.* DOI: 10.1038/s41586-020-2419-1

Structures and Surfaces Group

The Structures and Surfaces Group at Diamond Light Source comprises four beamlines: 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). These 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 focus this year has been on improving the user interface and accessibility for control of experiments to ensure that as many experiments as possible could be carried out remotely by users with the support of the beamline teams on-site. The success of the majority of these studies has been enabled by the strong partnership of the Diamond scientists with the user groups, leading to stronger collaborations and exceptional results. It has continued to be a busy year for beamline developments whilst also taking a strategic view for the future, in particular the important role that surfaces and interfaces play in broader research areas such as battery technology, photovoltaic structures, and catalytic/electrochemical systems under *operando* conditions. Expanding the techniques to these communities remains a key aim for the group.

Recent studies from this group include pioneering approaches in the design and production of renewable solar fuels and organic solar cells and developing new materials for data storage in solid-state electronic devices.

Discovering new catalysts for solar fuel production

In our current era of climate change, intensive international efforts are ongoing to develop carbon neutral processes that exploit renewable resources. One of the most promising areas of research is the production of solar fuels that can be made from common substances such as water and carbon dioxide and then stored for later use. Different photocatalytic materials are currently being used in developing photo-electrochemical cells to perform water splitting (to produce hydrogen and oxygen) or carbon dioxide reduction (to produce hydrocarbons). However, these materials suffer from severe limitations related to charge carrier recombination phenomena and inefficient light harvesting, and the search is on for more sustainable and efficient photocatalysts.

Spanish researchers are investigating the potential of metal-organic frameworks (MOFs) to act as photocatalysts. They used VerSoX (B07) at Diamond Light Source to provide detailed data on the charge dynamics processes and electrical properties in a new bismuth metal-organic-framework (MOF) to produce hydrogen. These studies, combined with spectroscopy, allowed the team to determine the structure of the photocatalyst and the mechanism behind the charge dynamic process and will allow further development of this exciting material.

Garcia-Sanchez A. *et al.* DOI: 10.1021/jacs.9b10261

Designing new high-efficiency organic solar cells

Organic solar cells are a type of photovoltaic cell that use a blend of carbon-based semi-conductor materials to produce electricity from sunlight. They offer the potential of cost-effective photovoltaics with low environmental impact when compared with inorganic cells such as silicon, but not all combinations of organic materials work efficiently, and many have had low efficiency, stability and strength.

Researchers in China and the UK carried out X-ray scattering experiments on Diamond Light Source's beamline I07, combined with other techniques, to explore the device efficiency of a blend of three different organic semiconductors. This so-called 'ternary blend' has the potential to enhance optical absorption, but selection of materials has been challenging.

These new measurements provide critical information on how adding a third component changes the molecular ordering of the blend. The research team were then able to correlate the thin film morphology with the electronic properties of the solar cell. Their results also allow predictions of whether a third component is likely to enhance device efficiency. Their work will help develop high-efficiency solar cells and is another step towards commercialisation of this technology.

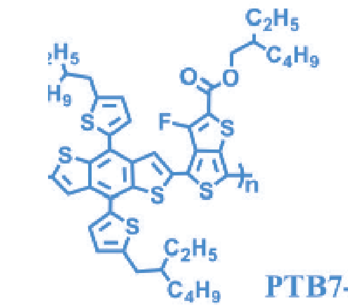
Li W. *et al.* DOI: 10.1063/1.5125438

Developing new materials for data storage

$PdCrO_2$ is a magnetic oxide metal with remarkably high conductivity, which consists of an alternating stack of Pd (palladium) and CrO_2 (chromium dioxide) layers. An international group of researchers wanted to study the unusual electronic properties of this layered lattice material which could have a significant impact on the design of solid-state devices for data storage and transfer. They performed initial studies using Angle-Resolved Photoemission Spectroscopy (ARPES) on beamline I05 at Diamond Light Source and observed some unusual spectral signatures. Theoretical calculations suggested that correlations and interlayer interactions had a significant role in their generation.

To understand the origin of these unusual spectral signatures, the team used the Surface and Interface X-ray Diffraction beamline (I09) to perform ARPES measurements. The combined nature of the study, with closely integrated work on the I09 and I05 beamlines applying different photoemission measurements, was crucial to the success of this work. This novel use of ARPES provides an approach to study materials that are incompatible with other, more conventional probes of spin-spin correlation functions. This potentially opens up new systems to experimental study, and an improved understanding of their magnetic properties will be important for real-world applications such as 2D spintronics.

Sunko V. *et al.* DOI: 10.1126/sciadv.aaz0611



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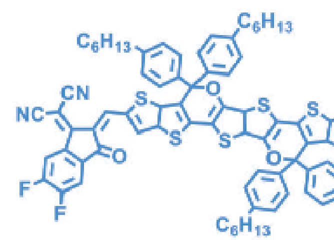

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Magnetic Materials Group

The Magnetic Materials Group at Diamond Light Source uses and develops a range of polarised X-ray probes including Resonant Elastic X-ray scattering (REXS), PhotoEmission Electron Microscopy (PEEM), X-ray Absorption Spectroscopy (XAS) and Resonant Inelastic X-ray Scattering (RIXS). Over the last year, our research community has gained fundamental insights into the electronic and magnetic degrees of freedom underpinning the physical properties of a host of materials using these probes. In this contribution, we present research demonstrating how PEEM can unveil the complex antiferromagnetic domain structure in CuMnAs thin films following intense pulsed electrical switching. We also present results reporting how soft X-ray scattering combined with soft X-ray imaging can reveal the tubular structure of magnetic Skyrmions in FeGe thin films. The versatility of high-resolution RIXS is showcased in a remarkable study of lithium-ion (Li-ion) battery cathodes, demonstrating how metal migration and molecular oxygen formation degrade the charge-discharge cycle. The results demonstrate how polarised X-rays can uncover a wealth of electronic and magnetic detail to aid the development of advanced materials in applications ranging from low-power consumption electronics to next-generation energy materials.

Pioneering the use of antiferromagnets in computing

The field of spin-based electronics (spintronics) is making huge strides in the development of computing and memory storage applications. Traditionally, the orientation of the magnetisation of ferromagnets has been intensively studied, but now researchers are turning additional attention to antiferromagnets due to their ultrafast dynamics, insensitivity to external magnetic fields and absence of magnetic stray fields. However, antiferromagnetism has been challenging to harness for applications.

