

SWIFT

(Spectroscopy WithIn Fast Timescales)

Prepared for Diamond SAC/DISCo

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2. Executive Summary

SWIFT is a high flux core-level spectroscopy beamline with a design that strikes an impressive balance between time and spatial resolution, enabling processes to be followed on timescales of tenths of milliseconds and sample heterogeneities to be investigated at the 20 μm scale. These features will enable science and engineering insights to be obtained that hitherto have been impractical to achieve, with economically important applications spanning manufacturing, energy, environmental management, chemical, aerospace and tourism. The science case provides examples in all these areas. SWIFT will contribute significantly to research that will meet the UK's Grand Challenges of ageing society, clean growth and future of mobility and will incorporate significant elements of AI and Big Data.

SWIFT is an essential development to maintain and enhance the capacity and capabilities for X-ray spectroscopy at Diamond- II, as the X-ray spectroscopy community will lose a beamline in the upgrade, and the core-EXAFS beamline (B18) is more than 3 times oversubscribed. However, the case for SWIFT is not about capacity per se, but also crucially about capability and being able to drive new research and innovation. SWIFT will enable Diamond to maintain its position as a state-of-the-art facility in the determination of the structure of materials under *operando* conditions. Together with the other complementary beamlines (B07, I08, I14, B18, I18, I20, I21, as well as the proposed BERRIES beamline) SWIFT will make Diamond the go-to facility for both industry and academia.

In short, SWIFT will be an essential piece of the research landscape and will ensure that the UK remains at the forefront in *operando* X-ray spectroscopy.

3. Scientific case

3.1 Introduction

The addition of SWIFT to the portfolio of X-ray Absorption Spectroscopy (XAS) instruments on Diamond-II will offer transformative capabilities for the study of materials in a wide range of disciplines including physics, materials science, engineering, chemistry and biology. SWIFT's high flux, time resolution and ability to make spatially resolved measurements at a 20 μm scale provides a step change in the ability to probe structure-property relationships in catalysis, batteries, nuclear materials, the environment, cultural heritage and enzymes. It is only through the fundamental understanding obtained, that processes and systems will be optimised and developed. This new beamline will increase the relevance of XAS in these areas and will be of significant benefit to both academia and industry.

The enhanced technical capabilities of SWIFT compared to the existing spectroscopy suite, will expand the user base significantly both in the UK and worldwide by providing increasingly detailed insight into processes and systems.

3.2 Science enabled by project

3.2.1 Chemistry and Catalysis

In all forms of catalysis (homogeneous, heterogeneous, bio and electro) a major challenge is the identification of the working active site and how these are affected by reaction conditions, reaction time and how these are distributed within the reactor as well as how catalysts are synthesised. In order to develop the required understanding of these systems, rapidly obtained spatially resolved measurements are critical as this enables an image of practical working systems to be obtained. High rates of data collection also provide a means to probe transient changes in the structure as a function of changing environment. This is of particular importance in catalysis as it will enable spectator and intermediate information to be differentiated. The new SWIFT beamline will facilitate these measurements and the importance of each are exemplified below.

SWIFT's exceptional time resolution will enable understanding of structure-property relationships in catalytic systems which have been, hitherto, extremely challenging and, often, impractical. The importance of transient measurements is also shown by the changes in atomic Cu sites which are key for CO oxidation, selective catalytic reduction (SCR) of NO_x and NH_3 oxidation (Fig. 1). SWIFT will allow observation of the transient species formed as a function of the changing environment on the ms timescale. For example, in these systems, $\text{Cu}(\text{NO}_3)_2$, which is thought to be a key intermediate under oxidising conditions during the NO_x SCR, has been observed.¹ This study highlights the importance of combining XAS with complementary techniques. Valence to core X-ray Emission Spectroscopy (XES) ($\text{Cu K}\beta_{2,5}$ and $\text{K}\beta''$) and High energy resolution fluorescence detection XAS (HERFD-XAS) has been used to probe the

