technopolis group

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Impact evaluation of European XFEL

Final Report

Version 3

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Final Report

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Table of Contents

1 Executive summary

The European X-Ray Free-Electron Laser (European XFEL) facility in Hamburg is a laser facility that generates ultrashort X-ray flashes – 27,000 times per second and with a brilliance that is a billion times higher than that of many conventional X-ray radiation sources. These characteristics allow users to study ultrafast processes such as chemical reactions, or the configuration changes of biomolecules.

European XFEL was founded in 2009 and the UK became a member state in March 2018, contributing approximately 2% (€26 million, 2005 prices) of the facility's construction costs. The UK also currently makes an annual contribution worth around 2% (c. €3 million) of the facility's operational budget, helping secure access for UK users and suppliers.

STFC appointed Technopolis to undertake an evaluation that would measure and demonstrate the impact from the UK's involvement in European XFEL since it became a member state. UK researchers have conducted a limited number of experiments with the facility thus far, as it only became fully operational in 2019 and the pandemic restricted access. Nevertheless, the study found that the UK's shareholding in and access to European XFEL has already delivered in a variety of areas, which are summarised below.

1.1 Unique capabilities enabling high volume, high quality UK science

- European XFEL provides UK researchers with access to an unparalleled laser facility, both in terms of the brilliance of the light available, and a high-quality sample preparation facility
- The UK is one of European XFEL's five heaviest users, with 86 different users since 2017
- UK scientists have used European XFEL's unique capabilities to deliver cutting edge-research, from the advancement of UK research in serial femtosecond crystallography (SFX), a novel approach to protein crystallography; to new methods for purifying water
- The majority of user survey respondents indicated that without European XFEL, many of their projects would simply have not been possible
- Since the facility's formation, UK researchers have been involved in 150 publications linked to European XFEL

1.2 Supporting diverse and multidisciplinary UK science

- The UK user base is diverse and includes those studying structural biology and matter under extreme conditions, as well as cross-discipline subjects such as methods and instrumentation
- Some 65% of UK publications linked to European XFEL have been multi or interdisciplinary, approaching double the value seen across all published academic papers
- While much of the UK's research at European XFEL has been pure science to date, some research also has clear real-world application in energy management and healthcare

1.3 Improving research skills and training the next generation of scientists

- European XFEL access has created strong skills benefits for UK researchers, particularly in improving their ability to work in international environments and international teams
- It has also provided a valuable opportunity to train early career scientists through both research projects, and facility visits. This in turn will help grow the nascent UK XFEL user community, improving the skills supply chain
- On-site facility usage has also enabled knowledge exchange across different research groups, and facilitated educational outreach activity

1.4 Supporting the UK research and innovation community

- European XFEL involvement and engagement has protected UK access to FEL facilities which are elsewhere over-subscribed or do not provide easy UK access
- Access to the facility also allows the UK to better understand the likely future demand for a UK XFEL, enabling more informed decision making on how best to support the community
- European XFEL helps STFC and UKRI meet its strategic goals to strengthen the UK's research and innovation community, in relation to early career researchers, and access to international networks and opportunities

1.5 Contributing to UK government priorities

- The UK's interactions with European XFEL have contributed towards wider government policy priorities including:
  - facilitating research that can help explore alternative energy sources (e.g. plasmas for nuclear fusion)
  - helping fulfil UK aims to become a science superpower by 2030, by enabling cutting-edge UK-led research
  - improving health (e.g. helping to understand new drugs and to develop new water treatment methods)

1.6 Enhancing the UK's international standing

- Involvement in European XFEL has increased international collaboration opportunities, with all but one of the UK-authored publications citing the facility having had at least one international partner
- The facility has also facilitated interaction between UK researchers and international funders, with authored publications typically receiving funding from three different countries
- The UK benefits from soft power gains, maintaining influence in international science decision making through its involvement in European XFEL

1.7 UK businesses winning contracts

- UK-based suppliers won contracts worth €700k with European XFEL, with goods and services provided including cameras and components, floor cranes and gas safety consultancy
- Outside the commercial sector, STFC has secured two flagship contracts to provide detectors and a laser
- These contracts have helped enhance the reputation of UK suppliers, as well as improving the country's skills base

1.8 UK industrial innovation and creating jobs

- Some UK businesses are already undertaking fundamental research at European XFEL, most notably the pharmaceutical firm, Heptares Therapeutics. We can reasonably expect greater UK industrial use of the facility going forward
- European XFEL has helped create and retain high value-added jobs. UK users reported that the ability to work on high-profile and cutting-edge projects has helped attract and retain skilled researchers and engineers to the UK

European X-Ray Free-Electron Laser Facility (European XFEL)

86 unique UK users (on average 2017-2022)

6 instruments in operation (currently)

160 UK user *visits* between 2017-2022

UK accounts for 5.5% of users compared to 2% of European XFEL costs

Key research activities at European XFEL

Structural biology, biocrystallography	34%
Matter under extreme conditions, warm dense matter, plasmas	25%
High-field science, non-linear X-ray Optics	11%
Femtochemistry	9%
X-ray scattering, X-ray optics	9%

European XFEL supports High Quality Research

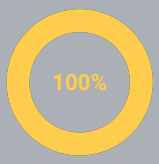
91% of UK European XFEL research concerned material science/physics

150 articles published (2009-2022)

Drives both scientific research as well as methods and instrumentation innovation

69% of papers were inter or multidisciplinary (Since 2017)

Facility was critical to pursuing key research questions



Facility was key to understanding their research area

European XFEL supports Skills and Knowledge

93% Indicated the importance of European XFEL on research skills development

Access improves research skills of users and their research teams

Supports key skills

- International collaboration
- Team working
- Project management
- Student/post-doc training

93% said European XFEL has broad impacts on the development of next generation researchers

Benefits to the UK at home and abroad

STFC Benefits

- Protect UK access to scientific facilities
- More informed decision about UK XFEL
- Strengthen UK research and innovation community

UK Government Objectives

- Helps to explore alternative energy sources, and help meet net zero and other climate objectives
- Supports aim of becoming science superpower by 2030
- Improves health through new knowledge of drugs and treatments

European XFEL supports International Collaboration

99% of UK papers included an international partner (2009-2022)

Germany was most common collaborator (87%)

Global Collaborators

European XFEL supports Suppliers

65 UK based companies supplied goods and services to European XFEL (2018-2020)

Combined, the contracts were worth £700k to UK firms

STFC itself is supplying detectors and lasers for new flagship projects at European XFEL

2 Introduction

This report presents the impact evaluation of the UK's involvement in the European X-Ray Free-Electron Laser Facility (European XFEL), and an evaluation framework for future monitoring.

2.1 The European X-Ray Free-Electron Laser (European XFEL) Facility

STFC aims to provide UK researchers with access to world-class research facilities. It manages and funds several major research infrastructures within the UK itself, including the Diamond Light Source, Central Laser Facility (CLF), and e-Merlin radio astronomy facility. In addition, STFC manages access for UK researchers to international science facilities, including European XFEL.

Founded in 2009 and having been operational since 2017, the Hamburg-based **European XFEL** is a laser facility that generates ultrashort X-ray flashes – 27,000 times per second and with a brilliance that is a billion times higher than that of many conventional X-ray radiation sources. These characteristics enable European XFEL users to study ultrafast processes such as chemical reactions, or the configuration changes of biomolecules. Research conducted at European XFEL has included mapping the atomic detail of viruses, taking 3D images of the nanoworld, and studying extreme states similar to those seen in the interior of planets and stars. There are only a handful of other XFEL facilities worldwide. European XFEL is the largest of these and has unique properties that set it apart.

The UK joined as a European XFEL member state in March 2018, contributing approximately 2% of the facility's construction costs. It currently also makes an annual contribution worth around 2% of the European XFEL's operational budget.[1] This financial contribution provides access to the facility for UK researchers. Beamtime is allocated based on the scientific excellence of proposals, but there are only limited circumstances in which users from non-member countries may apply. European XFEL will be changing its cost repartition model in 2024 to take account of usage as well as shareholding; this will increase the UK's annual contributions, based on its current usage levels.

There are two XFEL hubs in the UK which help domestic users prepare for their use of the Hamburg facilities, and indeed other XFELs worldwide. Diamond hosts the life sciences hub, developing relevant hardware and software for experiments and providing a sample environments lab and user access programme. The CLF hosts the physical sciences hub, offering training, support and networking, targetry and sample preparation, plus travel and subsistence.

The CLF is also a leading member of the Helmholtz International Beamline for Extreme Fields (HiBEF) User Consortium at European XFEL, where the user consortium is provided with priority access to beamtime in return for operating the instruments. The CLF and the University of Oxford also developed and built a high energy laser, DIPOLE 100-X, for HiBEF.

2.2 Impact evaluation of the UK's involvement in European XFEL

STFC appointed Technopolis to carry out an impact evaluation study of the benefits from the UK's investment and partnership in European XFEL (since it joined in 2018). There are a wide variety of impact types that we might expect the facility to produce, and therefore a range of different areas in which the UK may benefit from its shareholding and access. These include:

[1] https://www.xfel.eu/news_and_events/news/index_eng.html?openDirectAnchor=1435&two_columns=0

- **Scientific and research benefits:** including the role that European XFEL plays in advancing academic and commercial research, including through multidisciplinary and interdisciplinary research
- **Skills benefits:** including R&D skills amongst users and suppliers, as well as impacts on apprentices and students
- **UK policy and wider strategic objectives:** including meeting goals in STFC's Delivery Plan, and other wider government policy objectives
- **UK's international standing:** including the UK's ability to influence international science, and European XFEL's role in enhancing the UK's reputation as a centre of world-leading science
- **UK benefits from supplying the facilities:** including the additional revenue gained by firms from facility contracts, and benefits to their supply chains
- **Commercial and economic benefits:** including the sale of products based on research at European XFEL, or the production of spinouts from university research based at the facility

However, it is worth highlighting that full operations at European XFEL did not start until 2019 and then the pandemic prevented many in-person experiments in the early period. This means that the UK has only been involved in a limited number of experiments at the facility to date, as well as limited usage of European XFEL by UK industry. It was therefore expected that the study may only find limited evidence of impact from European XFEL at this stage.

Nevertheless, in Part 1 of this report we present the findings of our impact evaluation, examining each of the above impact pathways in turn. Part 2 then sets out an evaluation framework that STFC can use to monitor impacts going forward, helping to ensure it is well positioned to capture further evidence in future as the UK's involvement further develops.

A parallel study on the impact of the UK's involvement in the European Synchrotron Radiation Facility (ESRF) was also undertaken. The two studies are underpinned by a common workplan, assumptions and consultees. A joint methodology report is therefore provided separately.

Part 1: Impact Report

3 Scientific and research impacts

The most notable impact that European XFEL has had on the UK so far has been in advancing scientific research led by UK-based researchers. This section sets out the different ways that UK researchers have used the facility, the types of research that have benefited from the facility, and the specific ways that European XFEL has helped advance research.

3.1 Summary

- Over the last five years, the UK has accounted for approximately 5.5% of unique users and 4% of total visits to European XFEL. These rates are higher than the UK's shareholding in the facility, showing that there is strong demand form UK researchers, above the shareholding level
- Relative to other countries, UK researchers are heavy users of the High Energy Density (HED) instrument, which investigates matter under extreme conditions using radiation
- Access to European XFEL has already supported UK research in a wide range of scientific areas including structural biology and matter under extreme conditions
- UK researchers have been involved in 150 publications associated with European XFEL since its formation. These publications have covered a diverse range of disciplines, including material science and physics, life sciences, and computer sciences
- European XFEL has also supported a large number of UK authored research publications centred on methods and instrumentation, which will have cross discipline relevance
- The majority of UK-authored research publications citing European XFEL since 2017 have been multidisciplinary (69%), a level that is higher than would typically be expected
- European XFEL has been particularly helpful to UK researchers in adding to the pool of FELs that they can use. XFELs around the world are over-subscribed and the UK has no arrangement with them for researcher access. The UK's involvement in European XFEL ensures that UK researchers have quicker access to high quality research facilities
- European XFEL provides UK researchers with facilities that are not available elsewhere, including the brilliance of the light available, and a sample preparation facility on site (which helps mitigate against risks of sample deterioration during transit)
- UK researchers have also reported wider benefits from access to European XFEL, such as developing international connections.

3.2 Scale of European XFEL usage

As noted in the introduction, the UK contributes approximately 2% of European XFEL's budget. A study of the facility's monitoring data indicates that the UK's usage of the facility exceeds its shareholding, implying strong UK demand for the facility.

As shown in Table 1, over the last five years the UK accounted for approximately 5.5% of unique users and 4% of total visits,[2] both higher than the UK's 2% shareholding in the facility. It is also worth noting that the figures show usage from September 2017 even though the UK did not become a Member State until March 2018. Therefore, the UK's share of visits and unique visitors is likely to be even higher if one only considered the period after the UK's shareholding began.

While other countries like the United States may have seen a higher number of absolute unique users and total visits, the UK still compares favourably when we account for population. The UK

[2] The number of visits is larger than the number of unique users as a single unique users may have made multiple visits to the facility

had 1.3 unique users per 1 million people, ahead of the USA and significantly higher than the median across a sample of 32 other user counties in the world. Likewise, the UK accounted for 2.4 visits per 1 million people which is twice as high as the median for the group of 32 user countries shown in the table.

Table 1 Total number of European XFEL users and visits, by country, 2017 – 2022 (top ten countries by number of visits only)

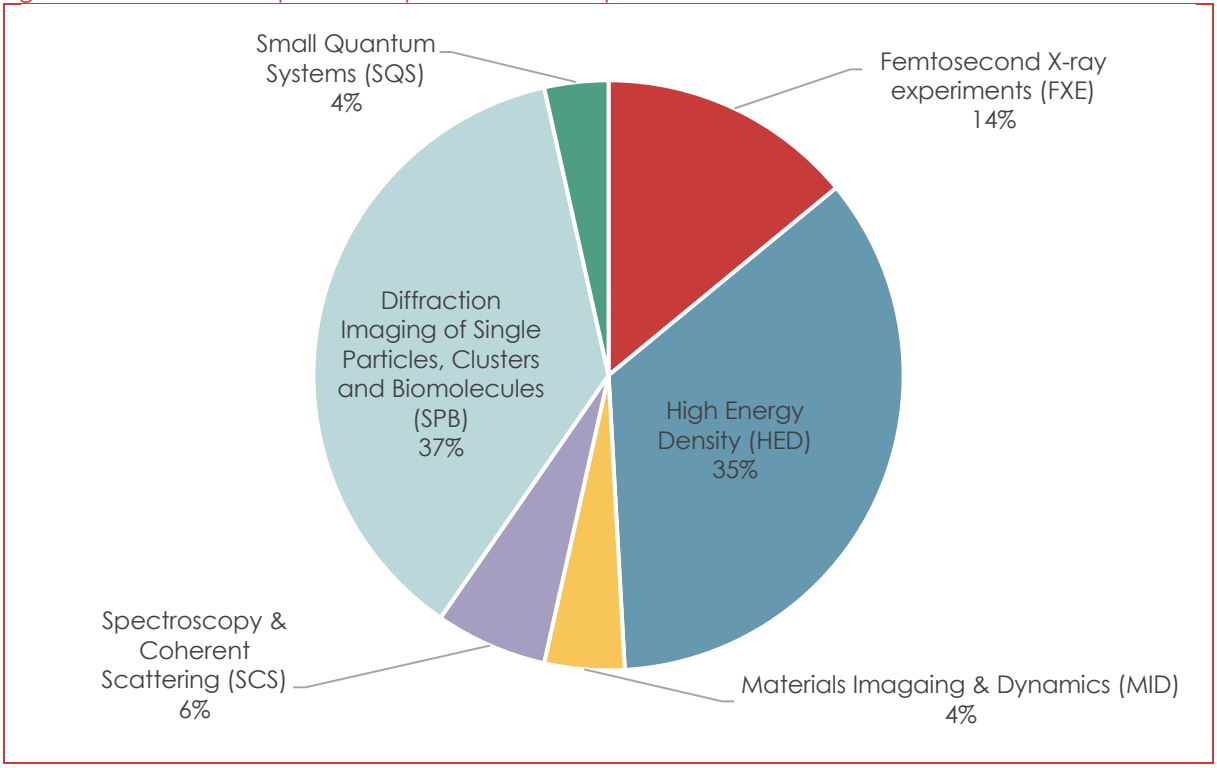
	Visits	Visits (%)	Visits per 1 million people	Unique users	Unique users (%)	Unique users per 1 million people
Germany	2,060	50.0%	24.6	631	40%	7.5
United States	818	19.8%	2.5	325	21%	1.0
Sweden	233	5.6%	23.1	87	5.5%	8.6
France	167	4.0%	2.6	85	5.4%	1.3
UK	**160**	**3.9%**	**2.4**	**86**	**5.5%**	**1.3**
Russia	144	3.5%	1.0	75	4.8%	0.5
Switzerland	124	3.0%	14.3	70	4.4%	8.1
Denmark	61	1.5%	10.5	28	1.8%	4.8
Australia	57	1.4%	2.2	21	1.3%	0.8
Italy	49	1.2%	0.8	31	2.0%	0.5

Source: European XFEL monitoring data

There are six different instruments in the European XFEL facility, each with different properties (e.g., in terms of wavelength and intensity) and adapted for a different purpose. All six allow for the study of ultra-fast processes, but only three (namely MID, SCS, and SPB) allow for the study of tiny structures, while two (HED and SQS) allow for the study of extreme states. These instruments became operational at different points in time: FXE (which enables research into rapid changes in molecules) and SPB opened in September 2017, while SQS and SCS opened in 2018, followed by MID and HED in 2019.