An international research team investigated the microscale antiferromagnetic order in copper manganese arsenide (CuMnAs) films. Use of PEEM on beamline I06 at Diamond Light Source enabled them to take images of the antiferromagnetic structures in microscale device structures. Electrical contacts on the sample allowed them to probe the magnetic state before and after applying current pulses.

The team showed that the electrical switching and relaxation behaviour they observed can potentially mimic the characteristics of biological neural networks, offering the potential to develop efficient and high-speed neuromorphic computing applications that mimic neuro-biological architectures present in the human nervous system. Because electronic and magnetoelastic fluctuations may accompany the strong magnetic disorder, charge and spin-sensitive imaging with higher spatial and temporal resolution may shed new light on the underlying physics of this effect.

Kaspar Z. *et al.* DOI: 10.1038/s41928-020-00506-4

Understanding the role of magnetic skyrmion tubes in data storage

Magnetic skyrmions are particles that can be found in some magnetic materials with exciting potential applications for data storage in electronic devices. Although skyrmions are typically portrayed as two-dimensional whirl-like objects, they have a vertical, tube-like structure. To date, this three-dimensional structure has not been observed and this would be important for understanding their stability in data storage.

A European research team were able to acquire the first direct observations of magnetic skyrmion tubes. They used the I10 beamline at Diamond Light Source to perform magnetic diffraction measurements on skyrmion material ~100 nanometres thick. The beamline's soft X-ray diffractometer, Reflectivity and Advanced Scattering from Ordered Regimes (RASOR), allowed them to perform the experiment while controlling the temperature of the sample and applying external magnetic fields. These breakthrough results allowed them to acquire images of skyrmions' vertical structure at X-ray imaging beamlines at the SOLEIL and BESSY II synchrotron facilities.

These new insights into the nanoscale mechanisms that govern the formation and destruction of skyrmions is a crucial step in ensuring that any data encoded in the form of skyrmions is not lost when any device is turned off.

Birch M. T. *et al.* DOI: 10.1038/s41467-020-15474-8

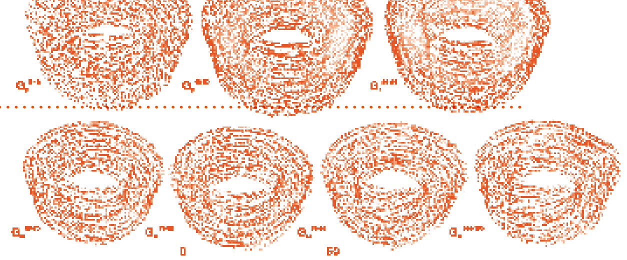
Optimising the efficiency of lithium-ion batteries

Lithium-rich cathode materials are being studied for the next generation of lithium-ion batteries as they potentially carry more charge than conventional cathodes. However, complex changes in crystal structure and a pronounced drop in voltage between the first charge and discharge (voltage hysteresis) could limit their use. Understanding the reversibility of these chemical processes is critical in determining how well a cathode material functions.

Researchers from the University of Oxford and Diamond Light Source used the RIXS beamline (I21) to study the chemical changes to the oxide ions at different stages of the battery charge-discharge cycle. Using high-resolution RIXS, they detected underlying vibrational fine structure that showed the oxidised oxide ions to be molecular oxygen. These oxygen molecules are trapped within the charged cathode material, but they can be reduced back to oxide ions on discharge. However, this process takes place at a lower voltage, giving rise to the voltage hysteresis.

With this increased knowledge, researchers can now devise strategies to suppress the release of oxygen, or prevent its formation, in next-generation lithium-ion batteries with higher energy density. Higher energy density batteries will extend the driving range of electric vehicles and increase the battery life of portable electronics between charges.

House R. A. *et al.* DOI: 10.1038/s41560-020-00697-2



Imaging and Microscopy Group

The Imaging and Microscopy Group at Diamond Light Source brings together eight experimental facilities (I08, J08, DIAD, I12, I13-1, I13-2, I14 and ePSIC, the Electron Physical Science Imaging Centre) which use electrons and X-rays to image samples under different experimental conditions across a diverse range of length scales and time scales.

Studies from the group this year included improving the imaging of Parkinson's disease, new insights into the movement and flow of magma, and optimising the manufacture of nickel superalloys used in the manufacture of high-temperature structural components.

Developing new ways of imaging Parkinson's disease

New synchrotron methods to characterise brain cell loss in Parkinson's disease could provide greater understanding of this disease and other related disorders.

Parkinson's disease involves the loss of a particular group of brain cells that produce dopamine. These cells contain a dark pigment called neuromelanin and post-mortem staging of the disease can be confirmed according to the relative loss of pigment. However, current methods of assessment are limited and often rely on additional chemical staining which constrains further analysis.

Researchers from the University of Warwick used synchrotron X-ray microscopy to visualise neuromelanin without relying on visible pigmentation or chemical staining. They performed spectromicroscopy on Diamond Light Source's beamline I08 using low energy X-rays allowing them to probe the organic structure of neuromelanin, which revealed a characteristic feature in its absorption spectrum. The team used this to create maps of neuromelanin distributions, which matched those observed in stained tissue sections. They also used nanoscale X-ray Fluorescence (XRF) with high-energy X-rays on beamline I14, which showed that neuromelanin could be identified by its elevated sulfur content. These new ways of mapping neuromelanin could hold significant potential for non-destructive studies investigating the relationships between depigmentation, metal binding and neurodegeneration in Parkinson's disease.

Brooks J. *et al.* DOI: 10.1002/anie.202000239

Understanding how magma moves

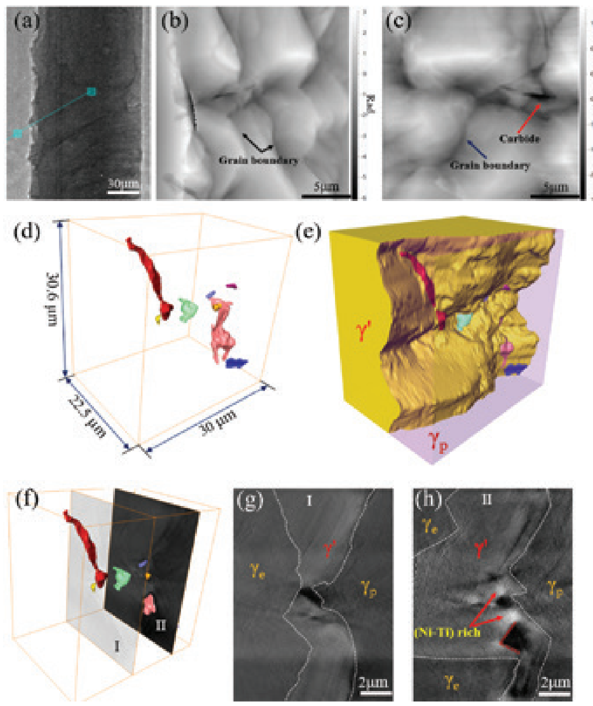
Laboratory-based studies at Diamond Light Source to better understand the behaviour and movement of magma will improve our ability to predict the impact of volcanic eruptions.