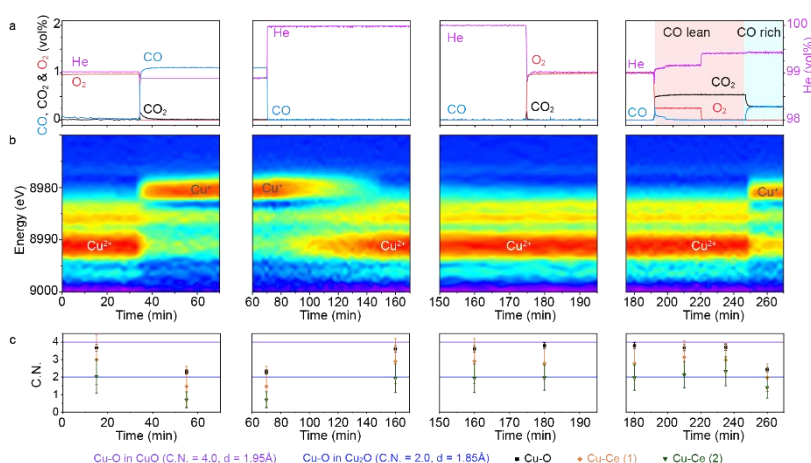


Figure 1. Operando XAFS at the Cu K-edge of 1wt% CuO-CeO₂. *a*, Gas concentration at the outlet of operando XAFS reactor as a function of time. *b*, Contour map of the first derivative XANES spectra, showing the continuous changes of absorption edge fine structure. *c*, Corresponding change of coordination number in Cu-O, Cu-Ce (1) and Cu-Ce (2) scattering as a function of time. The experiment was performed at B18 (DLS).

stable phase with precise coordination environment and thus, together with ms XAS, help to elucidate the redox mechanism of the Cu active site.

SWIFT's time resolution will also enable the study of the degradation of electrocatalysts. For example, the high potentials which occur during oxygen reduction electrocatalysts in PEM fuel cells as the result of start/stop cycling lead to the oxidation of Pt, causing Pt leaching and Ostwald ripening. The study