The two most popular instruments for UK users are SPB, which helps to determine the structure of single particles (42 users, 37%), and HED, which investigates matter under extreme conditions using radiation (40 users, 35%). Both instruments have a similar number of users, even though the former has been operational for two extra years. By way of comparison, when considering which instruments all European XFEL visitors have used (to September 2022), only 18% used HED, demonstrating a much stronger UK interest in this instrument relative to other countries.

Figure 1 UK users of European XFEL per instrument September 2017 - June 2022



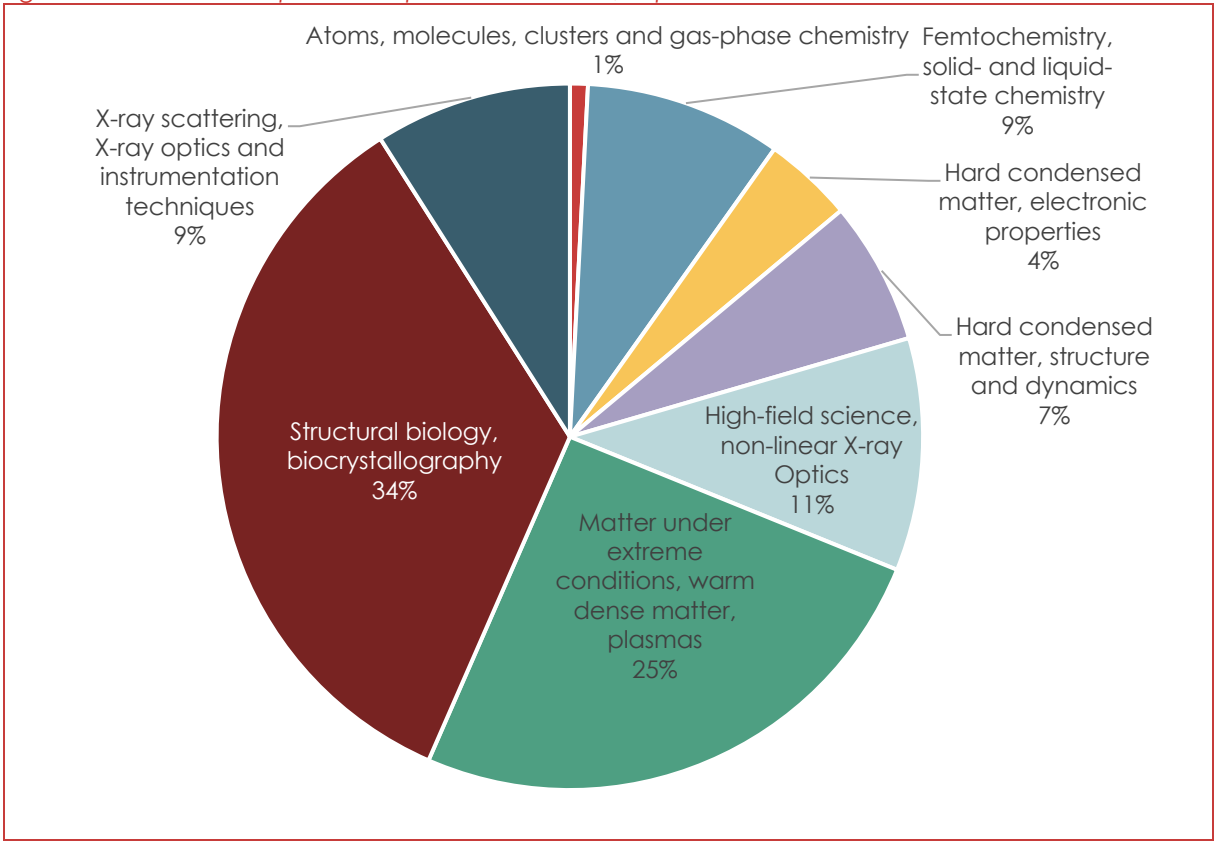
Source: European XFEL monitoring data (n=114)

3.3 Disciplines that have benefited from European XFEL

Access to the European XFEL has supported research in a wide range of scientific areas with important sector applications. The most popular area of scientific research for UK users is structural biology, which explores the structure of biomolecules and biological entities (e.g., proteins, cells) to support the development of pharmaceutical products and therapies (42 users, 34%). European XFEL has demonstrated superior performance over similar facilities in this field due to its ability to obtain higher resolution information from very small nanocrystals. For these reasons, stakeholders have described that European XFEL has been particularly important to those working in protein crystallography, and spectroscopy in chemistry.

Due to its properties, the laser has also been used to provide insightful explorations into the structure and behaviours of matter under extreme conditions, providing important applications in fields such as nuclear fusion and laboratory astrophysics (31 users, 25%). Overall, UK users pursuing research in these two fields account for more than half of all UK users.

Figure 2 UK users of European XFEL per scientific area, September 2017 - June 2022



Source: European XFEL monitoring data (n=122)

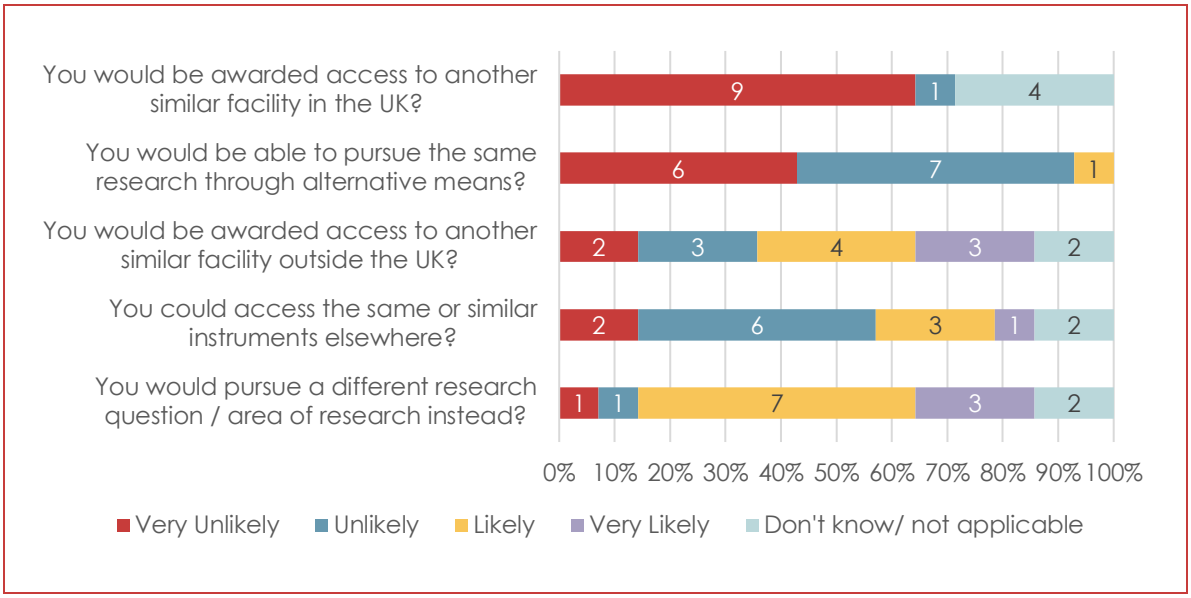
Very broadly speaking, the UK's usage of European XFEL has mirrored that of all users of the facility. The main areas of divergence are 'matter under extreme conditions' which accounted for 25% of all UK users but only 10% of all users, and 'atoms, molecules, clusters and gas-phase chemistry' which accounted for only 1% of UK users but 11% of all users.

3.4 Supporting research that could not occur elsewhere

The user survey evidence suggests that there are many cases where European XFEL has helped support research that would not be possible elsewhere. As shown in Figure 3, of the 14 respondents[3], 93% (13) stated that it was either "unlikely" or "very unlikely" that they would be able to pursue the same research they had undertaken at European XFEL through alternative means. Furthermore, 71% of respondents (10) indicated that without European XFEL access, it was "likely" or "very likely" that they would have pursued a different research question instead. This indicates that without European XFEL access, there are entire UK research areas that would be at risk, especially given that nearly 65% of respondents stated that it was very unlikely that they would be awarded access to another similar UK facility to continue their work.

[3] As set out in the separate methodology paper, these 14 responses equate to a 13% survey rate with the survey having been sent to 109 individuals registered as UK-based users by the facility. This response is broadly in line with typical response rates for online surveys of this kind.

Figure 3 Survey responses to: "If the UK were not a member of European XFEL, how likely is it that..."



Source: European XFEL user survey results

Stakeholder consultations have helped reveal reasons why some of the research undertaken at European XFEL is so difficult to undertake elsewhere.

Some spoke of how their research was only possible at XFELs, including European XFEL. They spoke of how facilities like Diamond and CLF don't offer the peak brightness and brilliance that XFELs do – therefore without XFELs, they would not have the means to continue their research.

An area where European XFEL offers added value relative to other facilities is in terms of the sample preparation facilities on site. Other XFELs lack such facilities, meaning that samples need to be prepared off site. Biological samples in particular start to deteriorate straightaway and if they are subject to customs delays following international travel, then the samples may not be usable by the time they reach the beamline. Being able to prepare samples on site at European XFEL mitigates against some of this risk and therefore can support some UK-based research much more easily than other international facilities might be able to.

The vignette below exemplifies the centrality of European XFEL to some ground-breaking UK-led science.

European XFEL and the UK's work in Serial Femtosecond Crystallography

Serial Femtosecond Crystallography (SFX) offers a new approach to protein crystallography, providing novel insights into the structure and function of molecular samples. European XFEL has helped a UK-based research group to advance SFX study, leading to a large number of research publications, and follow-on work including improved sample delivery.

Background

Serial Femtosecond Crystallography (SFX) is a relatively new discipline which has existed only for the last decade or so. It offers a new approach to protein crystallography. Traditionally, protein crystal studies using X-ray crystallography have involved rapidly freezing a large crystal and then rotating it while exposing it to a continuous X-ray beam. This one crystal yields many thousands of observations that are combined into a dataset, form which researchers can visualise nearly all the atoms within the crystal.

SFX offers a different approach. It involves exposing 10,000s to 100,000s much smaller samples (microcrystals) at room temperature in a sequential manner, each with a random orientation.

This means that each SFX dataset is built-up from thousands of samples at physiological temperature rather than a single, frozen sample. The technique enables scientists to study biological samples that are actively engaged in function during the data collection. It is particularly useful for rare, difficult to work with proteins, often involved in disease development, because many of these sample types only produce microcrystals.

A UK research group, led by Allen Orville at Diamond Light Source's XFEL Hub, a leading organisation in SFX science, has drawn on European XFEL considerably to advance the field of study.

How the facility has aided the research

Key to SFX research is being able to examine very small samples with very short X-ray pulses, as short as femtoseconds (a quadrillionth of a second). This approximately matches the time it takes to make or break chemical bonds. XFELs are thus a critical technology for SFX research, enabling scientists to create atomic-resolution 'movies' of complex chemical reactions. European XFEL is one of only a small handful of XFELs in the world, and it can deliver up 27,000 X-ray pulses per second, more than two orders of magnitude greater than others. According to research group representatives, UK SFX work has benefited from the geographic proximity of European XFEL's world class facility, including its state-of-the-art sample preparation facilities, helping make UK SFX research more time and cost efficient.

Impacts seen

European XFEL has enabled the UK SFX community to produce lots of novel data, often very quickly. This has led to a number of high-profile research publications which are now in the public domain. The work has also stimulated follow-on work for Dr Orville and colleagues, who are now working with European XFEL (and other facilities) to further SFX capabilities, such as the development of more efficient sample delivery.

There is a further element also of UK researchers not having as easy access to FELs as they do through European XFEL. Other FELs offer a very small portion of beamtime to international or non-subscribing members. UK researchers therefore have to compete with all other researchers from non-subscribing members for facilities which already have high demand as it is. The UK's membership to European XFEL helps provide easier access to FELs than is available elsewhere.

3.5 European XFEL and supporting high quality research

With journal articles having to go through peer review to enable publication, having a published journal article often indicates the presence of high-quality research. One indicator of European XFEL having supported high quality research is therefore the number of journal articles resulting from access to the facility.

Although the UK's involvement with European XFEL is relatively recent, there has still been sufficient time for it to help UK researchers produce published journal articles. UK researchers have been involved in 150 publications associated with European XFEL since its formation. The vast majority of these (136) involved UK-based staff at the facility, and most were published (105) from 2017 onwards when the facility become operational.

Looking firstly at UK staff publications (Table 2) our analysis[4] shows that the research reported in these publications has been across a diverse range of disciplines. While the vast majority of

[4] As the European XFEL monitoring dataset does not include information on the field of study, we assigned each publication to eight different scientific categories based on a list of key words provided in the LENS.org database, an open-source database with patent and scholarly work records. This list of key words was determined based on machine learning parsing of all accessible text in the research abstract of each record.

these publications (91%) centred on material science and physics, nearly half (49%) had a focus on methods and instrumentation which will have cross discipline relevance, while notable proportions of publications also covered other research areas such as chemistry, life sciences, and mathematics/computer science.