Researchers recreated flowing magma using a bespoke high temperature furnace and the XRheo rheological apparatus on the Joint Engineering Environmental and Processing (JEEP) beamline (I12). They used the high-speed X-ray imaging available on the beamline to watch the evolution of magmatic microstructure during flow for the first time.

The project developed the technical tools to look at magma at high magnification during deformation and flow. The 4D data (3 dimensions plus time) showed, for the first time, how much the distribution of the three phases of magma (bubbles, liquid and crystals) changes during flow, how many bubbles coalesce into larger bubbles, and how different regions of the sample behave very differently. The ground-breaking research opens up a new field in the study of magma rheology (movement and flow).

The methods developed in this study can also be used in other similar industrial systems with complex multi-phase fluids such as concrete, ceramics and certain foodstuffs.

Dobson K.J. *et al.* DOI: 10.3389/feart.2020.00287



X-ray ptychography image and tomography for the carbides in a superalloy sample.

Optimising the manufacture of nickel superalloys

Recent studies from a UK research group on both branchlines (I13-1 and I13-2) of beamline I13 at Diamond Light Source are helping to optimise the manufacture of valuable nickel-based superalloys and to reduce casting defects.

Nickel-based superalloys have been widely used to produce high-temperature structural components in aircraft and land turbine engines, rocket engines, nuclear power and chemical processing plants. Metal carbides are an important constituent in the microstructure and strength of these superalloys, and they allow excellent high-temperature stability, but this can also cause casting defects during the solidification process as well as crack initiation and propagation during plastic deformation. Until now, the nucleation and growth dynamics of metal carbides, especially the true 3D network structure and morphology of metal carbides formed in different solidification conditions, have not been fully understood.

The team used the two complementary synchrotron X-ray tomography techniques (microtomography and ptychography) on the branchlines to characterise metal carbide structures for the first time. These findings can assist scientists in ongoing quantitative measurement of crack initiation and propagation in metal carbides during plastic deformation and will help to ensure optimal design and manufacture of these important industrial components in the future.

Zhang Z. *et al.* DOI: https://doi.org/10.1016/j.scriptamat.2020.10.032

Crystallography Group

The Crystallography Group at Diamond Light Source 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). Bringing these beamlines together into one science group means we can fully exploit the technical and scientific expertise within its teams to provide the basis for future development and pioneering experiments.

Studies in the past year have included those to improve the capacity and function of lithium-ion batteries for electric vehicles, develop more accurate risk models of volcanic eruptions and optimise the design of Prussian blue analogues, an important family of materials used in a variety of industrial applications.

Improving performance of lithium ion batteries

Researchers are using Diamond facilities to make dramatic progress in the development of lithium-ion (Li-ion) battery technology. Although layered nickel-rich lithium transition metal oxides offer excellent energy densities when used as cathodes for electric vehicle batteries, this group of materials suffers from rapid performance loss. It is therefore essential to understand the degradation mechanisms at the material level, particularly during long-term ageing.

The team, from the Universities of Cambridge and Liverpool, the Faraday Institution and Diamond Light Source, used the Long Duration Experiments (LDE) facility on beamline (I11) to track the evolution of the crystal structure of battery materials *operando* over several months.

The results showed that a portion of the cathode material cannot reach the fully charged state progressively over time. Combining the results from multiple techniques, the team suggested that this was caused by a 'pinning' mechanism, where the crystal lattice of the material is pinned by its surface, preventing the material from being fully charged. These layered nickel-rich lithium transition metal oxides are likely to be the most popular cathode materials for the foreseeable future and so these findings will help in the development of strategies to mitigate degradation and optimise the function of Li-ion batteries.

Xu C. *et al.* DOI: 10.1038/s41563-020-0767-8

Predicting explosive volcanic eruptions

High viscosity magma often causes explosive and damaging volcanic eruptions. However, current knowledge of the mechanisms that regulate the style of volcanic eruptions fails to explain the anomaly that some volcanoes with low viscosity magmas have unexpectedly explosive eruptions.

Recent observations have shown that magmas may contain nanometric crystals (nanolites) 10,000 times smaller than the width of a human hair, whose formation and influence on both viscosity and bubble formation is unknown.

An international team of researchers used the Extreme Conditions beamline (I15) and the Small Angle Scattering & Diffraction beamline (I22) at Diamond Light Source to subject a basaltic magma that had been erupted explosively to X-ray diffraction measurements at high temperature (900-1500 Celsius) by varying the cooling rate. This allowed the *in situ* observation of nanolite formation and growth. Results showed that nanolites can form within milliseconds during rapid cooling, grow to ~50 nm in two minutes, and even aggregate. These new aggregates effectively disrupt the remaining free liquid flow, increasing the magma's viscosity and resulting in an explosive eruption. These important findings will provide data for new numerical models of volcanic eruptions that will provide risk scenarios in volcanic areas.

Di Genova D. *et al.* DOI: 10.1126/sciadv.abb0413

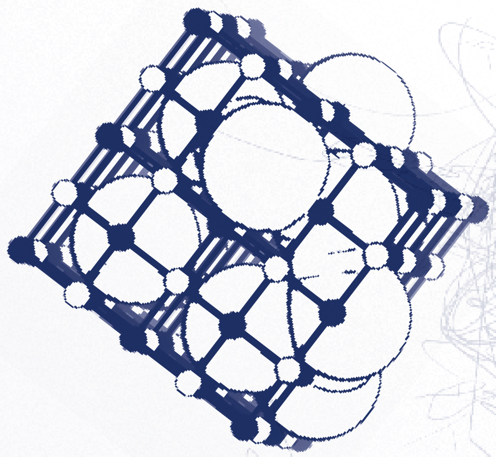
Optimising the design of catalysts, batteries and gas storage facilities

Studies on the Small-Molecule Single-Crystal Diffraction beamline (I19) at Diamond Light Source are providing the data needed to improve a variety of important industrial materials called Prussian blue analogues (PBAs). These are a broad family of microporous inorganic solids used in batteries, hydrogen gas storage and as catalysts to make high-value chemicals.