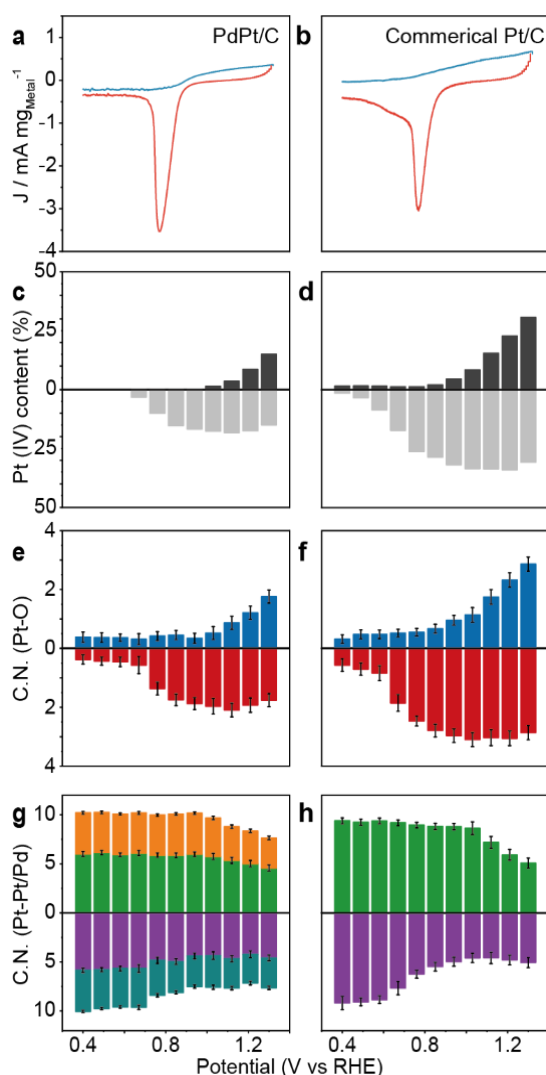


Figure 2. Pt oxidation states and Pt coordination environment during cyclic voltammetry. a, b, CV curves of PdPt/C (a) and commercial Pt/C (b) during *in situ* XAFS study. c to f, corresponding Pt(IV) content (%) and Pt-O C.N. for left-PdPt/C and right-commercial Pt/C. g to h, Pt-Pt (green and purple) and Pt-Pd (orange and teal) C.N. for left-PdPt/C and right-commercial Pt/C. Reversed charts are shown for the cathodic scans (lower charts). The experiment was performed at B18 (DLS).

of the Pt oxidation states at each potential at steady state reveals partial oxidation of Pt, a smaller Pt-Pt coordination number and a larger Pt-O coordination number (Fig. 2). However, these steady state structures are not representative of the conditions that occur during accelerated durability tests (ADT), when the potential is switched between 0.6 and 1.2 V vs RHE (reversible hydrogen electrode) within 10 s. SWIFT will enable the XAS measurement within one ADT cycle as function of potential, providing an understanding of the oxidation of Pt at high potentials under non-steady state conditions. Similarly, for oxygen evolution reaction (OER) electrocatalysts, high potentials cause rapid degradation. In acid electrolytes, RuO_x is the most active OER system, but it must be stabilised by Ir, whilst Ni, Fe, Co, and Mn are most promising in alkaline electrolytes. However, to date, only steady state XAS have been reported.²⁻⁴ In such highly dynamic systems it is important that the timescales of combined *operando* characterisation techniques are matched and the speed of the XAS measurements has proved to be limiting, especially when fluorescence measurements are required. SWIFT will transform these measurements with rapid fluorescence data collection on the second timescale.

The electrification of the chemical supply chain offers a route towards decentralised production. Two areas of particular interest are electrochemical CO₂ reduction (CO₂RR) and methane partial oxidation (CH₄OR). For the CO₂RR nanostructured Au, Cu, and Pd electrocatalysts provide high Faradaic efficiency at low overpotentials, but considerable advances are required to improve their activity and stability. *Operando* XAS measurements have proven to be invaluable in demonstrating the importance of Cu⁺ in the production of complex products⁵. However, the improved time resolution of SWIFT, especially for fluorescence measurements, will enable study of electrodes with more realistic loadings. The CH₄OR reaction to produce methanol has recently been demonstrated in alkaline

conditions at an electrode comprised of a physical mixture of TiO₂, RuO₂, and 5% V₂O₅, with redox cycling between V⁴⁺ and V⁵⁺ postulated as essential to the catalytic mechanism.⁶ Unfortunately the catalyst only lasted an hour. Here the time resolution offered by SWIFT will enable the study of such poorly stable

materials and provide the necessary mechanistic insights to aid further development.

To probe more challenging catalytic mechanisms, techniques which allow spectator species and intermediates to be distinguished are critical. Recently, modulation-excitation (ME)⁷ experiments have been used to correlate changes in structure with selectivity and activity data as a function of a transient change in the environment. To date, the ME measurements have limited time resolution under fluorescence mode. ME data taken at ms time resolution is of importance in exhaust catalysis including Three Way Catalysts (TWCs) for gasoline engines and low temperature NO_x adsorbers in diesel engines which operate using rapid changes in the gas atmosphere. Both systems typically contain low concentrations ≤ 1 wt% Platinum Group Metals (PGMs) supported on CeZrO₂, wash-coated onto ceramic monoliths. The high time resolution offered by SWIFT will enable a mapping of platinum group metals under these transient conditions allowing ME measurements to be undertaken, leading to the identification of the active species as a function of reactive gas or temperature, as well as obtaining a speciation profile into the catalyst monolith wall. Whilst ME measurements have been performed in gas phase catalytic experiments, they are rarely applied to liquid phase catalysed reactions that dominate the bulk, fine chemical, and pharmaceutical industries and include processes that are activated thermally, photochemically and electrochemically.⁸ SWIFT would allow ME experiments to be designed and applied to heterogeneous, homogeneous and bio-catalytic reactions taking advantage of the high flux and the beamline's time and spatial resolution.