Table 2 Research area of research publications published by UK staff at European XFEL (2009-2022)

Research area	Number of publications	% of all publications (n=136)
Material Science / Physics	124	91%
Methods and instrumentation	66	49%
Chemistry	23	17%
Life Sciences	22	16%
Mathematics / Computer Science	19	14%
Engineering	5	4%
Environmental and Earth Sciences	4	3%
Medicine	2	1%

Source European XFEL monitoring data. Some publications will be relevant to more than one area

Since 2018, when the UK became a member of the facility, UK-based researchers have contributed to a further 14 published papers which cited European XFEL. As with publications by UK-based European XFEL staff, the vast majority of these (79%) have focused on methods and instrumentation and will therefore be relevant across many different disciplines. Nearly all of the publications also covered material science / physics (as per Table 3)

Table 3 Research area of research publications published by UK researchers at European XFEL (2009-2022)

Research area	Number of publications	% of all publications (n=14)
Material Science / Physics	13	93%
Methods and instrumentation	11	79%
Life Sciences	4	29%
Chemistry	3	21%
Mathematics / Computer Science	3	21%
Environmental and Earth Sciences	1	7%

Source European XFEL monitoring data. Some publications will be relevant to more than one area

3.6 European XFEL supporting multidisciplinary and interdisciplinary research

Based on our analysis of UK research publications that have cited European XFEL, it is clear that much of the high-quality research supported has been multi or interdisciplinary. For example, since 2009, UK-based European XFEL staff have produced 88 multi-disciplinary publications, representing 65% of the total published. Furthermore, of the 105 produced just in the period since the facility became operational in 2017, 69% (72) have been multidisciplinary, showing a tendency towards greater multidisciplinarity over time.

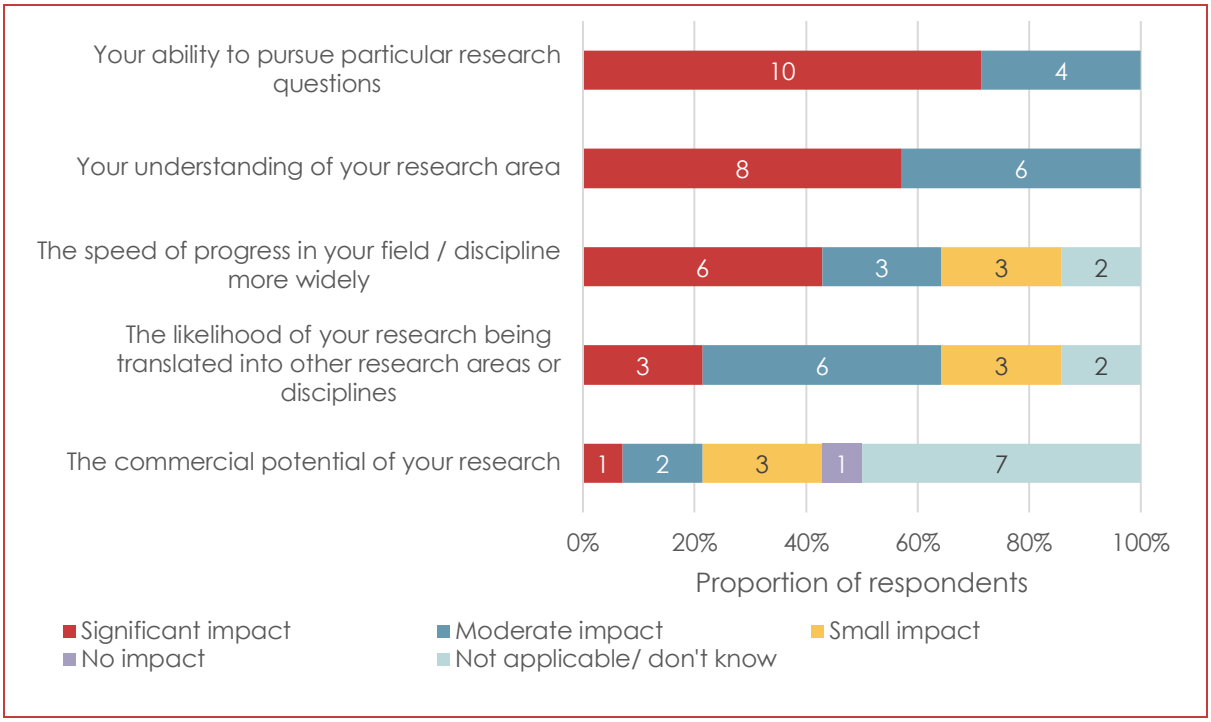
Levels of multi and interdisciplinarity appear stronger still amongst UK-based users of European XFEL. Of the 14 research publications involving UK-based researchers that have cited European XFEL, 12 (86%) had a multi or interdisciplinary focus.

By way of context for these figures, research by Fire and Guestrin (2019) found that between 2010 and 2014, 30% - 45% of all published academic papers were multidisciplinary.[5] This suggests that European XFEL has supported a higher amount of interdisciplinary research than might otherwise be expected.

3.7 Ways in which European XFEL has helped research

User survey respondents have helped indicate some of the specific ways that European XFEL access and usage has impacted on their ability to undertake their research. As shown in Figure 4, all respondents considered that European XFEL had either a significant or moderate impact on their ability to pursue particular research questions and on their understanding of their own research area. Also, more than 60% (9 respondents) stated that European XFEL has had at least a moderate impact on the speed of progress in their field and on the likelihood of their research being translated into other research areas or disciplines. 43% (6 respondents) also considered that European XFEL had at least a small impact on the commercial potential of their research.

Figure 4 Responses to "To what extent has European XFEL impacted on your own research activities?"

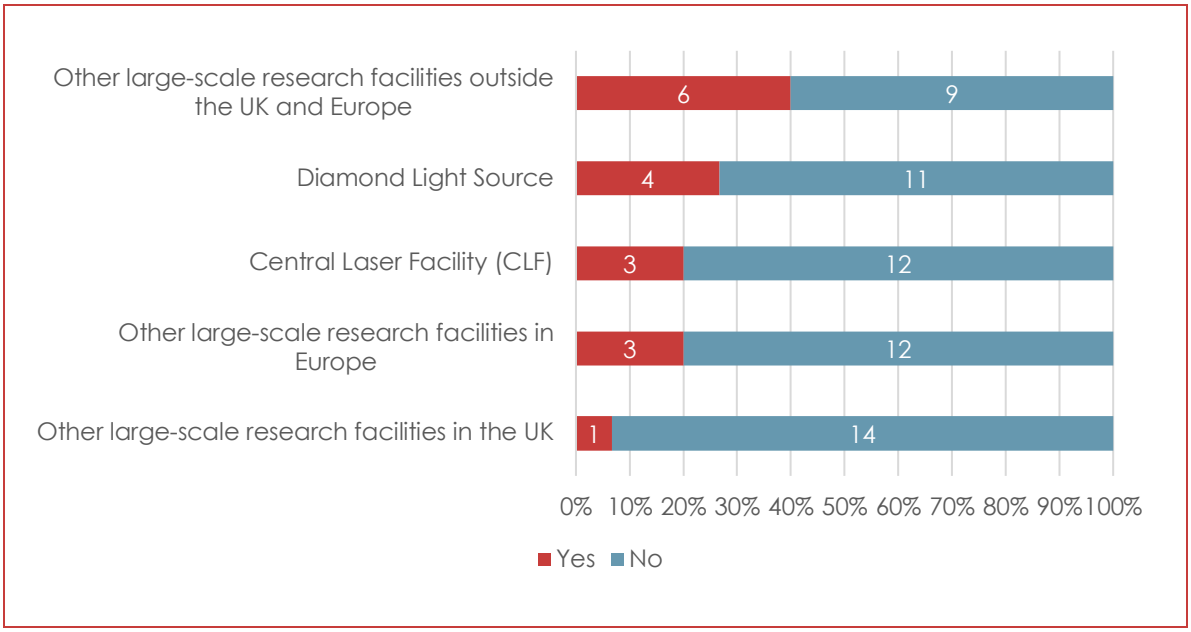


Source: European XFEL user survey results (n=14)

User survey respondents were also asked whether their research projects at European XFEL had also involved use of other facilities. This was the case for notable proportions of respondents: 27% (4) stated that they had used Diamond Light Source, 20% (3) indicated use of the Central Laser Facility, while 40% (6) said that they had used other large-scale research facilities outside the UK and Europe (see Figure 5).

[5] Fire, M. and Guestrin, C. (2019) 'Over-optimization of academic metrics: observing Goodhart's Law in action' in *GigaScience*, 8, 2019, 1-20.

Figure 5 Survey responses to "Has any of your research required the use of both European XFEL and any of the following together?"



Source: European XFEL user survey results (n=15)

Interviewed stakeholders provided some explanations as to the ways that European XFEL could help augment research taking place at other facilities, including those in the UK. One consultee spoke about the difficulties in securing time at other FELs. The need to reproduce experiments and results in a timely manner means that scientists may not be able to wait up to six months to secure beamtime in the same location where their previous experiment occurred. Access to European XFEL gives UK researchers more opportunity to secure beamtime to be able to re-run experiments. European XFEL also brought an advantage in terms of the number of pulses it can deliver to a sample in a given time period. This is especially important in the biological sciences where samples can deteriorate very quickly and therefore the ability to obtain multiple results from the same sample helps to make research more cost and time efficient.

It is clear from the evidence collected that involvement in European XFEL has already offered some additionality to the UK research community, despite its relative newness and issues with in-person access during the pandemic. The UK's XFEL user community undertakes specialist research, much of which is simply not feasible or possible at non-XFEL facilities. Certainly, interviewed stakeholders were clear that while UK facilities like Diamond and CLF could help support some research projects, these projects still had core experiments which required XFEL access. There are a very small number of XFELs across the world and all are over-subscribed – the UK's membership of European XFEL creates easier access to one XFEL for UK researchers that need it. European XFEL is also one of only two XFELs in Europe – the world's other XFELs are either in the USA or in East Asia. To that end, European XFEL also gives relevant UK researchers more geographically proximate facilities than would otherwise be possible, in turn helping make their research more time and cost efficient.

3.8 Wider benefits seen to scientific community

User survey respondents have also indicated that having European XFEL access had not only benefited their own research projects, but also wider activities that they had engaged in. There was a particular consensus on how working at European XFEL had brought benefits in terms of developing international connections. For instance, all 14 respondents to our user survey highlighted that European XFEL had at least a moderate impact on strengthening their international networks and relationships. Furthermore 95% and 85% of the 14 respondents also

confirmed at least a moderate impact on their ability to participate in international collaborations with European XFEL member states and on their national / international reputation, respectively.

The respondents have also noted a strong effect of working at European XFEL on their career progression, with all but two (12, 86%) highlighting a positive effect here.

Figure 6 Survey responses to "To what extent has European XFEL impacted on your own research activities?"

Source: European XFEL user survey results (n=14)

4 Skills impacts amongst users

In the previous section, we outlined how European XFEL usage has helped improve users' knowledge of their subject area. Primary research with European XFEL users and stakeholders has also demonstrated how facility usage has helped improve the broader scientific and research skills of research teams. This section explores these benefits in greater detail.

4.1 Summary

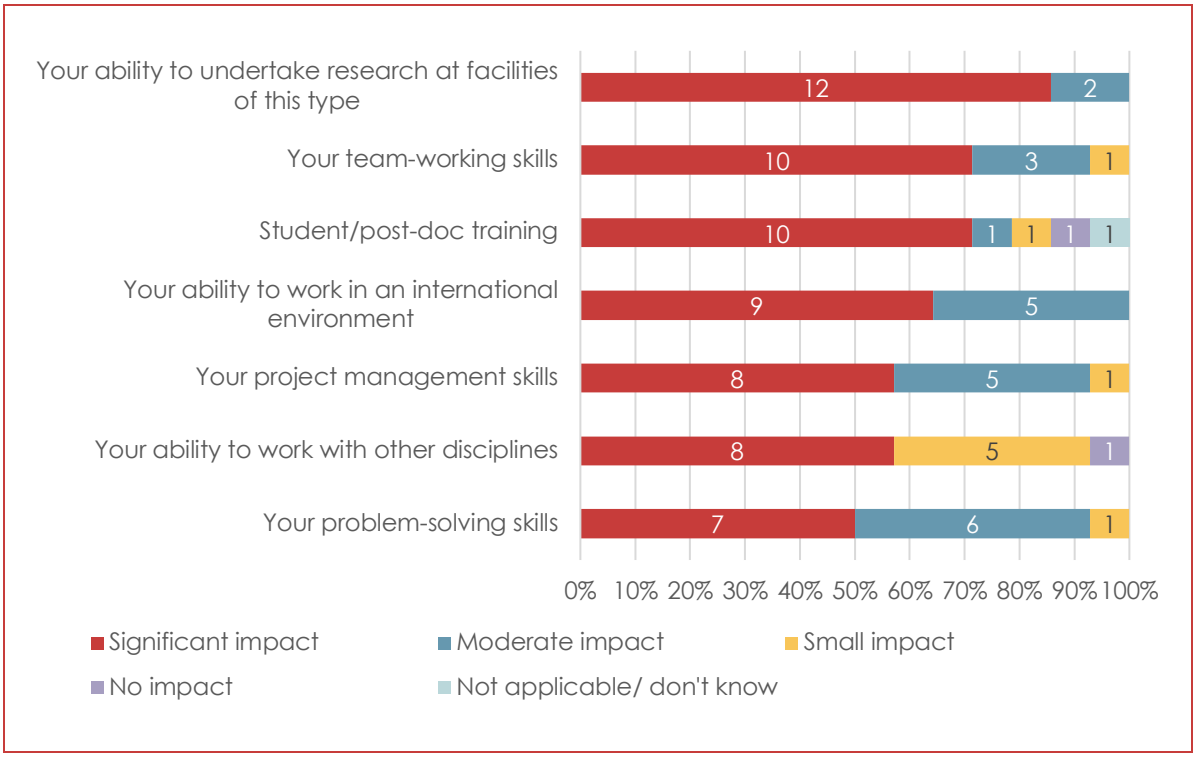
- European XFEL usage has played an important role in developing the skills and capabilities of UK-based researchers
- Commonly cited skills benefits include the ability to work in an international environment, team working skills, and project management skills
- Stakeholders have also said that European XFEL has provided a valuable opportunity to train early career scientists through funded visits there. This in turn will help to grow the nascent XFEL user community in the UK, thereby improving the skills supply chain
- European XFEL usage has also helped improve the skills and capabilities of the wider scientific community by enabling knowledge exchange across different research groups, and in facilitating educational outreach activity.

4.2 Improving user skills

As Figure 7 shows, the majority of respondents stated that their involvement with European XFEL had at least a small positive impact on them in all the listed skills and capabilities, as well as on their group or department. In particular, 70% reported a significant impact on their ability to undertake research at similar facilities. Interviewed stakeholders elaborated on this further, speaking of how access to European XFEL could help grow a nascent XFEL user community in the UK. On the one hand, it has helped more established researchers become more familiar with using XFELs, meaning they are better equipped to use European XFEL and other similar facilities in future. On the other hand, access to European XFEL has also provided a valuable opportunity to train early career scientists, thereby adding to the skills supply chain of UK researchers able to use such as facility. Consultees have spoken of how STFC has funded scientists to take PhD students with them to experiments at European XFEL, providing them with an opportunity to learn how to conduct research there.

The importance of European XFEL to the training of students and post-docs was emphasised in the user survey too, with over 70% of the 14 respondents indicating that the facility had had a significant impact in this area. Other commonly cited skills gained from facility usage were the ability to work in an international environment, team working and project management.