These materials have a disordered three-dimensional network of pores that allow ions or molecules to be moved or stored but until now this structure has not been identified. An international team of researchers investigated the pore structures of a range of PBAs to determine their characteristics. Using beamline I19 allowed them to measure the single-crystal X-ray diffuse scattering patterns of various PBA crystals.

Their results show that the pore networks of all PBAs, although disordered, are far from random. The patterns that persist within these non-random network structures affect the physical properties of the materials, such as their ability to store gases or the rate at which ions can be moved in and out. These findings suggest that there is scope for tuning the type of disorder present by varying the composition and synthesis route of the PBAs, and that this could produce improved materials for use in a variety of industrial applications.

Simonov A. *et al.* DOI: 10.1038/s41586-020-1980-y



Spectroscopy Group

The Diamond Spectroscopy Group consists of four beamlines; the Microfocus Spectroscopy beamline, I18, the Core EXAFS (Extended X-ray Absorption Fine Structure) beamline, B18, and the two independently operating branches of the Versatile X-ray Absorption Spectroscopy beamline, I20-Scanning and I20-EDE (Energy Dispersive EXAFS). These four spectrometers are complementary in the energy ranges they cover, the size of their focussed beam spots delivered to the sample, and the time resolutions they are able to reach. This complementarity means that they can support research across many different scientific disciplines, from chemistry and catalysis through materials science, condensed matter physics, environmental and life science, energy materials and cultural heritage.

In the past year a widely diverse range of studies have included investigating theories on the formation of mineral deposits on Mars, locating new sources of rare earth elements and designing new sustainable materials used in catalysis.

Understanding mineral formation on Mars

Jarosite is a common mineral on Mars but scientists have failed to explain how it could have formed as it requires liquid water, iron-rich minerals and an acidic-oxidative environment. A group of scientists proposed an 'ice-weathering model' where the mineral was formed under glaciers. To test this theory, they studied deep Antarctic ice deposits for the presence of jarosite.

An international team of researchers analysed samples of Antarctic ice on Diamond Light Source's beamline B18 using X-ray Absorption Spectroscopy (XAS) which allows data gathering on extremely diluted samples. The signature of jarosite was identified in X-ray absorption spectra, confirming that this mineral is present in Antarctic ice.

The mineral was not present in surface ice but increased rapidly as the depth increased and it became the most abundant iron mineral in the bottom sections of the ice core. This suggested that jarosite was not originally deposited in snow but that it forms in deep ice, thus supporting the Mars ice-weathering model. This is an important finding and increases understanding of the geological and geochemical processes and the role of glaciers that shaped Mars.

Baccolo G. *et al.* DOI: 10.1038/s41467-020-20705-z

Locating new sources of rare earth elements

Rare earth elements (REE) such as lanthanum and yttrium are essential for high-tech industries such as catalysts, magnets and rechargeable batteries. Over 80% of the world's current heavy REE deposits are found in clay deposits in China and extraction methods have been developed with little regard for the natural environment. Intensive international research is ongoing to understand how these deposits form and how REEs are bound to them. This will aid identification of further sites around the world and the development of more environmentally-friendly methods of extraction.

An international research team studied samples from China and a prospective site in Madagascar using Diamond Light Source's microfocus beamline I18 which allowed them to study the samples micron by micron. Combining X-ray Absorption Spectroscopy (XAS) with Scanning X-ray Fluorescence (SXRF) element mapping showed what surrounded the metals and their distribution in the sample. Although the rock samples from the two areas are different, the REE in both stick to the clay surfaces in an identical fashion. At the atomic level, the Madagascan clay deposits are the same as those currently exploited in China. These findings should allow us to develop easier, more environmentally friendly ways to extract these important elements and suggest that deposits may be more widespread than originally thought.

Borst A. M. *et al.* DOI: 10.1038/s41467-020-17801-5

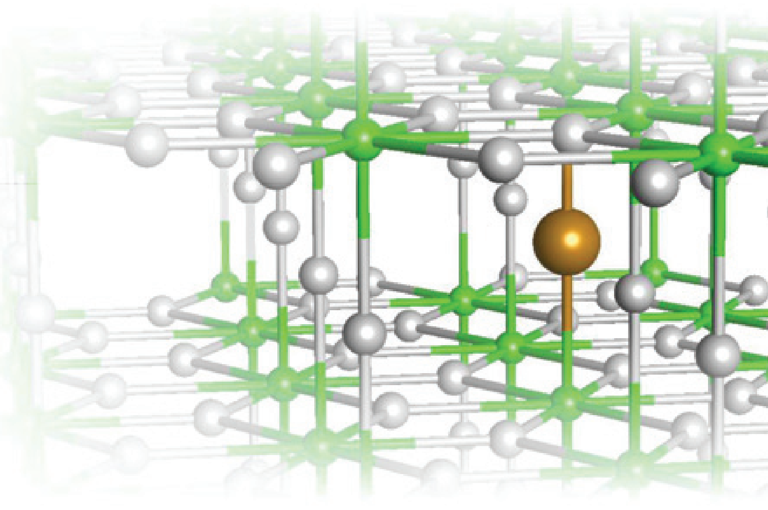
Designing new sustainable catalyst materials

Catalysts are set to play an important role in reducing carbon emissions and other environmental pollutants. Nitrous oxide (N_2O) is a by-product of fertiliser production, among other industrial processes, and has a global warming potential that it is approximately 310 times higher than carbon dioxide. The decomposition of N_2O is traditionally achieved using catalysts based on precious metals, but a promising alternative is to use perovskite structures of mixed-metal oxides such as lanthanum manganite ($LaMnO_3$).

This compound is currently prepared in a complex multi-step process at high temperature and researchers used Diamond Light Source's facilities to investigate its production with a novel ball milling method with the aim of improving its catalytic properties. They used the Energy Dispersive EXAFS beamline (I20-EDE) to monitor how the structure changes with increasing pressure, using X-ray Absorption Fine Structure (XAFS) measurements in real-time. Complementary measurements on the Versatile Soft X-ray (VerSoX) beamline (B07) provided information on the surface properties of the materials during catalysis.

This research provided important information on the conditions required to produce perovskite structures from ball milling, and shows the importance of synchrotron radiation methods in studying these materials, which is vital as researchers seek to develop sustainable methods for producing catalysts.

Blackmore R. H. *et al.* DOI: 10.1039/d0cp00793e



The structure of lithium nitride including an Fe impurity.