The combination of a small beam and high acquisition speeds offered by SWIFT is essential in the field of heterogeneous catalysis, enabling tracing of the kinetics of fast reactions and the dependency on gas feed and position in the catalyst bed. This is the case for the CO₂ activation in dry reforming and oxidative dehydrogenation reactions, recognized as key technologies which can de-fossilise the chemical industry without requiring large amounts of green hydrogen. Molybdenum carbides have been shown to facilitate these processes. The reaction conditions make it challenging to use laboratory-based techniques to monitor the fast (ms) allotrope interconversions as well as the phase changes to more oxidic species. Furthermore, deactivation is observed both through carbon deposition and re-oxidation. Laboratory studies suggest a gradual oxidation front moving through the catalyst bed. The ability to quickly map the catalytic bed will be enabled by the fast spatially resolved *operando* X-ray absorption spectroscopy (XAS) offered by SWIFT.

Another application can be found on the study of emission control catalysts, typically employing low concentrations of PGMs supported on rare earth oxides within ceramic monoliths. Due to the number of reactions that can occur as a result of the complex gas composition, spatial profiling along channels as a function of the gas environment is valuable and has been studied by spatially resolved mass spectrometry.⁹

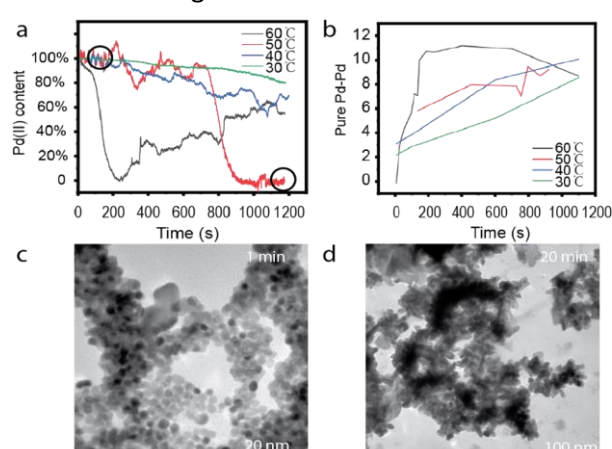


Figure 3. Growth of Pd nanoparticles in aqueous solution. (a) Pd(II) content as the function of time. **(b)** Pd-Pd coordination numbers for Pd particles. TEM images of Pd nanoparticles at 1 min **(c)** and 20 min **(d)** at 50 °C. The experiment was performed at I20-EDE (DLS).

However, further *operando* measurements as a function of the depth of penetration of gases through the wash-coat embedded in the monolith wall (in the order of 100-200 μm) as well as along the channel are critical. In the case of gasoline particulate filters, when the exhaust gases are forced to pass through the monolith walls to escape through an adjacent channel, there is also spatial variation in terms of catalyst wash-coat depth. Using the fast fluorescence capabilities and the 20 μm spatial resolution of SWIFT, rapid profiling of the cross sections of the monolith wall as a function of the transient conditions will be obtained, providing an understanding of the active sites and their relationship with the activity of the system.

A final example relates to the composition and structure of nanoparticles (NPs) during reaction and synthesis (Fig. 3). NPs are used as the active phase in

many catalytic systems, as their surface properties dominate material behaviour, leading to enhanced reactivity. XAS on the ms timescale benefits the determination of the critical initial nucleation and growth mechanisms, enabling rational design of the NPs. As an example, the SuperXAS beamline at the SLS has been used to obtain XANES data to monitor the reduction of Au^{3+} to metallic gold within the first 2 ms of NPs formation, while EXAFS data was used to monitor the size of the NPs over time.¹⁰ SWIFT will enable further increases in time resolution (sub ms), allowing the initial stages of nanoparticle nucleation and growth to be measured in more detail, including the observation of possible short-lived intermediates. In turn, SWIFT will enable experiments that will take full advantage of the development of microfluidics, by exploiting the spatial resolution to follow the synthesis of catalyst NPs, as described above, and other catalytic structures such as zeolites, MOFs or catalyst supports, where studies are still limited.