Figure 7 Survey responses to "To what extent has your involvement with European XFEL had a positive impact on the skills and capabilities of you and your group/department, in terms of:"



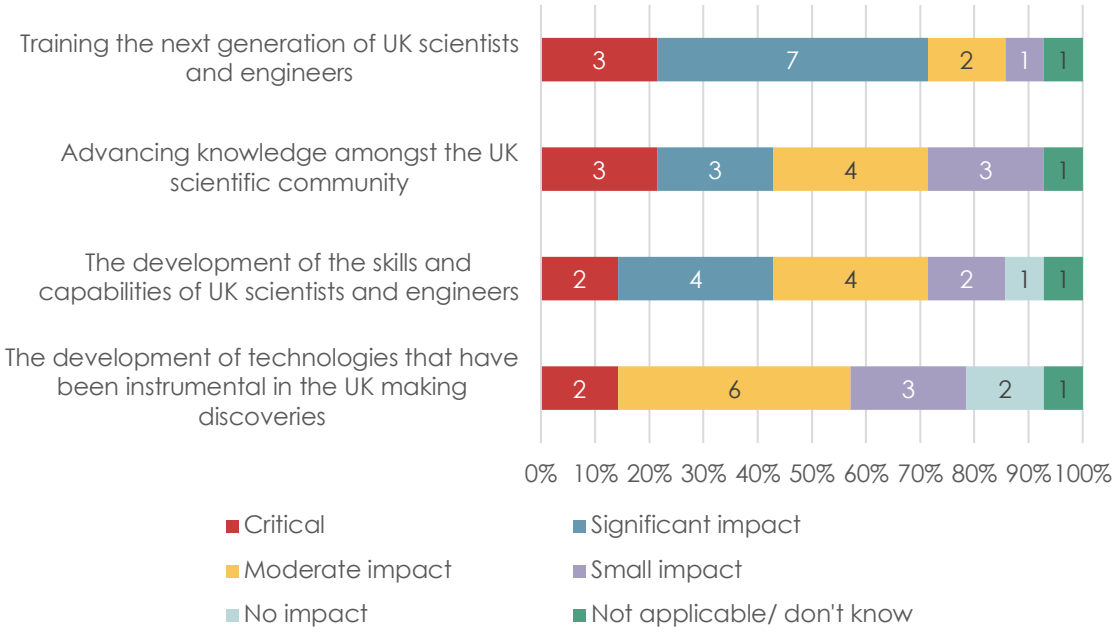
Source: European XFEL user survey results (n=14)

4.3 Improved skills and capabilities amongst the wider scientific community

Respondents to the user survey have also spoken of how UK access to European XFEL has contributed to an improvement in the wider skills base outside of the research groups using the facility. As shown in Figure 8, nearly all the respondents believed that European XFEL had had at least a 'small impact' in relation to training the next generation of UK scientists and engineers, something which the PhD training opportunities referred to above will have contributed to. Likewise, nearly all the respondents also felt that European XFEL had had at least a small impact in relation to advancing knowledge amongst the UK scientific community.

It also appears that the facility has helped share knowledge outside the UK scientific community too, with half of 14 respondents indicating that they had used their European XFEL-enabled research to support educational outreach activity. One example of such work comes from the XFEL Hub based at Diamond where STFC has funded researchers with the UK's serial femtosecond crystallography community to take early career researchers to European XFEL to see experiments being run there.

Figure 8 Survey responses to "How important has European XFEL been to the following?"



Source: European XFEL user survey results

5 Tackling wider UK policy & strategic objectives

Although not originally anticipated as a central impact pathway during the scoping phase, as the study has progressed, it has become clear that European XFEL has played an important role in contributing to wider policies and strategies. In particular, in meeting the strategic goals of STFC (particularly around securing the UK's involvement in and access to international infrastructures), but also in relation to other broader government policies.

5.1 Summary

- The UK's involvement in European XFEL has contributed to STFC being able to meet its strategic objectives around:
  - Protecting UK interests in international science facilities
  - Making an informed decision about a potential UK XFEL
  - Strengthening the UK's research and innovation community
- The UK's interactions with European XFEL have helped contribute towards some long-standing policy priorities, including finding alternative non-fossil fuel energy sources, improving health, and helping fulfil aims to become a science superpower by 2030.

5.2 European XFEL's contribution to protecting UK access to scientific facilities

As noted in their 2022-2025 Strategic Delivery Plan, one of STFC's strategic objectives is "*championing and promoting UK interests*" in world-leading international facilities.[6] Several consultees have spoken of how UK access to European XFEL contributes towards this goal, particularly in protecting the UK's interests with regards to XFEL science. Some stakeholders also spoke of how XFEL science is a research area that is gaining much more traction and interest. For example, consultees have spoken of how European XFEL is already over-subscribed and that there is a growing community of FEL scientists in the UK and globally more generally. However, the current geopolitical climate means that the UK may not necessarily have guaranteed access to other XFELs around the world. For instance, one consultee spoke of how China is currently constructing an XFEL in Shanghai, but it is uncertain whether the UK will have access to this. The UK's membership of European XFEL ensures that UK researchers have access to an XFEL at a time when increasing demand and geopolitical constraints may create difficulties in gaining beamline time elsewhere.

5.3 Enabling more informed decision making about a UK XFEL

As noted above, there is growing interest amongst UK scientists in XFEL science, so much so that in 2019 STFC published a peer-reviewed, science case for a UK XFEL. The 2022 STFC Strategic Delivery Plan takes this one step further, committing to undertaking a conceptual design and options analysis of a UK-based XFEL.[7] However, even interviewed supporters of a UK XFEL have acknowledged that the current community of XFEL scientists is currently very small and will need to grow before there is a strong case for a UK facility. The UK's membership of European XFEL ensures that UK researchers have access to a cutting edge XFEL and provides a basis for growing the UK XFEL community further. Rather than committing resources to a UK XFEL now, it gives policy makers an opportunity to assess how far and how quickly UK demand for XFEL science is increasing, and whether this is sufficient to justify expenditure in the UK. In other words,

[6] Science & Technology Facilities Council (STFC) and UK Research and Innovation (UKRI) (2022) *Delivery Plan*, p.13. Available at https://www.ukri.org/wp-content/uploads/2022/09/STFC-010922StrategicDeliveryPlan2022.pdf (accessed 8 November 2022)

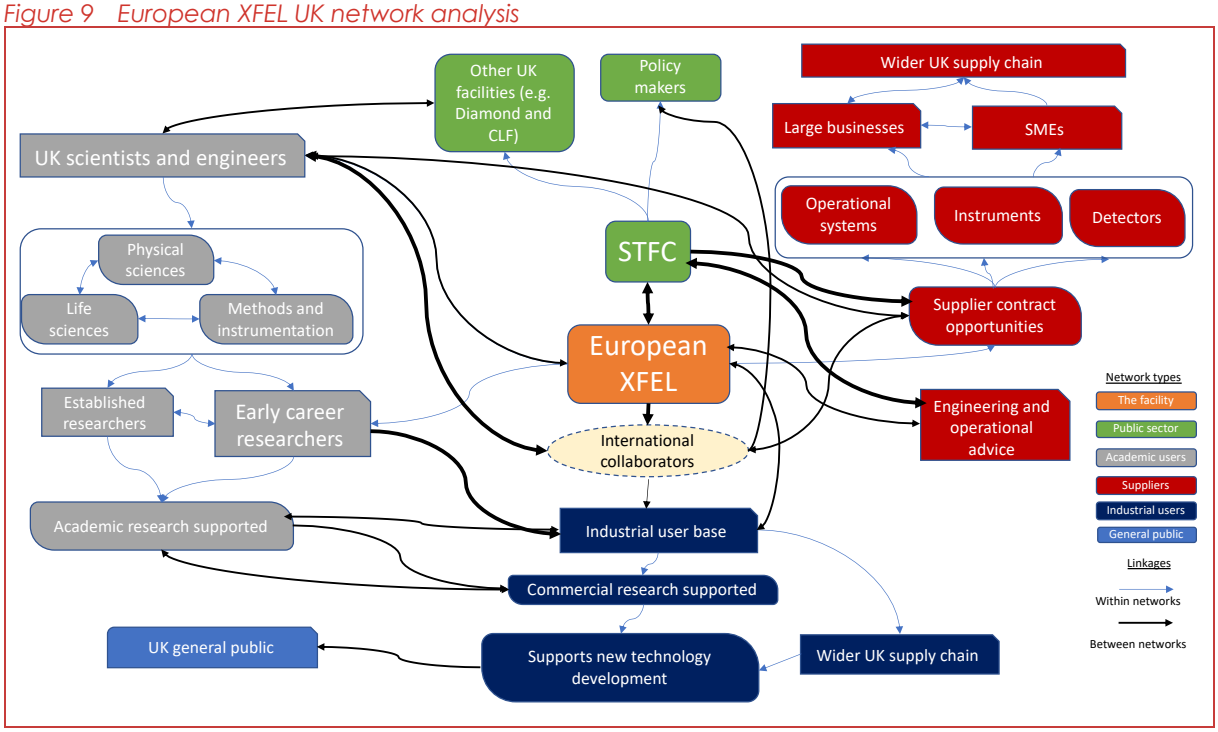
[7] Ibid. p. 34

having access to European XFEL helps give policy makers time to make a more informed decision as to whether there is strong case for a UK-based XFEL.

5.4 European XFEL's contribution to building stronger research and innovation partnerships

STFC's 2022 Delivery Plan also states ambitions for creating "*The conditions for an outstanding research and innovation system.*" This includes creating thriving ecosystems, better connected industry and academia, and creating better links between research and the general public.[8] European XFEL has played an important role in this, helping create a more joined up scientific community within the UK, as well as enhancing connections internationally. Figure 9 provides a network analysis for European XFEL, summarising the different UK networks that have benefited either directly or indirectly from European XFEL access, as well as the links that have formed between different network communities.

Figure 9 European XFEL UK network analysis



Source: Technopolis. Note that thicker arrows denote more important and stronger links

There are a number of mechanisms that are central to this community existing in the way it does:

- **Centrality of STFC**: STFC has a number of links to European XFEL which creates knock-on benefits for others, both in the public sector and in other networks. As a strategic partner of European XFEL, STFC has been able to share knowledge and ideas with researchers and management staff at European XFEL which can inform wider strategies, including a future UK XFEL. STFC has also created links for the suppliers' network. Not only is STFC an important supplier of European XFEL in its own right (including engineering and operational advice), it is also a conduit and facilitator for bidding opportunities for UK suppliers.

[8] Science & Technology Facilities Council (STFC) and UK Research and Innovation (UKRI) (2022) *Delivery Plan*, p.7. Available at https://www.ukri.org/wp-content/uploads/2022/09/STFC-010922StrategicDeliveryPlan2022.pdf (accessed 8 November 2022)

- **The interaction of UK scientists and engineers across multiple networks**: European XFEL has played a pivotal role in supporting the development of knowledge, skills, and capabilities of UK scientists and engineers in fundamental science. Fundamental research provides the building blocks for a variety of different applications, meaning that multiple networks have sought to draw on their European XFEL-developed expertise. UK scientists and engineers have contributed to outputs for the academic community, but have worked closely with European XFEL suppliers, and industrial users, both of whom have valued access to improved fundamental knowledge.
- **The role of early career researchers**: as noted in previous sections, early career researchers have been amongst the groups that have benefited the most from having access to European XFEL. They have had a chance to contribute to high profile research projects by working at European XFEL, and have also had an opportunity to learn new scientific and work skills. Much of this knowledge and skills are relevant to industry, meaning that industry is often keen to take on those that have trained at European XFEL.
- **The importance of international collaborators**: arguably one of the most important players in this research community are international collaborators, be they international researchers, or science policy makers in other countries. From a research perspective, European XFEL has been an important conduit in ensuring the UK has access to international collaborators, which has helped shape the outputs generated across all the other UK-based networks.
- **Development of societally relevant research:** European XFEL has enabled both academia and industry to undertake research on themes that are commercially relevant, addressing everyday issues such as healthcare, and clean energy. To that end, the UK's involvement in European XFEL is contributing to tackling societal concerns that the UK general public faces.

5.5 Meeting government policy priorities

The UK's involvement in European XFEL has also contributed towards addressing several wider government policy priorities, including:

- **Helping explore alternative energy sources**: In 2021 the UK government published a fusion strategy, setting out a desire to demonstrate the commercial viability of fusion as a sustainable low-carbon energy source, and to develop a world-leading fusion industry within the country.[9] Stakeholders have spoken of how fusion science can only be explored and better understood in facilities like FELs. The X-ray flashes they provide can for instance, help to analyse plasmas that could be exploited in future fusion reactors.[10] To that end, access to European XFEL will give the UK a means to develop its fusion science capabilities, and inform the development of new long-term energy low-carbon energy sources.
- **Becoming a science superpower**: In March 2021, the Government set an ambition to be recognised as a Science and Technology Superpower by 2030, "remaining at least third in the world in relevant performance measures for scientific research and innovation, and having established a leading edge in critical areas."[11] Stakeholders inside government have spoken of how they view European XFEL as being a valuable asset to the UK, helping enable the UK to achieve this science superpower goal.

[9] BEIS (2021) *Towards Fusion Energy: The UK Government's Fusion Strategy*

[10] https://www.xfel.eu/science/energy/index_eng.html (accessed 13 September 2022)

[11] HM Government (2021) *Global Britain in a competitive age: The Integrated Review of Security, Defence, Development and Foreign Policy*, p. 7

- **Improving health:** UK researchers have worked on projects that have used European XFEL to better understand new drugs, while a research project led by the University of Sheffield has also used the facility to test ways of potentially treating water using copper and light, as showcased in the vignette below.

European XFEL and research into light activated antibacterial water treatment

A research group based at the University of Sheffield has used the FXE instrument at European XFEL to understand the structural changes that occur when copper complexes absorb light. This has helped improve their understanding of which copper complexes will be most effective as a cheap and easily scalable form of water treatment.

Background

Copper complexes have potential applications in water purification. When a copper complex absorbs light, it is promoted to a higher energy state, and if it interacts with oxygen in this high energy state then it is able to convert oxygen into a much more active and reactive form. This more reactive form of oxygen is in turn more able to kill pathogens such as bacteria. It has been shown by the Weinstein group at the University of Sheffield, in collaboration with Prof David Kelly's group and Prof Mike Ward's group, that one of the complexes achieves the threshold, set by the World Health Organisation, to be classified as a "highly protective" method for water treatment.

There has been growing interest into light-driven processes involving copper complexes - understanding these processes will enable the development of more efficient copper complexes for antibacterial applications in real world settings. A research group, led by Professor Julia Weinstein at the University of Sheffield, has looked to examine these questions, seeking to understand how the structures of different copper complexes lead to change in the excited stage (i.e. when they absorb light), and how long these changes last for. The research group has used the FXE instrument at European XFEL to help examine what changes occur at the molecular level in real time.

Research impacts

Use of European XFEL has helped Professor Weinstein and her research group understand the structural changes that occur when copper complexes absorb light. They have used the facility to help examine geometry changes in real time, and are using this information to help determine which complexes are best suited for application in antibacterial water treatments going forward. Thus far, they have examined the capabilities of these complexes in a laboratory, showcasing efficient killing of bacteria including methicillin resistant S. Aureus (MRSA) and E. Coli. They are currently investigating the complexes involved in the processes but will be investigating optimal setups for delivering this water treatment.

Wider impacts

Analysis by UNICEF and the World Health Organisation (WHO) in 2019 found that 1 in 3 people globally did not have access to safe drinking water. The hope is that Professor Weinstein's research will contribute to addressing this issue. The research is hoping to better understand the mechanism by which the copper complexes produce reactive oxygen species needed to kill bacteria. By understanding which copper complexes work best, the research will help develop more effective water treatment systems in the future. In addition, the research team has recognized that copper is a cheap and readily available metal. This means that solutions developed through the research could be more easily scaled up, and more cheaply implemented worldwide.

6 UK's international standing

The UK's involvement in European XFEL has helped contribute to the UK's international standing within the scientific community. As outlined below, facility access has helped secure the UK's involvement in international collaborative research projects, as well as providing the country with diplomatic and 'soft power' advantages too.

6.1 Summary

- European XFEL has played an important role in fostering and enabling international collaboration opportunities for UK researchers. Nearly all of the UK -authored publications that have cited the facility have had at least one international partner
- The facility has also facilitated interaction between UK researchers and international funders, with UK-authored publications that are citing European XFEL typically receiving funding from three different countries
- Stakeholders have commented that such international collaborations are now more difficult following the UK's departure from the European Union, and potential departure from the Horizon Programme. European XFEL therefore provides a vital conduit for pan-European collaborations, and also helps give UK research greater profile
- Involvement in the facility also helps showcase the UK's best practice in research management and governance, and gives the UK influence over international science policy and decision making.