Soft Condensed Matter Group

The Soft Condensed Matter Group at Diamond Light Source is comprised of the High Throughput Small Angle X-ray Scattering (SAXS) (B21), the MultimodeInfrared Imaging and Microspectroscopy (MIRIAM) (B22), SAXS and Diffraction (I22) and the Circular Dichroism (CD) Microspectroscopy (B23) beamlines at Diamond Light Source. This unique portfolio of instruments enables studies of non-crystalline materials at micro to meso-scale resolutions that include two-dimensional thin-films (photovoltaics), living mammalian cells, three-dimensional matrices (e.g. metal-organic frameworks, gels and waxes) and nano-particles in non-crystalline states. The group now offers mail-in services for SAXS and CD measurements through UAS (User Administration System) announcements. In addition, I22, B22 and B23 offer off-line access to IR microscopy and imaging, CD spectroscopy and SAXS measurements.

Studies this year have included observing the cellular impact of drug treatments, developing vaccines that do not require refrigeration for storage and transport, and identifying a new cost-effective approach to Alzheimer's Disease therapy.

Viewing the effect of drug treatment in a single cell

A fundamental part of pharmaceutical development is to be able to detect the metabolic changes taking place inside a cell following drug treatment. Currently, most techniques require staining to reveal chemical changes, but this may alter the natural process and produce misleading results. Infrared (IR) microspectroscopy can probe chemical changes in biological matter without the use of dye but the images produced to date are too coarse to see clearly inside a single cell.

A team of researchers investigated a new Synchrotron IR spectroscopic imaging method, developed on the Multimode InfraRed Imaging And Microspectroscopy (MIRIAM) beamline (B22) at Diamond Light Source to probe the molecular changes inside macrophages. These white blood cells produce many tiny fatty droplets when exposed to drugs, but the exact reason for this response is not clear.

The study results showed that IR nanospectroscopy can measure a drug's effect inside a mammalian cell by clearly identifying the chemistry changes within the fatty droplets before and after the application of the drug. This powerful new molecular imaging tool can now be used to understand the responses of macrophages exposed to different drugs. This will help identify new drug candidates and improve the chance of success in delivering better medicines in the near future.

Chan K. L. *et al.* DOI: 10.1021/acs.analchem.9b05759

Developing vaccines that do not need refrigeration

Almost all vaccines require refrigeration for storage and transport and a vaccine cold chain has been developed to distribute vaccines worldwide. However, this poses problems in developing nations due to the availability of refrigerators, electricity, infrastructure and staff training.

An international team of researchers has developed a novel method of making existing vaccines thermally stable so that they will not depend on cold chain distribution. The process, called ensilication, uses silicon dioxide to create layers of inorganic materials around individual vaccine components which protects the vaccine from temperature degradation. The research team aimed to gain further understanding of the ensilication mechanism by use of *in situ* Small Angle X-ray Scattering (SAXS) on the time-resolved SAXS & Diffraction beamline (I22) at Diamond Light Source. They studied tetanus toxin C fragment, an inactive component of the tetanus toxin present in the diphtheria, tetanus and pertussis vaccine and were able to show that ensilication maintained the vaccine effect through a three-stage process – nucleation, rapid growth and aggregation.

This study explains the mechanism of ensilication of vaccines and how to control the process effectively. This research provides a potential solution for biopharmaceutical stabilisation and could help to increase vaccine transport and administration in all countries around the world.

Doekhie A. *et al.* DOI: 10.1038/s41598-020-65876-3

Assessing a potential new treatment for dementia

There is currently no cure for Alzheimer's disease, which is associated with the formation of large protein plaques (amyloid-β and tau proteins) in the brain that kill neurons. One therapeutic approach is to block or impair the formation of these plaques and a research group from Lancaster University and the team on the Circular Dichroism beamline (B23) at Diamond Light Source used high-throughput screening techniques to analyse the impact of 88 potential compounds on stabilising protein deposition. The results showed that epinephrine (adrenalin) was superior to the other compounds. Further investigations of chemically similar compounds showed that salbutamol, the well-established asthma drug, interacts with the tau protein substantially, preventing the formation of abnormal tangled clumps that at the early stages are thought to damage brain neurons and progressively induce dementia. Salbutamol could, therefore, be a potential treatment for Alzheimer's disease and now requires *in vitro* and eventually a full *in vivo* evaluation as a potential therapeutic for Alzheimer's disease.

Developing new drugs is slow and very expensive. It is far quicker and cheaper to repurpose clinically approved drugs for other diseases. There is now potential for this approach to be applied to other neurological disorders (such as Parkinson's and Huntington's diseases) and any other disorder associated with protein deposits including type 2 diabetes and cancer.

Townsend D. J. *et al.* DOI: 10.1021/acschemneuro.0c00154

Integrated Facilities and Collaborations

Diamond Light Source collaborates closely with neighbouring research institutes and companies on the Harwell Science and Innovation Campus and beyond. The integrated facilities at Diamond present academic and industrial users with a one-stop-shop for research opportunities. These facilities and partnerships bring together expertise from UK universities, research institutes and industry to help tackle 21st century challenges.

Integrated Facilities

The Membrane Protein Laboratory (MPL)

The MPL is a state-of-the-art facility for membrane protein research and is open to user applications from anywhere in the world. Since its inception, the MPL has supported visiting researchers in investigating proteins that are embedded in cell membranes. 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 will help develop future disease therapies.

The MPL has a dedicated laboratory close to the experimental end stations and electron microscopes, which greatly enhances scientists' ability to characterise these targets. A recent study[1] used MPL facilities to investigate a series of Archarhosdopsin-3 (AR3) structures which opens the way for the development of new tools in the fields of neuroscience, cell biology and beyond. Another study used *in vitro* and *in cellulo* approaches to characterise disulphide bonding in the major outer membrane protein (MOMP), an important Chlamydia vaccine target[2].

References:

1. Bada Juarez J. F. *et al.* DOI: 10.1038/s41467-020-20596-0
2. Danson A. E. *et al.* DOI: 10.3390/biology9100344

Fragment screening (XChem)

The XChem facility stayed open throughout lockdown for experiments aimed at accelerating development of new treatments for COVID-19. Early in the pandemic, XChem joined a collaboration to identify fragment compounds bound to the Main protease, a key enzyme in the life cycle of the SARS-CoV-2 virus, to provide templates for designing bespoke molecules to block the enzyme. The data stimulated much interest, and XChem became a founding partner of the COVID Moonshot, a global non-profit initiative aiming to develop a novel antiviral drug by crowdsourcing designs of new inhibitors from chemists worldwide who could mine the Diamond data. The project continues to release its data in real-time, which has driven rapid progress.