3.2.2 Battery materials

Operando XAS techniques are key to understand the complex transformations and degradation processes occurring in battery cycling, given the amorphous nature of some of the intermediates formed during insertion/extraction of ions.¹¹ Currently, battery chemistry relies extensively on layered transition metal oxides containing Ni, Co, and Mn, as these metals do not tend to migrate into lithium positions when Li is deintercalated during battery charging¹². Challenges remain in assessing local structural changes at higher nickel-content cathodes which offer higher energy densities. Furthermore, with a move to more earth-abundant elements for battery cathodes, such as Li_2MnO_3 , there is an increasing interest in materials where the intrinsic disorder on the cation lattice can mitigate structural degradation upon cycling. However, fundamental questions remain for this class of materials, including an assessment of the redox behaviour of the transition metals and the effects of anion substitution, and their elucidation is key to improve materials performance. The UK has significant strength in this area for both lithium and post-lithium ion batteries supported by the Faraday Battery Challenge, a £274M funded investment in battery technology. We expect that SWIFT will have a major role to play in this field, by enabling measurements of the spatial distribution and the dynamics of systems under real conditions.

The capability of monitoring the electronic and geometrical structure of materials during fast electrochemical reactions even for dilute systems offered by SWIFT is important in the study of fast ion transport properties in battery electrodes optimised for power density, where fast charging and discharging can make the study of fundamental processes governing ion diffusion challenging. This new instrument will enable the investigation of the dynamics in *fast* battery systems of interest to the transport industry that operate at high ionic (de)intercalation rates, such as LiFePO_4 (Fig. 4)¹¹ and the more recently discovered niobium tungsten oxides¹³. Similarly, relevant structural information may be obtained on supercapacitors. SWIFT will also allow rapid local structural determination of battery materials containing elements with different absorption energies. This is the case of high-performing and environmentally friendly negative anodes based on BiSb (Sb K-edge 30.5 keV and Bi L_3 -edge 13.4 keV), or multi-element cathode materials, such as high-entropy disordered rocksalts,¹⁴ structurally designed to allow fast Li-ion mobility within the structure. Here, the speed of SWIFT will enable an *almost* simultaneous determination of the local environment and oxidation state of the different transition metals contained in these oxides during *operando* studies, allowing to derive the correlation between electrochemistry and

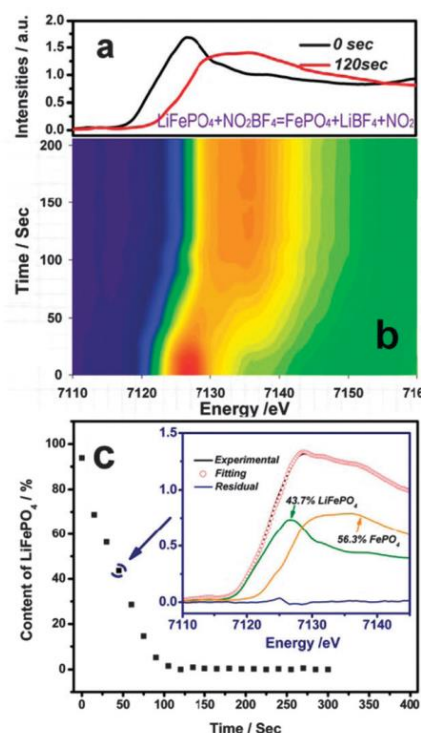


Figure 4. Dynamics of high rate lithiation in LiFePO_4 using 30s acquisition times (taken from ref. 12)

structure. Additionally, simultaneous XAS and powder X-ray diffraction collection capabilities implemented in SWIFT will provide crucial insights into the charge compensation mechanisms occurring in this family of battery materials.