6.2 Creation of international collaboration opportunities

A study of the UK-authored publications that have cited European XFEL provides evidence that access to the facility has facilitated collaborations between the UK and researchers from across the world. As Table 4 shows, from the list of 150 publications with UK authors (either UK staff at European XFEL, or UK-based users), all except one included at least one international partner. On average, UK researchers have worked with approximately five international collaborators but roughly a quarter of publications reported a higher number of international collaborators than this. UK researchers were most likely to collaborate with authors from Germany and the United States, with 99% and 87% of publications co-authored with researchers from these two countries.

Table 4 Number of European XFEL publications co-authored with UK researchers/staff, 2009 - 2022

	Staff	Users	All
UK researchers only	**1**	**0**	**1**
United Kingdom	**136**	**14**	**150**
Germany	135	14	149
United States	116	14	130
France	55	6	61
Sweden	30	3	33
Czechia	27	3	30
Australia	15	7	22
Russia	19	0	19
Poland	17	1	18
Netherlands	17	1	18
Japan	14	2	16

Italy	13	3	16
Switzerland	12	3	15
China	13	1	14
Ireland	12	2	14
Hungary	9	3	12
Spain	9	2	11
South Korea	9	2	11
Canada	6	0	6
Austria	5	0	5
Slovakia	4	1	5
Singapore	4	1	5
Norway	4	0	4
India	4	0	4
Slovenia	2	1	3
Portugal	2	0	2
Romania	2	0	2
Denmark	1	0	1
Finland	1	0	1
Belgium	1	0	1
Greece	1	0	1
New Zealand	1	0	1
Mexico	1	0	1
Turkey	1	0	1
Saudi Arabia	1	0	1

Source: European XFEL monitoring data

Table 5 provides further evidence that European XFEL supports international collaboration. It shows, UK authored publications that have cited European XFEL have on average, received funding from three different countries. Furthermore, approximately 36% of publications had more funders than this average. In terms of the funding sources, two-thirds of all publications have benefited from US funding, and 57% have received funding from European institutions, including the European Research Council, and the European Commission.

Table 5 Countries providing funding for European XFEL research with UK involvement

	Staff	**Users**	**All**
UK funders only	**8**	**0**	**5**
United States	88	12	100
European institutions	75	11	86
United Kingdom	**69**	**4**	**73**
Germany	57	12	69
Singapore	40	7	47
France	13	4	17
Czechia	13	1	14
Russia	11	0	11
Poland	8	1	9

South Korea	7	2	9
Japan	7	0	7
Sweden	6	1	7
China	6	0	6
Switzerland	4	1	5
Italy	3	2	5
Australia	3	2	5
Hungary	4	0	4
Netherlands	4	0	4
Spain	2	0	2
Portugal	2	0	2
India	2	0	2
Slovakia	1	0	1
Slovenia	1	0	1
Ireland	1	0	1
Romania	1	0	1
Norway	1	0	1
Canada	1	0	1
New Zealand	1	0	1
Turkey	1	0	1

Source: European XFEL monitoring data

6.3 Greater international influence

Feedback from interviewed stakeholders is that membership of European XFEL has helped give the UK greater influence within the global scientific community. They argued that in part, this improved influence came from the fact that European XFEL provides international collaboration opportunities, such as those outlined above. Stakeholders spoke of how the UK's departure from the European Union and potential departure from the Horizon Programme means it is more difficult (at least in the short term) to secure European collaborations. While the Government is pursuing bilateral agreements for joint working with other nations, membership of European XFEL does facilitate access to more pan-European research groups too.

One stakeholder spoke of the role that European XFEL plays in helping showcase the UK's abilities at leading and managing international science projects effectively and efficiently. By sitting on the European XFEL Council, STFC is able to showcase its best practice in research management and governance, for instance, the plans it has in place to become net zero by 2040.[12]

6.4 Maintaining science diplomatic relations with other nations

Stakeholder interviews have also highlighted the fact that policy makers and key decision makers within the UK scientific community view membership of European XFEL as a valuable policy asset. The UK's involvement provides some 'soft power' and influence with other countries in science policy decision making and helps to confirm the UK's commitment to collaborating in research in Europe, following Brexit. The UK for instance, meets with France and

[12] See https://www.ukri.org/news/green-transformation-for-uk-science-estate/

Germany every year to discuss the three nation's participation on research infrastructures, including possible financial contributions going forward. The UK's involvement in European XFEL helps give it some leverage in such discussions that it would not otherwise have. The UK's shareholding in the facility has also meant that it has been able to contribute to discussions around future access that some nations will have to European XFEL. Such are the diplomatic benefits of facility membership that one stakeholder went so far as to say that were the UK to withdraw from European XFEL, there would definitely be a diplomatic fallout for the country.

7 Benefits to the UK in supplying European XFEL

A number of UK organisations have benefited from securing contracts to supply European XFEL with goods and services. This chapter summarises the types of benefit they have seen.

7.1 Summary

- European XFEL estimates that in the period 2018 to 2020, 65 UK-based companies supplied goods and services to the facility. Between them, these suppliers had contracts worth €700k
- The goods and services that UK suppliers have provided have varied considerably, including cameras and components, floor cranes, and gas safety consultancy
- Outside the commercial sector, STFC has secured two high profile contracts to provide European XFEL with detectors and the DiPOLE D100-X Laser. Both are flagship projects that have helped enhance STFC's reputation, and helped improve the organisation's skills base.

7.2 Businesses that have worked for European XFEL

Currently, available data does not provide precise information on the number of UK organisations that have secured contracts with European XFEL. In large part, this is due to the way that European XFEL captures data on its suppliers, recording the home country of a contractor's headquarters, rather than the location of the contractor's division that has secured the contract. Therefore, if a UK-based division of a French company, for example, wins a European XFEL contract, it is unlikely to be recorded as UK-won contract. Likewise, UK-headquartered businesses may win contracts that are serviced in another country.

Nevertheless, according to European XFEL's own internal analysis, during the period 2018 to 2020 (the latest available data), there were 65 companies that had supplied the facility that were either operating in the UK or were headquartered in the country. The types of goods and services that UK suppliers have provided have varied considerably, including cameras and associated components, heavy duty folding floor cranes, maintenance services, and gas safety consultants.

As part of separate analysis, the Industrial Liaison Office at European XFEL has estimated that the facility had given €700,000 worth of contracts to UK suppliers in 2020. Assuming that the facility awarded similarly valued contracts in both 2018 and 2019 too, then it suggests an approximate contract value was €30,000 per UK supplier. Of the 65 UK suppliers to European XFEL in the period 2018-2020, 10 (15%) have received more than €50,000 in funding commitments, demonstrating the facility has also given some organisations access to either repeat, or much larger value contracts still.

The Industrial Liaison Office at European XFEL highlighted the following UK-based contractors as being particularly important to them:

- FMB Oxford Ltd – the company has been involved in five mirror system projects that have involved the design, delivery and installation of European XFEL's Day Two instrument (D2). FMB Oxford has developed new, technically advanced designs that allow the cradling and bending of mirrors, as well as active cooling control and detectors.[13]
- Lasermet Ltd – the company has developed a laser interlock safety system for the SASE3 instrument. Lasermet has needed to develop a new system that is a departure from the ones they commonly develop[14]

[13] https://fmb-oxford.com/2741-2/

[14] https://www.lasersystemseurope.com/feature/beam-blockers

- Korvus Technology Ltd – the company has developed the HEX-L deposition system for the HED instrument, a film deposition system which enables the preparation of samples at European XFEL, ready for characterisation.[15]

Vignettes for FMB Oxford and Lasermet below set out in more detail the types of benefit that UK businesses have seen.

Supplier benefits – FMB Oxford

Background

FMB Oxford, has nearly 30 years of experience in synchrotron beamline development. Employing around 60 scientists and engineers, FMB Oxford offers services for the development of beamline components, control systems, monochromators, mirror-systems, and detectors. Given its expertise, the company was contracted by European XFEL to produce components for XFEL instruments. The involvement particularly focused on the high precision positioning system and development of mirrors, mounts, and benders.

Work for the facility

By 2016, FMB had conducted three projects to develop mirror systems (U-bender mirror) for European XFEL's SPB/SFX instrument. Among these was the work on mechanical bender system for mirrors, allowing for mirror support without gravity compensation, and for small corrections to be made to the shape of the mirror. Developed for high calibration and precision, FMB Oxford's work on the instrument's mirror systems led to the identification of possible flaws in measurements that could arise due to temperature differentiation. To address this, FMB conducted further work to introduce cooling controls leading to higher stability in the research environment.

Commercial and economic impacts

To service their European XFEL contracts, FMB Oxford needed to invest in new equipment and infrastructure, which in turn has left them better placed to secure other contracts elsewhere. For example, to meet the specifications for supplying the initial contracts to European XFEL, FMB upgraded their cleanroom to meet ISO6 particle free cleanroom specification required by European XFEL. Thus, engagement with European XFEL led to expansion of manufacturing infrastructure to meet higher quality specifications, and has also opened new commercial opportunities.

An FMB representative also acknowledged that signing contracts with European XFEL positively impacted their international visibility and standing in the international synchrotron market.

Skills impacts

According to an FMB representative, the collaboration with European XFEL required the team to develop new skills to approach issues related to the cooling system. The development of the new thermoelectric coolers likewise produced new know-how at FMB.

[15] European XFEL (April 2021) *Annual Report: ILO Report*

Supplier benefits – Lasermet

Background

Lasermet are a Bournemouth-based company that specialises in laser safety products and solutions. They have worked with European XFEL to develop safety systems for the SASE3 x-ray light source.

Work for the facility

Lasermet has developed an interlock safety system for SASE3. Lasers are commonly contained in a single laboratory, making it more straightforward to keep it in a single place and ensure they are not present in unintended areas. With European XFEL however, there are multiple rooms with multiple sources, being delivered to multiple targets. This makes it much harder to keep track of where a laser is – unintended exposure could lead to serious injury to users. Lasermet has been closely involved in the development of an interlock safety system for European XFEL which will help determine whether a laser (and associated radiation) is in a room or not, and ensure that beams cannot enter a room until a series of hardware-based safety procedures have first been met.

Benefits seen

It appears that the contract has helped raise Lasermet's profile. European XFEL's ILO team has already highlighted Lasermet as having been an important UK supplier to the facility, while the company's work for European XFEL has also featured in trade articles.[16]

7.3 STFC as a supplier to European XFEL

Outside the commercial sector, STFC has also experienced substantial benefits as a supplier to European XFEL. In September 2020, it secured a €160,000 contract to provide spare parts, maintenance and support to European XFEL. It was the twelfth largest contract awarded by European XFEL between July and December 2020. As shown in the following two case vignettes, STFC has also undertaken two other particularly high-profile contracts for European XFEL: the inputs by the Rutherford Appleton Laboratory to the Large Pixel Detector (LPD), and their work on the DIPOLE D100-X Laser. In both instances, the contracts have helped enhance the reputation of the UK's scientists with them being engaged in flagship and cutting-edge work. The advanced technical nature of both contracts has also helped improve the skills base amongst STFC's research team, and also played a role in maintaining the activeness of research and development skills in the UK.

Construction of the Large Pixel Detector

European XFEL required a detector with specific characteristics and therefore appointed STFC's Rutherford Appleton Laboratory (RAL) to deliver and design a detector that could meet these. The work has allowed RAL to improve its internal capabilities (including quality assurance processes) and helped give them the expertise to serve large scale projects at other facilities.

Background

With a repetition rate of 27,000 times per second and a unique timing structure, European XFEL required a unique detector with appropriate time-response characteristics to yield precise

[16] See for example article in Electro Optics: Electro Optics (2017) *Safe Surgery*. Available at https://www.electrooptics.com/feature/safe-surgery (accessed 10 January 2023)

results. However, when the European XFEL project was first launched, no commercial imaging detectors existed.

The Research Project

In 2006, STFC's Rutherford Appleton Laboratory (RAL) secured the 10-year contract to design and deliver a new detector capable of meeting the facility's requirements. Led by RAL's Detector and Electronics Division, the project included the design and fabrication of the first fully functional Large Pixel Detector (LPD) X-ray detector, including the development of a tile that can be butted on four sides and a new readout chip (ASIC) to handle the demands of the system.

The LPD was installed at European XFEL's Femtosecond X-Ray Experiments (FXE) instrument in 2017. With a total sensitive area of 250,000 cm^2, the LPD is a 1 megapixel detector containing 16 super modules and was the first X-ray detector to record at a rate of 4.5 MHz - 4.5 million pictures per second. This instrument is unique to European XFEL and enables researchers to observe ultrafast reactions and processes, including the formation and breaking of molecular bonds.

Impacts from research

Given the experimental nature and novelty of the detector, a substantial proportion of the project supported R&D activity. As a result, RAL has benefited from improved internal capabilities, developed to overcome the technical challenges relating to the instrument's hardware and construction, and software relating to operating the instrument and handling data. Due to the size and number of supermodules required, RAL also made improvements to their quality assurance process, e.g. through creating an auditable trail on quality and parts. The project also needed to develop supermodules that were easily swappable for servicing and maintenance. This allowed RAL to improve its capabilities in building safer and more user-friendly X-ray detectors.

Without the European XFEL contract, RAL believes it would not have developed large detectors. Prior to its European XFEL contract, RAL had not developed X-ray detectors of this scale. The project has therefore also given them additional capacity and capability to deliver future large-scale projects not only as part of follow-on activities at European XFEL, but also facilities like Diamond Light Source which has already used the Front-End Module (FEM) card developed for the LPD on a detector on its I13 Coherence beamline.

UK Participation in the HiBEF Consortium

The UK is a key player in the Helmholtz Beamline for Extreme Fields (HiBEF) consortium which develops experimental setups at European XFEL's High Energy Density (HED) beamline. STFC and EPSRC funded work into the DiPOLE 100 laser for the consortium, with the project helping showcase STFC and CLF capabilities, as well as helping forge relationships with international partners.

Background

The Helmholtz International Beamline for Extreme Fields (HiBEF) consortium works to contribute and operate different experimental setups at the High Energy Density (HED) beamline of the European XFEL. The consortium was established to extend the scope of research that could be carried out at the European XFEL beyond baseline instruments by pooling consortium members' equipment and resources. Founded in 2013 by DESY and Helmholtz-Zentrum Dresden-Rossendorf (HZDR), HiBEF involves a user consortium involving more than 350 scientists

at 60 research institutions in 16 countries, including the UK Science and Technology Facilities Council (STFC).

The Project

The UK contributed to the HiBEF User Consortium by constructing the DiPOLE 100 laser (Diode Pumped Optical Laser for Experiments) which was jointly funded by STFC and the Engineering and Physical Sciences Research Council (EPSRC). The laser was manufactured, assembled, and tested by the STFC's Central Laser Facility (CLF), before being shipped to Germany and installed on the HED instrument in 2019. As the first user experiments will begin in the spring of 2023, the instrument has not yet supported any material outputs.

The development and installation of the laser was driven by demand from the user community for a high-energy laser for compression experiments. The unique combination of the European XFEL and the DiPOLE laser will generate conditions similar to the interior of Earth-like exoplanets. Using this instrument, researchers will be able to probe the atomic structure and dynamics of materials under the extreme conditions found within the core of a planet, potentially opening up a new field of laboratory astrophysics. The conditions generated are also relevant to other research fields, including examining the fundamental science of the strength of materials under rapid deformation, and the potential synthesis and recovery of novel materials.