Along with collaborators, the XChem team performed screens against a further seven COVID-19 proteins, to trigger further productive drug discovery efforts. By April 2021, combined international efforts had discovered 234 fragment compounds that directly bind to sites of interest on the surface of this cohort of seven proteins. Many of these data are already public, providing large numbers of starting points for designing compounds as antivirals.

Highlighted publications

- Douangamath A. *et al.* DOI: 10.1038/s41467-020-18709-w
- Chodera J. *et al.* DOI: 10.1038/s41557-020-0496-2
- Schuller M. *et al.* DOI: 10.1126/sciadv.abf8711
- Newman J. A. *et al.* DOI: 10.1101/2021.03.15.435326

XFEL (X-ray Free-Electron Laser) Hub

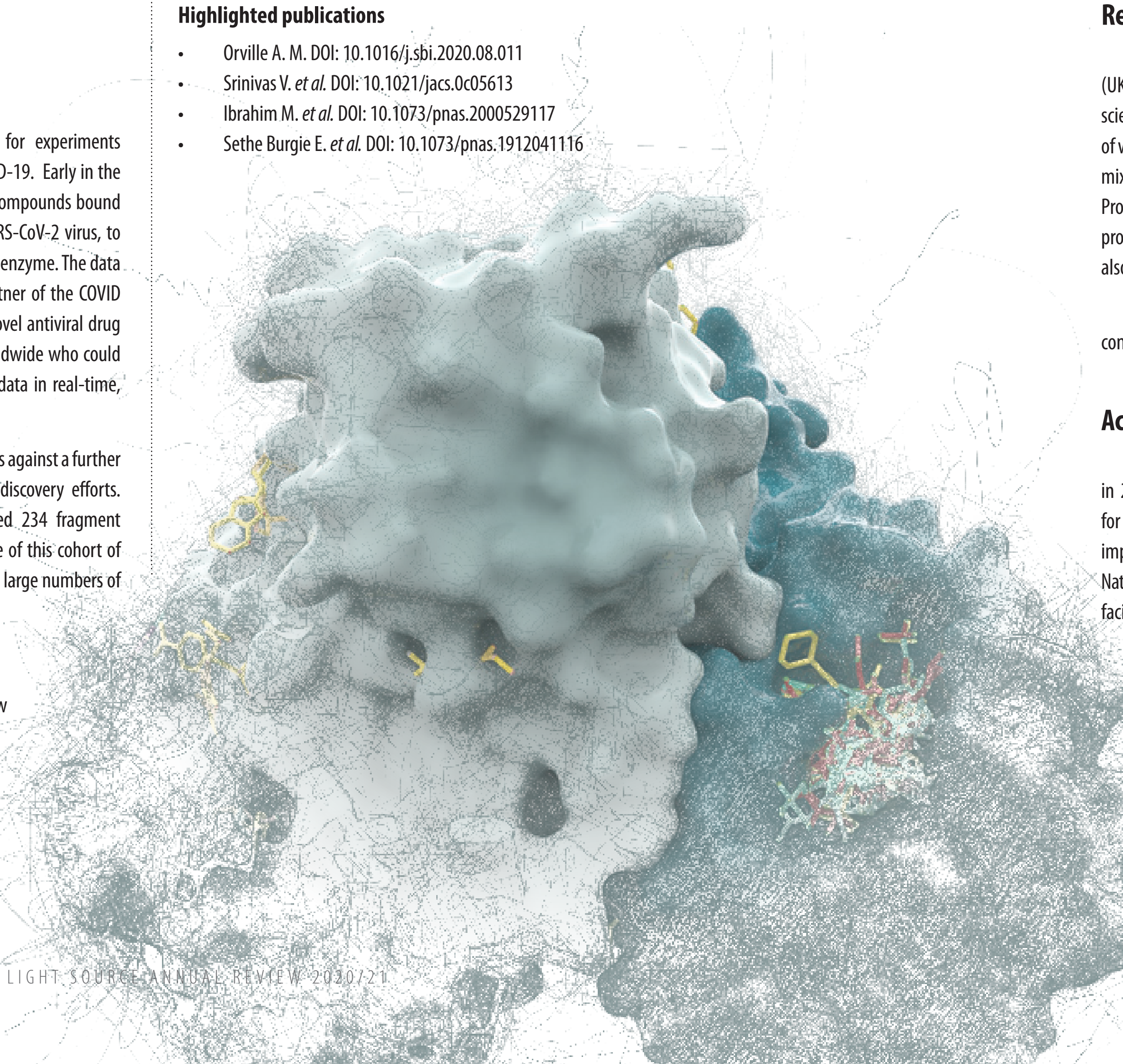
The XFEL Hub continues to provide expertise and support to the UK community engaged in serial crystallography and XFEL-related life science research. The Hub also organises the Block Allocation Group 'Dynamic Structural Biology at Diamond and XFELs' for serial crystallography and time-resolved studies.

Nearly all XFEL beamtime awards over the past year have been impacted by the COVID-19 pandemic. Since February 2020, our XFEL activities included more than a dozen beamtime awards fielded at XFELs SACLA (Japan), PAL-XFEL (South Korea), LCLS (USA), and the European XFEL (Germany). From August 2020 the Hub participated in all XFEL beamtime through remote connections, including the Hub-led COVID-19 experiments at LCLS and the European XFEL. The Hub also initiated major projects to establish strategies for time-resolved Macromolecular Crystallography studies with on-demand sample delivery and reaction initiation methods that can be correlated with X-ray Emission Spectroscopy.

Dr Allen Orville and team created an updated science case for a UK-based X-ray Free Electron Laser (UK-XFEL). More information can be found at: *www.clf.stfc.ac.uk/Pages/UK-XFEL-science-case*

Highlighted publications

- Orville A. M. DOI: 10.1016/j.sbi.2020.08.011
- Srinivas V. *et al.* DOI: 10.1021/jacs.0c05613
- Ibrahim M. *et al.* DOI: 10.1073/pnas.2000529117
- Sethe Burgie E. *et al.* DOI: 10.1073/pnas.1912041116



Representation of the chemicals binding to the main protease of the SARS-CoV-2 virus.

Collaborations

The Rosalind Franklin Institute

Diamond is a founding member of the Rosalind Franklin Institute (The Franklin) with ten universities and UKRI-STFC. The Institute is dedicated to bringing about transformative changes in life science through interdisciplinary research and technology development. Last year the Wellcome Trust awarded The Franklin, along with partners MRC Laboratory of Molecular Biology (MRC LMB) and Diamond, a £25m grant to support the development of three new electron imaging technologies that will have the capacity to revolutionise how we see life, pushing the boundaries of imaging in life science. Diamond's share of the grant is to fund the development of a Hybrid electron X-ray Instrument (HeXI), which is set to play a major role in drug discovery efforts. HeXI will make electron diffraction accessible to Diamond's existing life science users as well as attract new users to study pharmaceutical compounds and their binding.

Other collaborations include:

- The Amplus project with Thermofisher Scientific to develop instruments to deliver a revolution in cryo-electron tomography – using electron microscopy to build up three-dimensional models inside the cell.
- SPT Labtech and Diamond are developing methods for sample preparation using SPT Labtech's chameleon, an automated system for next generation cryo-EM sample preparation.

Research Complex at Harwell (RCaH)

RCaH is a joint venture between Diamond and UK Research and Innovation (UKRI) and provides a research hub on the Harwell campus for the physical and life sciences. It currently has over 180 researchers from UK universities working in a mix of wet and dry laboratory space supported by research grants. In addition, there is a mix of research facilities or consortia based at RCaH including Diamond's Membrane Protein Laboratory (MPL), the Central Laser Facility (CLF), CCP4 and CCP-EM. RCaH provides the majority of the wet laboratory space for Diamond group leaders and also hosts the UK XFEL Hub, XChem and the Harwell crystallisation facility.

The last year has been extremely busy for RCaH to allow COVID-19 research to continue, including the first fragment screening data from Diamond.

Active Materials Building

Construction of a new dedicated Active Materials Building (AMB) started in 2020. The new facility, which should open later this year, will provide space for radioactive materials research, enabling experiments that were previously impossible in the UK. This new laboratory is part of phase 2 of the Government's National Nuclear User Facility (NNUF) project to provide state-of-the-art experimental facilities for research and development in nuclear science and technology.

The University of Manchester

Diamond has joined a new partnership of UK universities to help researchers carry out experiments using X-ray Computed Tomography (XCT). Funded by the Engineering and Physical Sciences Research Council (EPSRC), the National Research Facility for X-ray Computed Tomography (NXCT) provides world class 3D imaging facilities and data analysis, research knowledge and technical experience.

NXCT's mission is to provide access and expert support for both academia and industry. Diamond will work with NXCT to help guide potential users toward the right facilities for their studies. NXCT users will access Diamond via the standard routes and will benefit from the support of a joint appointee between Diamond and Manchester, a post funded 50% by the EPSRC grant to specifically support NXCT activities.

The University of Manchester at Harwell (UoMaH) is hosted by Diamond and provides the interface with the Harwell national facilities. The core technical team specialises in developing sample environments and equipment in support of experiments, involving high risk materials and extreme sample environments, fielded at the national facilities. UoMaH also has a growing contingent of research fellows based at Harwell. They strengthen the University's link with Harwell by bringing their research, networks and new users from Industry and Faculty academics to Diamond.

The Faraday Institution

Diamond is involved in several Faraday Institution projects including:

- The displacement and strain with battery electrodes and developments in super-resolution techniques and machine learning to enhance correlative imaging.
- The Faraday CATMAT project to increase understanding of cathode materials, in particular using oxygen-redux materials to increase cathode energy density using the I21 beamline. The project is also developing 3D spectroscopic and structural imaging on beamline I14 to aid characterisation of these materials.
- The Degradation project uses high-resolution X-ray Powder Diffraction on beamline I11 to obtain valuable information on the structural evolution of novel, high energy-density electrode materials, *in situ*. The Long Duration Experiment (LDE) facility has been used to perform long-term, *in operando* cycling experiments, providing a better understanding of the degradation mechanisms leading to battery capacity loss and poor cycle life.
- I15-1, the X-ray Pair Distribution Function (XPDF) beamline, is a collaborator in the Recycling, Degradation and SOLBAT projects. Recent developments in cell design at I15-1 will facilitate fast *operando* XPDF studies for Faraday researchers investigating next generation cathodes, solid-state batteries and recycled battery materials.

Industrial Liaison

This has been a year like no other, and while we mourn those lost and remember those struggling, we also want to take time to recognise some of the most positive moments.

We have moved the operations of the Industrial Liaison Office (ILO) to home offices. Through many hours of Zoom and Teams calls we have been welcomed into our clients' lives, meeting their families and their pets! Shared understanding of the pressures and a strong desire to collaborate in extraordinary circumstances have brought the most human elements of scientific research to the fore.

From mid-March 2020, Diamond's operations were restricted to COVID-19 research, but the ILO XChem team had already spent much time working on Diamond's collaborative COVID-19 research projects. This work has contributed to understanding of the SARS-CoV-2 virus and the design of potential therapeutics. Industrial life science services were able to resume in May.

Years of optimising remote working on Diamond's life science beamlines has ensured a smooth transition during this period. Data management systems are in place to support sample shipments and tracking and secure external access, making preparations from the client side simple and straightforward. State of the art robotics and automation enable fast, accurate and reliable instrument control from labs, offices and kitchen tables all over the world. Cryo-electron microscopy, macromolecular crystallography, fragment screening and small angle scattering services have been in high demand and the industrial programme is thriving.