Impacts

The UK's work on the DiPOLE laser has helped to showcase the work and capabilities of the CLF, as this laser enables data collection at rates thousands of times greater than at other competitor FEL facilities in the USA and Japan. There have also been some important skills benefits for CLF staff, as there have been considerable design challenges in adapting DiPOLE to fit alongside the HED end-station.

There have also been some more internationally dimensioned benefits, with the UK's participation in HiBEF providing the platform to build stronger collaborative relationships with EU facilities and research partners, and for researchers to explore novel, cutting edge areas of research.

8 Commercial and economic impact from users

As well as generating academic and research benefits, UK-based European XFEL users have also generated commercial and economic benefits for the UK, both in terms of generating economic activity, and in helping attract and retain skilled talent within the country.

8.1 Summary

- There is evidence of some UK businesses already undertaking fundamental research at European XFEL. These have potential to generate revenue benefits in the future
- As the UK user base at European XFEL grows over time, it is reasonable to also expect greater industrial use of the facility, either directly or indirectly
- At a macroeconomic level, research groups have found it easier to attract and retain talented and high skilled scientists because the research group has used European XFEL.

8.2 Usage of European XFEL for commercially focussed purposes

Data are not systematically collected on the number of industry users that have accessed European XFEL, nor the number of academic users that are conducting research on behalf of or in collaboration with industry. Nevertheless, we are aware of some UK businesses that have conducted research at European XFEL, thereby demonstrating the potential of the facility to generate economic activity within the UK.

A notable example is the Cambridge-based Heptares Therapeutics who, since 2019, has collaborated with European XFEL staff on a research project to better understand G protein-coupled receptors (GPCRs), structure-based drug design and targeted drug delivery.[17] While the work at European XFEL has focused on fundamental research, drugs developed for this human protein account for almost 40% of all prescription drugs on the market to date. Therefore, it is perfectly possible that the research developed will be translated to new or improved pharmaceutical products in future. To that end, we can expect to see some additional sales and revenue that is at least partially attributable to the work at European XFEL.

While we have to date found limited instances of the UK being engaged in commercially focused work via European XFEL, we can reasonably expect greater commercial activity to emerge in the future. Stakeholders commented that they expect the user community to grow, and for there also to be new opportunities emerge for collaboration with industry.

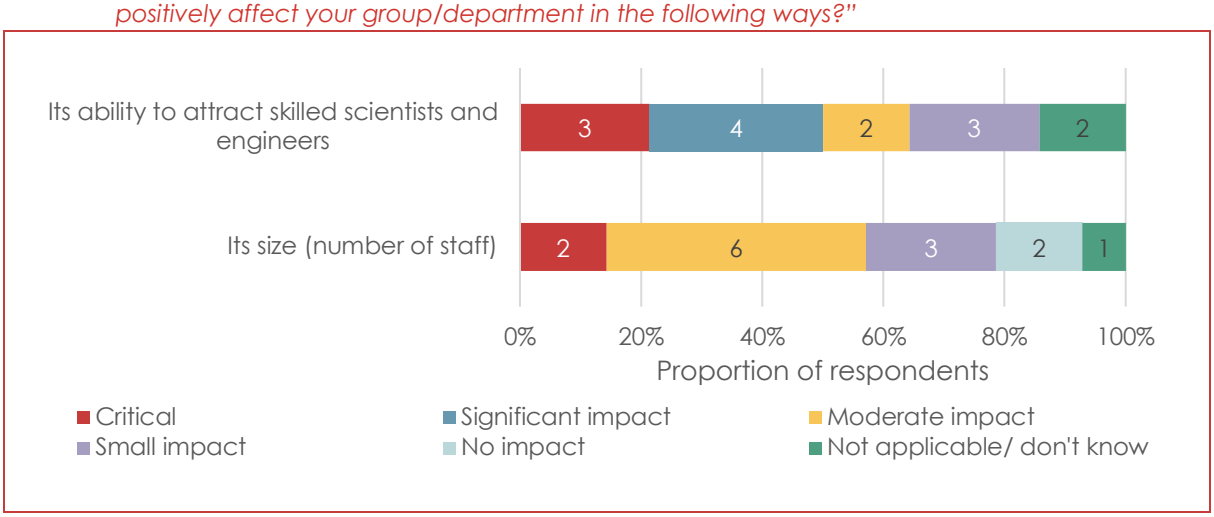
8.3 Impacts on the wider economy

Evidence from the user survey also suggests that activity by academics and industry at European XFEL has generated some labour force benefits for the UK economy. As shown in Figure 10, 85% of respondents (12) have seen at least a small impact on their ability to attract skilled scientists and engineers to their group or department. Indeed, three of the 14 respondents (21%) indicated that European XFEL had been 'critical' in attracting a skilled workforce, again emphasising the facility's importance in helping secure a certain talent base in the UK economy. Additionally, 60% of the 14 respondents indicated that European XFEL membership may have had a moderate impact on employment, stating that their workforce would have been smaller in the absence of the facility. The results, however, should be treated with an element of caution. There is no evidence to suggest that all of this cited employment will be additional, and one would certainly expect a certain level of deadweight and

[17] European XFEL (2020) *European XFEL Annual* Report, p. 75. Available at. https://www.xfel.eu/sites/sites_custom/site_xfel/content/e35178/e56171/e56388/xfel_file136638/AnnualReport_2020_DigitalVersion_eng.pdf (accessed 19 September 2022)

displacement. Nevertheless, it would be reasonable to expect at least some levels of additionality associated with the employment generated.

Figure 10 Survey responses to "To what extent does UK membership of/involvement in European XFEL positively affect your group/department in the following ways?"



Source: European XFEL user survey results (n=14)

9 Summary and conclusions

9.1 The UK's involvement in European XFEL

- Founded in 2009 and operational since 2017, the Hamburg-based European XFEL is a laser facility that generates ultrashort X-ray flashes. This enables users to study ultrafast processes such as chemical reactions, or the configuration changes of biomolecules
- The UK joined as a European XFEL member state in March 2018, contributing approximately 2% of the facility's construction costs, and making an annual contribution worth around 2% of its annual operational budget
- Full operations at European XFEL did not start until 2019. This, coupled with the pandemic preventing many in-person experiments, means that the UK has only been involved in a limited number of experiments per year thus far
- Nevertheless, our analysis has shown that the facility has already generated benefits to the UK in the following areas:
  - Scientific and research benefits
  - Commercial and economic benefits
  - Skills benefits
  - UK benefits from supplying the facility
  - UK's international standing

  The main findings of the study in each area are summarised in the sub-sections below.

9.2 Science and research benefits

- The UK's usage of European XFEL has exceeded its shareholding, showing the country has used the facility more than would be expected
- European XFEL supports a diverse range of disciplines in the UK. While a lot of work has focused on structural biology and matter under extreme conditions, a substantial amount of work on methods and instrumentation has also been undertaken, which has cross discipline relevance
- European XFEL has also supported the UK in producing high quality research, being cited in many UK-authored research publications. The majority of these publications have been multidisciplinary (69%), a proportion that is larger than would typically be expected
- European XFEL has offered unique capabilities to UK researchers, enabling experiments which are not feasible at other facilities. XFELs around the world are over-subscribed, so European XFEL has also been useful in providing UK researchers with additional capacity.

9.3 Skills benefits

- European XFEL has played an important role in developing the skills and capabilities of UK-based researchers, particularly in being able to work in an international environment and gaining opportunities to exchange knowledge and ideas with international researchers
- European XFEL has provided a valuable opportunity to train early career scientists. This in turn will help grow the nascent UK XFEL user community, improving the skills supply chain

9.4 UK policy and wider strategic objectives

- The UK's involvement in European XFEL has contributed to STFC being able to meet its strategic objectives around:
  - Protecting UK interests in international science facilities

- Making an informed decision about a potential UK XFEL
- Strengthening the UK's research and innovation community

- The UK's interactions with European XFEL have also contributed towards some long-standing wider government policy priorities, including finding alternative non-fossil fuel energy sources, and helping fulfil aims to become a science superpower by 2030.

9.5 The UK's international standing

- European XFEL has played an important role in fostering and enabling international collaboration opportunities for UK researchers. Nearly all of the UK-authored publications that have cited the facility have had at least one international partner, while UK-authored publications have also on average received funding from three different countries
- The ability to collaborate internationally also has helped make UK research at European XFEL more impactful
- Involvement in the facility also helps showcase the UK's best practice in research management and governance.

9.6 Benefits from supplying the facility

- European XFEL estimates are that between 2018 and 2020, 65 UK-based companies supplied goods and services to the facility. Between them, these suppliers had contracts worth €700k. These suppliers have provided a wide variety of different goods and services including cameras and components, floor cranes, and gas safety consultancy.
- Outside the commercial sector, STFC has secured two high profile contracts to provide European XFEL with detectors, and the DiPOLE D100-X Laser. Both are flagship projects that have helped enhance STFC's reputation, and helped improve the organisation's skills base.

9.7 Commercial and economic benefits

- Stakeholder feedback is that there has been relatively little industry usage of European XFEL to date. However, there is evidence of some UK businesses undertaking fundamental research at European XFEL. These have potential to generate revenue benefits in the future.
- At a macroeconomic level, research groups have found it easier to attract and retain talented and high skilled scientists because the research group has used European XFEL.

Part 2: Evaluation framework

10 European XFEL future monitoring and evaluation framework

In this chapter, we present our proposal for a monitoring and evaluation framework that STFC could use as the basis for tracking the benefits flowing from the UK's involvement in European XFEL. The framework is also designed to support future independent evaluations by ensuring a more wide-ranging and complete record of achievements across each impact pathway.

10.1 Design assumptions

The framework draws on the approach adopted for the current study, which has been shown to provide useful and reliable evidence as to the impact of European XFEL membership for the UK. We have however, simplified and consolidated some of impact areas proposed, and provided a clearer elaboration of the role for STFC in creating and collating information.

Table 6 Overall structure for impact areas – benefits from UK investment in European XFEL

Area	Benefits to UK
1. World-class science and research	1.1 Pushing the frontiers of human knowledge & understanding, enabling further scientific progress 1.2 Sustaining the UK's research excellence & leadership through access and opportunities at European XFEL 1.3 Supporting the UK's involvement in multidisciplinary and interdisciplinary activity 1.4 Attracting investment & talent via improved perceptions of the UK as a leading research nation
2. World-class skills	2.1 Increased skills and capabilities of the UK workforce 2.2 Increased (future) UK STEM workforce
3. The UK's international standing	3.1 The UK's influence in the international science and technology landscape 3.2 Improved diplomatic relations and engagement 3.3 The UK's image as a 'great science and innovation nation' 3.4 The UK's ability to engage with and/or lead international research collaborations
4. World class innovation	4.1 UK benefits from the wider application of European XFEL-derived technologies 4.2 UK benefits from wider application of European XFEL-supported research 4.3 Spillover benefits to other UK research facilities 4.4 Increased performance amongst UK suppliers to European XFEL

We have assumed that the framework will support STFC in monitoring the full extent of UK involvement with European XFEL. It should also provide an improved platform for future evaluations, allowing evaluators to concentrate on analysing the range of additional wider benefits attributable to European XFEL, and less on basic data collection and compilation.

In developing this framework, we have also reflected on our experiences of undertaking this study, and in particular some of the methodological limitations and constraints faced. A notable methodological deviation from this framework and our study is the use of a list of European XFEL suppliers rather than the STFC CRM used for this study. Owing to resource constraints at European XFEL, and time pressures associated with the study, we were unable to obtain a full list of UK-based suppliers to European XFEL as well appropriate contact details from them. As such, the suppliers survey was not as well targeted as it may have been, and the survey may not necessarily have reached all of the intended audience. We expect that STFC will have greater time to establish the relationships needed with European XFEL to obtain the required supplier details from them, and thus ensure that future monitoring activity has better quality evidence it can draw on.

An added consideration for European XFEL monitoring is securing feedback from users. For this study, we sought this feedback via an online user survey. Data protection concerns about sharing email addresses with us meant that European XFEL administered the survey on behalf of the study team. This approach yielded a response rate that was comparable to ones seen

in similar studies. Nevertheless, the lack of email addresses meant that we could not send targeted reminders to non-respondents, potentially preventing us from fully maximising response rates. We have assumed that STFC will be able to work with European XFEL to sign a data sharing agreement which will include the transfer of contact details for researchers. This will enable future researcher surveys, as recommended in the framework below, to have maximised response rates.

Another key consideration in the development of this framework is the feasibility of the data collection requirements. While we acknowledge that the framework is an ambitious one, we also believe it is a realistic and achievable one should a reasonable level of resource be available to STFC. Nevertheless, we appreciate resource levels may be uncertain going forward and have therefore highlighted the indicators that STFC should prioritise for collection.

10.2 The Framework

The following tables present a list of possible indicators against the four impact areas and 14 pathways described above. The implementation column discusses where the data may be sourced from and by whom. It also includes various suggestions for measures to strengthen the STFC-European XFEL monitoring system in order to provide future evaluations with a more comprehensive and robust evidence base. The list of performance dimensions is shorter and simpler than that explored in the current evaluation, reflecting lessons learned about what is available, what is important for understanding contributions, and what is feasible within the context of a typical, broad-ranging evaluation (covering all impact pathways) such as this.

Table 7 European XFEL monitoring and evaluation framework: proposed indicators for world-class science and research

Impact pathway	Indicator	Implementation (who, what, how)	Frequency of data collection
1.1 Pushing the frontiers of human knowledge & understanding, enabling further scientific progress	Annual presentation (list / case studies) of notable scientific and technological advances	• STFC already seeks to identify and showcase notable scientific and research advances realised through European XFEL involving UK-based scientists. While key individuals are aware of this list of examples, it is not captured in a systematic or consolidated manner • STFC should look to maintain a list of notable examples, updating on an annual basis. The list of case studies presented for this study could act as a starting point. • These individual items could provide the basis for the development of longer and more structured 'scientific advances' case studies, developed periodically either by STFC or by external contractors. The ambition should be to produce 4-5 scientific case studies a year out of a longer list of promising items • This portfolio of cases should be developed to reflect STFC's strategic commitment to both (i) frontier research and (ii) its underpinning technology. They should also present not only the research result, but also say more about the significance of its implications for wider science (and ideally also for wider society and the economy).	Annual
1.2 Sustaining the UK's research excellence & leadership through access and opportunities at European XFEL	Number of UK researchers accessing European XFEL facilities	• Annually, STFC should work with European XFEL to obtain and collate statistics on the number of UK users, and the number of UK associated with the facility. Where possible, this should include the amount of time requested and awarded to UK-based researchers, at an instrument level • Information on other Member States (if available), or at least on all countries combined, would provide a useful benchmark.	Annual
	Bibliometrics – Annual number (and UK share) of publications on European XFEL research – Share of UK papers in the 10% most highly cited papers that have used European XFEL – Annual number of publications citing	• The engineering and physical sciences make extensive use of journal articles, and as such bibliometrics provides an efficient means by which to track the volume of UK-related European XFEL research outputs and assess its international standing. • The analyses might be kept very simple, such that STFC could run the analytical exercise internally every year using an online platform and based on the list of publications citing European XFEL that European XFEL itself records centrally. Otherwise, there are a number of firms providing bibliometric analytical services reasonably economically. Such services could be contracted, perhaps alternating from one year to another between a simple computation of three or four standard citation metrics and a more wide-ranging analysis of the UK's international standing in various disciplines in comparison with benchmark countries. • The in-depth bibliometric analysis could also seek to capture references to European XFEL research in other disciplines, reflecting its influence in other areas of research.	Annual

Impact pathway	Indicator	Implementation (who, what, how)	Frequency of data collection
	European XFEL papers, UK share		
	List of UK-based scientists / engineers that have won major scientific prizes in recognition of European XFEL research	• STFC is already tracking prizes, some of which are showcased in the STFC Annual Impact Report. • This could provide the basis for a European XFEL-specific account of prestigious awards, which could be reported in a separate paper as well as being picked up as appropriate in corporate publications.	Annual
1.3 Supporting the UK's involvement in multidisciplinary and interdisciplinary activity	Proportion of all papers citing European XFEL and involving UK authors, that cover more than one subject area of topic	• The methodology used in this study could be replicated every 3-4 years to help show the progress made against this indicator • STFC should work alongside European XFEL to obtain a list of the DOIs of academic papers involving UK authors of facility staff from the UK which have cited European XFEL. These can then be combined with subject/topic categorisations of each paper, as provided in LENS.org, which can be used to determine whether papers have covered multiple topics or not • This analysis could also examine which subjects collaborate with each other the most • This is a labour-intensive exercise and therefore should occur on an infrequent basis. It may also be best done by external contractors	Every 5 years
1.4 Attracting investment & talent via improved perceptions of the UK as a leading research nation	List of international researchers locating in the UK to take advantage of UK strengths relating to European XFEL	• STFC may be able to orchestrate this monitoring activity, drawing on its pre-existing network of contacts in key institutions. • This would involve STFC engaging annually with a shortlist of (~15) individuals from the stakeholder community with a good view of the UK's involvement overall with European XFEL (e.g., representatives from key university departments and laboratories). • This could take the form of an interview or feedback form, requesting examples of notable investments, inward movement of researchers, and the latest developments in their field. Indicative examples could then be pursued for further detail as necessary.	Every 2-3 years

Table 8 European XFEL monitoring and evaluation framework: proposed indicators for world-class skills

Impact pathway	Indicator	Implementation (who, what, how)	Frequency of data collection
2.1 Increased skills and capabilities of the UK workforce	UK-based researchers and students' participation in European XFEL-related activities	• An annual report should be produced, presenting an overview (count) of the UK population conducting research at or working with European XFEL. European XFEL itself is able to provide this data, plus data on UK staff employed at the facility. • Determining the impact on skills will require additional work to systematically and routinely poll researchers on the skills and social capital they acquire through their work at/with European XFEL, e.g. looking at a range of domain, technical and management skills. Group leaders could also be asked how many PhD theses have been delivered with European XFEL as a central focus/data source, and how many PhD students are working on European XFEL projects • It will also be useful to establish a career tracking capability to begin to follow the progress of European XFEL alumni through their future careers, across job titles, sectors and borders. This may be tackled best in collaboration with European XFEL	Annual
2.2 Increased (future) UK STEM workforce	Impact on student subject selection	• STFC should consider developing a STEM uptake observatory, which would run periodical studies of students to track their engagement with European XFEL (and other similar facilities) and their views on science and their choice of subjects, higher education decisions and careers.	Every 5 years

Table 9 European XFEL monitoring and evaluation framework: proposed indicators for the UK's international standing

Impact pathway	Implementation (who, what, how)	Frequency of data collection
3.1 The UK's influence in the international science and technology landscape	• A chapter could be included within an annual STFC report, detailing notable developments and more generally itemising all such highlights (through European XFEL and other facilities). • The material would need to be identified internally within STFC, via researcher surveys and through discussions with European XFEL and those UK individuals in key positions with European XFEL (e.g. representatives on the Council or committees). Occasional examples could be highlighted in the annual report, while the most promising could be prepared into fuller science diplomacy case studies	Annual
3.2 Improved diplomatic relations and engagement	• STFC could develop a tool for inviting its scientific partners to provide feedback on the experiences of collaborating with UK-based scientists. This could help understand areas where the UK is strong or less strong is, and where STFC could provide training or encourage different behaviour. • To obtain a more rounded view of perceptions, STFC will need to commission international research to determine the views of scientists, scientific administrators, professionals and the public in European XFEL member countries. This is the type of work could occur alongside the science and innovation	Every 2-3 years

Impact pathway		Implementation (who, what, how)	Frequency of data collection
		councillors in the UK embassies. However, it may be too burdensome for them to implement fully, making the appointment of a consultant a better option. • Data collection will also need to be done at sufficient scale to allow the analysis to test for links between UK work at European XFEL, and perceptions of UK science more generally, perhaps through selected critical incidents.	
3.3 The UK's ability to engage with and/or lead international research collaborations	Number of UK-authored academic papers that cites European XFEL which also involve international collaborators	• European XFEL's publication database already contains the addresses of all authors which can be used to determine their host country. These data should be analysed on an annual basis • Similar analysis should occur with publications that have authors from another country to help provide a benchmark	Annual

Table 10 European XFEL monitoring and evaluation framework: proposed indicators for world-class innovation

Impact pathway	Indicator	Implementation (who, what, how)	Frequency of data collection
4.1 UK benefits from the wider application of European XFEL-derived technologies	List / case studies of technologies developed at or for European XFEL, which have come into wider use	• STFC should look to produce a list of relevant technologies (with wider application) and update this annually. This should include new additions in the past 12 months, and a longer list of previous success (the stock). • This could draw on several sources, including Gateway to Research, a survey of European XFEL suppliers (which could be based on the one developed for this study), and work that STFC does more generally in tracking achievements (as set out in 1.1). • STFC should also develop one or two examples into fuller impact case studies each year, exploring the wider benefits to the UK. They could then disseminate these via social media platforms.	Annual
4.2 UK benefits from the wider application of European XFEL-supported research	List / case studies showcasing the application of European XFEL research, which has come into wider use elsewhere	• STFC should keep under review any news about the application of European XFEL research in other areas of relevance to the UK, such that it might develop one or two impact case studies annually. • These cases may need to be prepared – or at least approved by the affected UK-based researchers and should therefore follow the structure of Research Excellence Framework (REF) 2021 case studies to minimise any burden on the research community.	Annual

Impact pathway	Indicator	Implementation (who, what, how)	Frequency of data collection
		• A long list of candidate cases might best be prepared based on several sources, including a new researcher survey, as well as the work of STFC in tracking UK achievements at European XFEL more generally. REF 2021 submissions may also provide a useful starting point. This exercise might be accompanied by an examination of the wider use of UK-based European XFEL research in other fields / countries (using bibliometrics).	
4.3 Spillover benefits to other UK research facilities	Knowledge transfer between European XFEL, CLF and Diamond	• STFC should look to engage with key contacts and senior stakeholders at CLF and Diamond each year, using this as the basis to compile a list of the main areas of interaction between the two facilities, and the key outcomes from this • STFC may also want to co-ordinate an annual survey of all new staff at CLF and Diamond to determine if they have previous work or research experience at European XFEL too • It may also be beneficial to incorporate as part of any bibliometric analysis, an examination into whether there has been any co-authoring of papers of papers between European XFEL staff and/or those from CLF or Diamond.	Every 5 years
4.4 Increased performance amongst UK suppliers to European XFEL	List/value of products / services brought to market by UK firms, which stem from research carried out at European XFEL	• As noted in the main report, European XFEL does not systematically record which of its contracts have been awarded to UK-based offices. Previously, European XFEL's Industrial Liaison team compiled their own analysis of the estimated value of contracts awarded to UK suppliers. STFC should work with European XFEL to have this analysis updated every year or two. • STFC may wish to supplement this with a biennial survey of suppliers named in the annual European XFEL ILO report. STFC could approach the named contact for each of these firms as they appear in STFC's own CRM.	Every 2-3 years
	International competitiveness of UK-based suppliers to European XFEL	• STFC might want to carry out a biennial analysis of the competitiveness of UK-based suppliers, to determine if European XFEL contracts have helped them secure contracts with other facilities, and helped them bring new products to market (and any turnover or employment associated with it) • This exercise is more involved than simply tracking sales and employment and does need additional primary data on exports and profitability. It also requires some level of econometric analysis to take account of different contractual histories and also to allow for a comparison of European XFEL suppliers with the performance of matching groups of firms in order to estimate the size of any statistical differences.	Every 2-3 years
	UK industrial return in goods and services	• Currently, industrial return for European XFEL is not available owing to the difficulties in working out whether contractors are UK-based or not. STFC should work with European XFEL to see if there is any data which they, or external consultants could use in the future to help determine the industrial return for the UK.	Every 2-3 years

Impact pathway	Indicator	Implementation (who, what, how)	Frequency of data collection
		• More fine-grained information on individual contracts (and contractors), as well as unsuccessful bids would also offer further insight. This level of detail should be available from European XFEL on request for successful applicants at least, although further confirmation will be needed on the availability on data on unsuccessful bids • There would however be merit in doing more: a more disaggregated analysis in order to inform STFC as regards the effectiveness of its various promotional efforts (analysing bids too, if possible, as well as contract awards). STFC will no doubt want to continue its efforts to raise awareness among prospective bidders and may also want to trial new approaches such as producing more success stories to show businesses that contracts are winnable and can deliver benefits even with low margins, or more proactively sharing tenders with CRM members. – A fuller, sector-specific analysis would allow STFC to determine the relative effectiveness of its various business development efforts. A survey of suppliers could also provide feedback on company experience of the contracting process, STFC support and views on 'best practice' or 'lessons learnt' to share with organisations interested in bidding.	
4.5 Commercialisation of research	Generation of intellectual property following research undertaken at European XFEL	• We understand that STFC already plans to use Researchfish data to collect information on patents, copyrights and trademarks that have been created as outputs of research they have supported. • STFC should look to capture this information on UK research conducted at European XFEL, working with the facility as needed to secure any additional information needed.	Every 5 years
	Spin-out activity	• We understand that STFC is also planning to capture spin-out companies initiated as outputs of STFC-supported research as part of its benefits and realisation framework. It will look to use Researchfish data for this. • STFC should look to capture this information on UK research conducted at European XFEL, working with the facility as needed to secure any additional information needed. • STFC should look to capture not only the number of spinouts initiated, but the number of STFC staff employed as a member of the company.	Every 5 years

The framework presented above points to the need for several **additional data collection activities**, including new surveys (e.g. of UK-based European XFEL suppliers, of new CLF and Diamond staff), bibliometric analyses and the collation of examples of technology development. These suggested additional activities, discussed further below, could constitute part of an enhanced monitoring system, run on a continuous basis by STFC or its contractors, with the results informing operational oversight and periodical external evaluations.

10.3 Monitoring arrangements

In addition to continuing the current monitoring and reporting arrangements, including working closely with European XFEL to determine what relevant information they are able to share, we recommend STFC considers implementing **several additional data collection / analytical activities** to strengthen the monitoring system.

- Researcher survey: Implement an annual or biennial survey of all UK-based European XFEL researchers (which might be targeted just at PIs awarded beam time), to obtain feedback on notable achievements in each of the four impact pathways.
- Supplier survey: Implement an annual or biennial survey of UK-based European XFEL suppliers to obtain feedback on their experience and capture information about specific capability benefits, innovations, wider sales and exports, plus competitive advantage. This exercise could be extended to all applicants (successful and unsuccessful) and seek to capture wider insight and feedback or focus just on those awarded contracts. In either case, requesting information on specific applicants / contractors from European XFEL, rather than relying on STFC's more general CRM, might improve response rates.
- Engaging with Diamond and CLF stakeholders: We recommend an annual consultation exercise with Diamond and CLF stakeholders to help identify the various ways that the facilities have collaborated with each European XFEL. These should be recorded in single repository, which also set out the relevant impact pathways that the example covers. This repository can be drawn on as needed, with particularly noteworthy examples being used as part marketing and communications activities. Stakeholder engagement might also involve a short survey every year of new joiners to the Diamond and CLF staff base, to help determine whether they have previously worked at or with European XFEL, either as part of their academic training, or as an employee of the facility.
- Cataloguing individual achievements: There are numerous instances of individual successes in each of the four impact pathways, and STFC and European XFEL are already capturing some of these, albeit in an ad hoc and unsystematic manner. It would be helpful, however, if STFC could broaden its search for notable achievements. The current arrangements mostly capture information about scientific advances, but there is likely to be more to report on industry and skills and working systematically across all four impact pathways may be helpful. It would be good to record all of these items in a single repository or database, tagged with the relevant impact pathways and performance dimensions. This would produce a much longer list of interesting facts than can be presented in an annual report or newsletter, showcased in rolling communication activities, as well as support further analysis and feed into future evaluations.
- Case studies: STFC should then identify and develop a selection of examples from each impact area into fuller case studies, based on additional discussion and desk research. These cases could aim for two pages (500 words plus images) and follow a reasonably standard structure (from European XFEL-related activities, through the outputs and outcomes of this work, on to potential/realised wider socio-economic benefits). The

resulting cases could then be used in a number of different ways, to support STFC annual reporting and periodical external evaluation of UK participation in European XFEL.

- Biennial review of UK science at European XFEL: There would be benefit in carrying out regular bibliometric analyses to gauge the international standing of UK-based scientists on the one hand and the citation of their work on the other. This would also allow STFC to understand the changing geography of UK cooperation and selective international benchmarking with other leading scientific countries. It would also enable an assessment of the level of international collaborations occurring, as well as the amount of multi and interdisciplinary research occurring.

We understand that STFC is currently developing a benefits and realisation framework to use across its entire portfolio of work. There may already be plans to incorporate some of the elements above into this, but STFC may also need to undertake a mapping exercise to determine whether any of these activities need adding to the planned framework.

10.4 Assessing the counterfactual

Assessing the counterfactual is always difficult when examining the impact of research infrastructures such as European XFEL. The facilities tend to cater for relatively small and niche areas of the scientific community, meaning that there is not a large pool of well-matched non-users which could form a robust control group. An alternative counterfactual approach could be to study the outcomes and impacts generated at other research facilities that UK researchers use, using this as a basis for deciding whether the UK is getting more out of European XFEL than it could do otherwise. However, there are few comparable alternatives to either facility that could be used for this basis. Furthermore, our research has found that many users use alternatives alongside European XFEL rather than instead of it. To that end, it was not practical to separate facilities into control or treatment groups given the significant overlap of users between them.

Consequently, we suggest that future evaluation activity relies on self-reported additionality. This is an approach that has worked well in this study – consultees have been able to gain insightful comments from users and suppliers alike to more qualitative questions around the difference the facility has made to them, and what (if anything) they might have been able to achieve without the facility. This approach, is used in the framework too, will be in keeping not only with this study, but also with other previous impact studies of research infrastructures, including Technopolis' 2021 impact study of Diamond Light Source.

10.5 Evaluation arrangements

The experience of conducting the current study has uncovered gaps in evidence and research/analysis methods to support a holistic, robust assessment of European XFEL's impact on the UK. A strengthened STFC monitoring system that focuses on documenting activities, outputs, and outcomes will help with this. The evaluation itself should be able to build on this improved monitoring system, corroborating data and extending the benefits-realisation perspective to the wider effects on science, innovation and skills. It should also be able to identify, quantify and monetise more of the total spectrum of European XFEL benefits than was possible with this evaluation The framework will enable a more systemic monitoring of the quantum of benefits achieved under each impact pathway whereas this study has had to rely on the view of stakeholders and degree of serendipity to find high impact examples (meaning that that our analysis may have missed some notable examples that consulted stakeholders are not aware of). The framework also incorporates additional quantitative analysis such as bibliometric analysis which was out of scope for this study. This framework will therefore the evaluators closer to being able to carry out a cost-benefit analysis that provides a more complete and fair account of European XFEL-derived benefits for the UK.

The timing of future evaluations is a matter for discussion, as there is no clear advice in existing UK evaluation guidelines and the periodicity and scope of the government's comprehensive spending reviews is rather changeable. Historically, the grant-awarding research councils and their research institutes were subject to 5-yearly, or quinquennial reviews, and while this is no longer the case, the periodicity feels appropriate to a major science programme (three years is arguably too short, and 10 years is arguably too long).