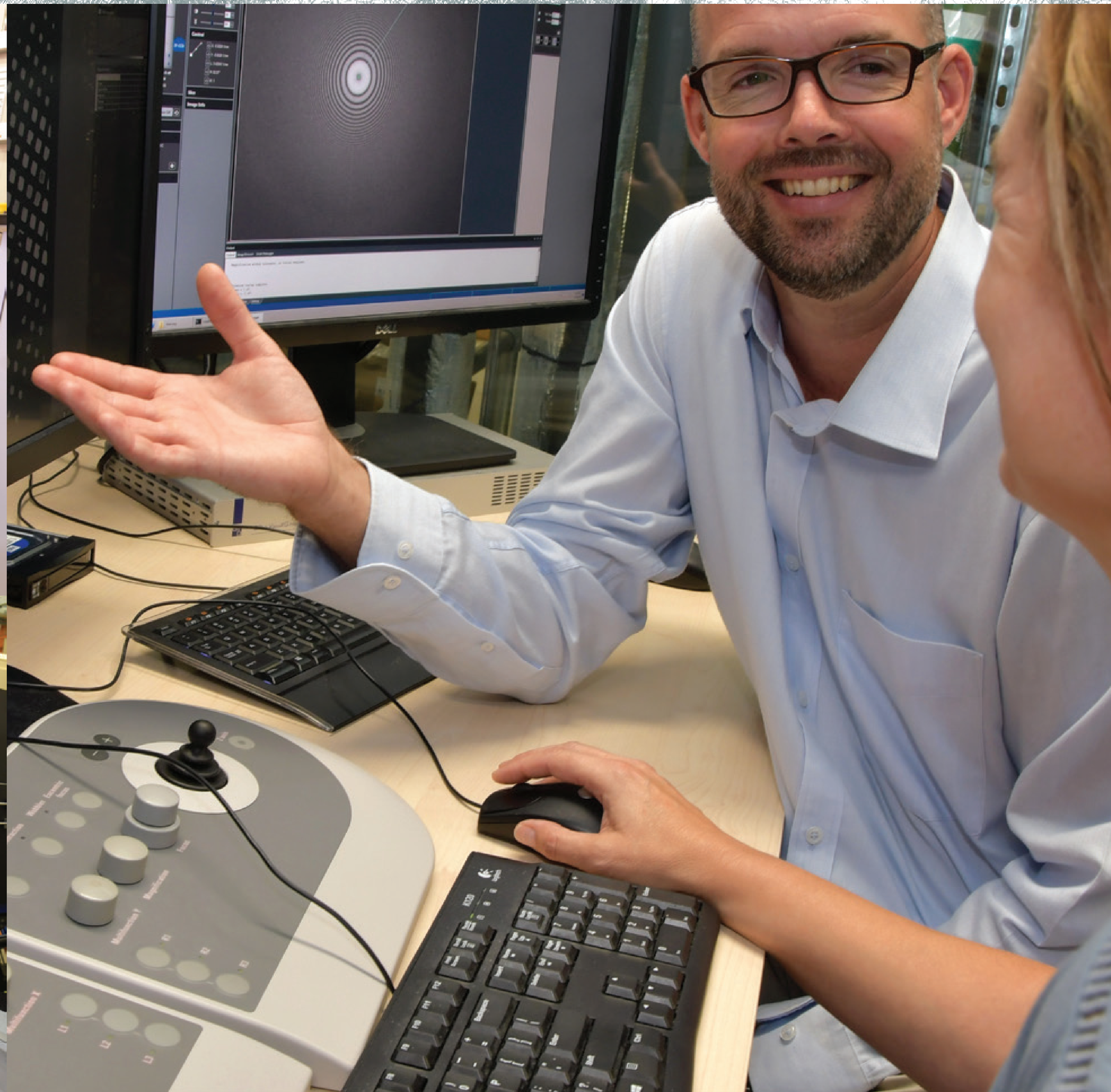
Our mail-in data collection services continue to be very popular and samples can be prepared and shipped directly to us for experiments. Samples can then be prepared by our staff or proceed directly to data collection. Years of experience in designing and delivering mail-in experiments have allowed us to accommodate any additional challenges presented by the pandemic. Although there has been a limited operational timetable, reduced demand from academia during restricted university lab access has created opportunities for greater flexibility and access for industry.

Physical sciences experiments resumed for industrial clients in the late summer of 2020. As restrictions were relaxed, more complex experiments with increased staff requirements became possible. Diffraction, imaging, small angle scattering and spectroscopy services are now running regularly to support our clients.

The ILO team have used their unique blend of experience, expertise and excellent communication to assist in designing complex experiments during this time. Our Diamond colleagues have been instrumental in ensuring that industrial beamtime has had the minimal possible disruption during this time.

We have updated our marketing and communications information so please visit our website at www.diamond.ac.uk/industry or follow us on LinkedIn (Diamond Industrial Liaison Group) or Twitter (@DiamondILO) for more information.

If you have a project in mind or an analytical need to discuss, please get in touch on industry@diamond.ac.uk and we will do our best to make it a reality.



Members of the ILO team pictured at Diamond, pre-pandemic.

Education, Training and Engagement

Engaging with and inspiring the public continues to be a key part of the Diamond Light Source vision. We have been able to continue our vision to engage and inspire, with new remote and virtual activities through the pandemic. During the year we had over 9,600 significant interactions (30+ minutes) with 'virtual' visitors, including researchers, students, school pupils, the general public, and VIPs or stakeholders.

Public and schools

We have developed a new series of family webinars and new video technologies have been used to deliver virtual tours of the facility. A range of media resources now allows visitors to our website to virtually explore Diamond for themselves.

> ***"It was great to be able to see inside the beamline and the experimental hutch. Thank you so much, it's difficult to do much extra-curricular at the moment so this is a real treat."***
>
> *- A schoolteacher at a virtual schools' visit*

Virtual schools' events and work experience has expanded our outreach, and in July 2020 we were able to welcome over 100 students to three days of events to give students a real insight into the variety of careers available.

> ***"I have very much enjoyed the experience and would encourage other people to do this work experience. Lots of information, detailed, in-depth and fascinating!"***
>
> *A work experience student*

We reinforced our commitment to widening participation and diversity within STEM subjects (Science, Technology, Engineering and Mathematics) and partnered with the Social Mobility Foundation and with BBSTEM (Black British Professionals in STEM) in various activities. Our core programme and partnership activities continued to deliver a range of events including virtual stargazing, a 'Science in your future' event for girls, and particle physics masterclasses. The online nature of activities has also helped us develop new partnerships.

Higher Education engagement

Training of students through our undergraduate placements and PhD programmes continues to be one of our core engagement activities. Despite the pandemic we were able to support our current PhD and Year in Industry students and allowed access to beamtime and laboratories to PhD students, as part of the priority access route. We welcomed 32 new PhD students bringing the ongoing PhD studentships to 104, with 24 new students expected in October 2021.

Although we had to cancel the 2020 Summer Placement programme these students have the opportunity to join the 2021 cohort. After a brief delay we were able to welcome the Year in Industry students to Diamond via a series of virtual events and these projects are ongoing. We were also able to support 11 virtual visits from university groups.

Scientific workshops and conferences

We ran a broad range of online scientific and technical workshops, training courses and conferences tailored towards the needs of our staff and user community and attendance was increased by 57% on 2019/20.

> ***"This was an overall fantastic workshop. To date, I think this is the most valuable training I could have obtained as someone who is earning their PhD based in X-ray crystallographic research."***
>
> *- PhD student attending the Diamond-CCP4 Data Collection and Structure Solution Workshop, Dec 2020*

We also delivered 13 community engagement webinars as part of the Diamond-II proposed upgrade programme.

Zoom attendees of a Diamond-CCP4 Data Collection and Structure Solution Workshop, late 2020.

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