Appendices: Case studies

Light activated bacteria killing Case Study

1.1 Summary

As part of their broad research in ultrafast photochemistry of photoactive metal complexes, a research group led by Professor Julia Weinstein has been studying the antibacterial properties of Cu(I) complexes in water. The FXE instrument at European XFEL has been central to this research, using the controllability of the light beam's power and frequency to study femtosecond level changes in the geometry of different materials in an excited stage (i.e. when they absorb light). The research project has helped Professor Weinstein's team understand the fundamental science that explains the behaviour of different molecules under these conditions. They believe the research can contribute to the broad international efforts in the development of cheap and scalable forms of water treatment in the developing world. The research group also has also benefitted from being able to discuss ideas about data analysis with European XFEL staff, and the facility access has also helped early career scientists gain hands-on experience in conducting X-ray experiments which are unique.

1.2 Background

Copper complexes have potential applications in water purification. Martin Appleby, a Chemical Physics graduate who embarked on a PhD supported by Grantham Center for Sustainable futures at the University of Sheffield, hypothesised that such complexes have potential to kill bacteria in water. When Copper absorbs light, the complex is excited into it takes on a high energy state, and if it interacts with oxygen in this high energy state then it is able to convert this oxygen into a much more active and reactive form. This more reactive form oxygen species is in turn more able to kill pathogens such as bacteria. The efficiency of one of the complexes has been shown by the Kelly and Weinstein groups at the University of Sheffield to achieve the threshold set by the World Health Organisation to be classified as a "highly protective" method for water treatment.[18]

The next step was to understand the mechanism of light-driven processes of these complexes, which is a general focus of research in Professor Julia Weinstein's group at the University of Sheffield. The research group looks at all aspects of interaction of light with matter in condensed phases, conducting studies in Sheffield in the Lord Porter Laser Laboratory, and have used research infrastructure in the UK (STFC), Europe and worldwide.[19]

1.3 The Research Project

There has been growing interest into the potential applications of photoactive copper complexes such as in antibacterial water treatment – understanding these processes will enable the development of more efficient applications in real world settings. Professor Weinstein's research project has looked to examine these questions, seeking to understand how the structure of different complexes leads to changes in the higher energy, excited state (formed when they absorb light), and for the timescales these states exist for. The research group has used the FXE instrument at European XFEL to help examine what changes occur at the molecular level in real time.

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[18] Appleby, M., Walker, P., Pritchard, D., van Meurs, S., Booth, C., Robertson, C., Ward, M., Kelly, D., and Weinstein, J. *Cu(I) diamine complexes as immobilised antibacterial photosensitisers operating in water under visible light*. 'Material Advances'. 2020, 1, 3417

[19] https://www.sheffield.ac.uk/chemistry/people/academic/julia-weinstein

1.4 Impacts generated

1.4.1 Scientific and research

Use of European XFEL has helped Professor Weinstein and her research group understand the structural changes that occur when copper complexes absorb light. They have used the facility to help examine these changes in real time and are using this information to help determine which complexes will be best suited for development for water treatments going forward. This is an important contribution to our fundamental understanding of photoactive metal complexes. Thus far, they have examined the capabilities of these complexes on a laboratory scale, showcasing efficient killing of bacteria including methicillin resistant S. Aureus (MRSA) and E. Coli.

Professor Weinstein's work has already led to some follow-on plans. They are currently investigating the complexes involved in the processes but will be investigating optimal setups for delivering this water treatment in the future.

1.4.2 Commercial and economic

While there have been no commercial or economic benefits from the research yet, there is potential for future impact here. The research team is looking for industrial support to help scale up their research, and examine how materials fare in the presence of bacteria. The research team already has a commercial application in mind for their research (provision of cost-effective water treatment) and are looking to further their research with this use in mind.

1.4.3 Skills benefits

Working at European XFEL has allowed members of the Professor Weinstein's research group to develop new skills. As part of this research project, the group had a fully funded PhD position which was co-funded by the University of Sheffield, and the UK XFEL hub. Central to this student's work was conducting experiments at European XFEL, and collaborating with staff there. The student, Rory Cowin, a Chemical Physics graduate from the University of Sheffield, has just finished their second year of the PhD and because of the work conducted at the facility, they have been able to attend a wider variety of conferences, and have become part of an active FEL user network in the UK and internationally.

The research team more generally has also benefited from interactions with European XFEL staff, drawing on them to help improve not only research skills but data analysis skills too.

1.4.4 Other impact areas

Analysis by UNICEF and the World Health Organisation (WHO) in 2019 found that 1 in 3 people globally did not have access to safe drinking water.[20] The hope is that Professor Weinstein's research will contribute to addressing this issue. The research is hoping to better understand light-driven processes involving Cu(I) complexes in an effort to produce more efficient complexes for antibacterial applications. By understanding which copper complexes work best, the research will help develop more effective water treatment systems in the future. In addition, the research team has recognized that while copper complexes are effective catalyst for killing bacteria with light, copper is nevertheless a cheap and readily available

[20] https://www.who.int/news/item/18-06-2019-1-in-3-people-globally-do-not-have-access-to-safe-drinking-water-unicef-who

metal. This means that solutions developed through the research could be more easily scaled up, and more cheaply implemented.

1.5 The importance of the facility in achieving impacts

European XFEL has been central in enabling Professor Weinstein's research in how light affects the structural properties of molecules. Studying light absorption and its effect on chemical structures means having to study phenomenon occurring in the space of femtoseconds. FELs are unique in that they produce beams of photons which carry much higher energy, and are much shorter in time than in a synchrotron. This means that facilities like European XFEL have enabled the research team to study the very first steps of molecular behaviours at the femtosecond level, something which synchrotrons cannot do.

European XFEL has provided added value in other areas too, interacting with other groups at XFEL, and becoming part of the ever-broadening XFEL community. The research group has particularly valued the outstanding quality of European XFEL staff who have provided incredible amount of support every step of the way, including data analysis after the beam time. The beam time initiated what is likely to become a long-term scientific collaboration.

FMB Oxford and D2 Instrument Case Study

2.1 Summary

FMB Oxford, a manufacturer and supplier of beamlines and beamline component, was appointed to produce mirror systems (U-bender mirror) for European XFEL's SPB/SFX Instrument. Developed for high calibration and precision, FMB Oxford's work on the instrument's mirror systems led to the identification of possible flaws in measurements that could arise due to temperature differentiation. To address this, FMB conducted further work to introduce cooling controls leading to higher stability in the research environment. FMB benefitted from new engineering know-how while tackling the work for the SPB/SFX instrument.

2.2 Background

FMB Oxford, has nearly 30 years of experience in synchrotron beamline development. Employing around 60 scientists and engineers, FMB Oxford offers services for the development of beamline-components, control systems, monochromators, mirror-systems, detectors. Given its expertise, the company was contracted by XFEL to produce components for XFEL instruments.[21] The involvement particularly focused on the high precision positioning system and development of mirrors, mounts, and benders.

2.3 Work for the facility

By 2016, FMB had conducted three projects to develop mirror systems (U-bender mirror) for European XFEL's SPB/SFX instrument. Among these was the work on mechanical bender system for mirrors[22], allowing for mirror support without gravity compensation, and for small corrections to be made to the shape of the mirror.[23] The testing of the system revealed sensitivity to temperature variations. FMB addressed this through cooling controls aimed at ensuring a high stability environment for research utilising the mirror system.[24] Further work by the company involved the development of experimental detector positioning structures. FMB continues to provide new technologies for XFEL, including the development of attenuators and steering.

Additionally, FMB has also provided services to contractors that have also worked for European XFEL. Recently FMB was in the process of finalising the design for a new high-resolution monochromator[25] – a contract for the University of Jena which will subsequently be supplying the HED Instrument in European XFEL.[26]

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[21] XFEL (2017). The High Energy-Density instrument at the European XFEL. Available at: https://www.xfel.eu/sites/sites_custom/site_xfel/content/e35165/e46561/e46886/e46963/e63038/xfel_file63079/Posters_merged_eng.pdf

[22] XFEL (2016). Update: European XFEL optics, diagnostics and operation schemes. Available at: https://indico.cern.ch/event/536269/contributions/2344034/attachments/1361873/2061177/Photon_A2016Oct24_01_H.Sinn.pdf

[23] Vannoni M., Mart I., Sinn H, (2016). Characterization of an X-ray mirror mechanical bender for the European XFEL. Available at: https://fmb-oxford.com/wp-content/uploads/bsk-pdf-manager/paper_mechanical_bender_rev.compressed-2_39.pdf

[24] FMB (2016). European XFEL projects. Available at: https://fmb-oxford.com/2741-2/

[25] A monochromator is an optical device that separates polychromatic light (such as sunlight or light coming from a lamp) into individual wavelengths (monochromatic light). This then allows for individual wavelengths wo be selected and directed.

[26] EFEXL (2021). The HED Instrument at the European XFEL Status in 2020. Available at: https://www.xfel.eu/sites/sites_custom/site_xfel/content/e35165/e46561/e46886/e46963/e127531/xfel_file127533/210120_Appel_HEDHIBEF_UM_satellite_v1.0_web_eng.pdf

2.4 Impacts generated

2.4.1 *Scientific and research*

Work with European XFEL has allowed FMB to further develop new parts and approaches relevant for all synchrotrons. The analysis conducted in the development of the U-bender system and the subsequently identified issues that might arise (i.e., fluctuations due to temperature differences) led to FMB developing a new specialised cooling system using thermoelectric coolers. This system allows for scientific work to be conducted with: "ultra-high precision mirrors within a high stability environment".[27] According to an FMB representative this stability is achieved because the thermoelectric cooling system removes the transfer of vibrations to the optics that would result from older cooling system design. This new approach to cooling systems has resulted in other synchrotron facilities contacting FMB to discuss the design and collaboration.

In 2016, the Group Leader of X-ray Optics at European XFEL acknowledged the benefits of FMB Oxford's work, stating that FMB Oxford provided: "useful suggestions about the implementation and tuning of the instrumentation" used by XFEL to: "control and to adjust in a closed-loop a bendable X-ray mirror using displacement-measuring devices".[28]

2.4.2 *Commercial and economic*

To service their European XFEL contracts, FMB Oxford needed to invest in new equipment and infrastructure, which in turn has left them better placed to secure other contracts elsewhere. For example, to meet the specifications for supplying the initial contracts to European XFEL, FMB upgraded their cleanroom to meet ISO6 particle free cleanroom specification required by European XFEL.[29] Thus, engagement with European XFEL led to expansion of manufacturing infrastructure to meet higher quality specifications, and has also opened new commercial opportunities.

An FMB representative also acknowledged that signing contracts with European XFEL positively impacted their international visibility and standing in the international synchrotron market.

2.4.3 *Skills benefits*

According to an FMB representative, the collaboration with European XFEL required the team to develop new skills to approach issues related to the cooling system. The development of the new thermoelectric coolers likewise produced new know-how at FMB.

2.4.4 *UK benefits to supplying the facilities*

The work with European XFEL also meant that FMB required suppliers for various parts (i.e., detectors, power sources) which resulted in other UK businesses being integrated into the overall supply chain.

2.5 The importance of the facility in achieving impacts

Representatives both at European XFEL and at FMB have spoken of the importance of the relationship between the two organisations in generating the impacts outlined above. The

[27] FMB (2016). European XFEL projects. Available at: https://fmb-oxford.com/2741-2/

[28] Vannoni M. et al (2016). Calibration and optimization of an x-ray bendable mirror using displacement-measuring sensors. Available at: https://opg.optica.org/oe/fulltext.cfm?uri=oe-24-15-17292&id=347974

[29] FMB (2016). Official Opening of the New Cleanroom. Available at: https://fmb-oxford.com/official-opening-of-the-new-cleanroom/

European XFEL contracts have directly led to the development of new instruments which FMO was not previously engaged in. FMB has also considered the collaboration to be very successful, allowing both teams to develop new engineering know-how while working on the SPB/SFX instrument.

XFELs and the UK's work in Serial Femtosecond Crystallography

Background

Serial Femtosecond Crystallography (SFX) is a relatively new discipline developed over the past decade to make use of entirely new X-ray sources called X-ray free electron lasers (XFELs). These new facilities and data collection strategies offer new approaches to protein crystallography. Protein X-ray crystallography was developed more than 50 years ago by UK researchers, among others. Traditional studies now involve "freezing" a single "large" protein crystal and then carefully rotating it about one or more axis while exposing it to a continuous X-ray beam. This one crystal yields many thousands of observations that are combined into a dataset, from which researchers can visualise nearly all the atoms within the crystal. Crystallography is so powerful, it now underpins more than 90% of all new drugs.

SFX offers a different approach. It involves exposing 10,000s to 100,000s very small samples (microcrystals) at room temperature in a sequential manner, each with a random orientation, and from which only a very small subset of the whole dataset is obtained. Because the XFEL X-ray pulse is so brief, the microcrystal is essentially stationary during exposure to the incredibly intense X-ay beam, which vaporises the sample. Consequently, each SFX dataset is built-up from thousands of samples at physiological temperature rather than a single, frozen sample. This is particularly advantageous in time-resolved studies wherein the biological samples are actively engaged in function during the SFX data collection – a long standing frontier challenge in the field. It's also especially useful for rare, difficult to work with proteins, often involved in disease development because many of these types of samples only produce microcrystals. Studying smaller samples under natural and functional conditions yields new insights into atomic structure and function – and all from the same samples. The results are so compelling that similar serial crystallography methods, which have been developed and enhanced, creating huge synergetic value are now also conducted at most synchrotrons, including Diamond Light Source.

A UK research group, led by Allen M. Orville at Diamond's XFEL Hub, is a leading organisation in SFX science, has used the European XFEL in Germany and all of the other XFEL facilities around the world to considerably advance the field of study. Critical to these efforts, he and his group are supported by the STFC UKRI, Diamond, Wellcome, and the Royal Society.

How XFEL facilities have aided research

A key to SFX research is the ability to examine very small samples that may include their reactions with very short X-ray pulses, as short as femtoseconds (10^{-15}, a quadrillionth of a second). This approximately matches the time it takes to make or break chemical bonds. XFELs and the European XFEL are thus a critical, enabling technology. Scientists often use XFELs to make observations with exquisite temporal resolution while reactions are happening, and thereby create stop-motion, atomic-resolution movies of complex reactions. A critical consideration is how to trigger the reaction of interest, which is often integrated into the sample delivery strategies used in SFX studies. As each new sample is delivered into the X-ray interaction region, reactions are initiated by one of several means that include light activation and/or adding reagents. After an appropriate reaction time, the sample is probed with the X-ray beam. SFX data from several delay times spread across the whole reaction cycle creates the stop-motion movie.

The European XFEL is one of five XFELs in the world (USA, Japan, South Korea, Switzerland, and Germany), and because of the scientific impact, they all support SFX research. The European XFEL in Germany can deliver up 27,000 X-ray pulses per second, more than two orders of

magnitude greater than the others. Thus, it is a geographically proximate and world class facility, that includes state-of-the-art sample preparation and characterisation facilities. These features helped make UK SFX research more time and cost efficient.

Impacts seen

XFELs enable the UK SFX community, who collect lots of novel data, often very quickly. Several high-profile research publications are now in the public domain, Diamond alone has produced 23 publications of which 9 relate directly to SFX science. The XFEL Hub and the SFX community have also worked to transfer technologies between facilities meaning the symbiotic relationship between facilities is benefited from technological enhancements, which has stimulated many new science capabilities world-wide. Perhaps most generally enabling are the Hub's developments of very sample-efficient delivery and reaction initiation strategies for time-resolved serial crystallography experiments at XFELs and synchrotrons. Thus, the next generations of researchers will routinely make 'molecular movies' of biology in action.

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