The high flux on SWIFT will also enable studies where elements are present at low concentration. Such measurements are critical to examine the nature and behaviour of low concentration dopants which improve the stability in batteries or cathode materials that experience a small proportion of cationic migration during cycling. For example, in layered cathodes containing small quantity of Fe^{3+} ions, these migrate from their original octahedral sites to tetrahedral sites upon cycling.¹⁵

3.2.3 Earth, environment, cultural heritage and planetary sciences

One of the key goals for the “geosciences” is to understand the dynamic processes that have shaped our planet and the Solar System, including the geodynamic behaviour deep within Earth and the range of environmental systems upon Earth’s surface, both natural and anthropogenic. The ultimate challenge remains to identify and understand at the microscopic scale the fundamental mechanisms that control these systems and drive change within them. The capabilities of SWIFT represent a step change in the ability to quantify dynamic systems under realistic geological and environmental conditions and non-destructively analyse irreplaceable natural and culturally significant materials.

Spatially resolved rapid scanning at 20 μm resolution on SWIFT will enable the chemical imaging of both large and small areas of samples. Combining spectroscopy and imaging of dilute elements within large geological or palaeontological objects allows exploration of the evolution and biodiversity of life and key anatomical adaptations (for example the vertebrate skeleton), as well as informing mechanisms of preservation and identifying residual compounds and breakdown products of the original biochemistry.¹⁶ The small beam is vital for the analysis of radioactive samples, which often require size-reduction due to their hazardous nature. This will give us the ability to rapidly measure the local coordination of actinides and other elements within nuclear waste simulants during heating (and cooling)¹⁷, or irradiated tritium breeder materials^{18,19} (to observe changes as radiation-induced defects are annealed).

Dynamic *in situ* and *operando* experiments are limited in scope on B18 or I18. Challenging studies of transient inclusions and localised chemical species, or reversible correlated changes in chemical-state and phase under realistic deep Earth conditions (low concentrations, extreme P, T, strain, etc) within furnaces, diamond anvil, multi anvil and deformation rigs become possible. Adsorption-desorption and precipitation-dissolution reactions in spatially targeted areas for key polyvalent toxic elements, contaminants, and radionuclides can be experimentally quantified in real time^{20,21,22}. Multiple interactions of elements can be monitored across the mineral-fluid and geo-bio interfaces in soil, contaminated land, ore, and agricultural systems can be modelled. Similarly, the ability to perform spatially resolved *operando* analysis on dilute metallurgical systems opens up the development of sustainable extractive technologies utilising bio-, liquid-liquid, DES, and electro- methods on complex heterogeneous ores. Moreover, analysis at high frequency on dilute systems will enable the application of cutting-edge *operando* cyclic voltammetry to a range of geochemical, geomicrobiological and radiochemical-induced redox transformations.

SWIFT will enable the study of corrosion phenomena on ms timescales with chemical sensitivity, including the formation of inhibited interfaces and protective corrosion scales, as well as the local breakdown of passive films and coatings. In addition, the 20 μm beam size is well matched to the microstructure of many alloys. For example, data from solution species interacting with the ferrite and pearlite phases of carbon steel could be collected, to directly test hypotheses that the latter phase is the location of cathodic chemistry. Such insight may underpin new routes to corrosion control, such as grain boundary engineering.

One of the biggest hindrances to research in this area relates to beam induced damage to the material being studied. The nature of such beam-sensitive phases is varied and includes non-crystalline materials such as amorphised phases, borosilicate and volatile-containing silicate glasses, hydrated or

organometallic compounds and materials comprising photosensitive polyvalent elements^{23,24}. In all these cases, ms data acquisition with a spatially resolved beam as provided by SWIFT is essential. Rapid scanning is particularly important for the study of complex degradation phases relevant to science-based conservation of culturally important artefacts, specimens and paintings, that are known to photo-reduce/oxidise or devolatilise within seconds on I18 (and even B18). Indeed, the danger of inducing beam damage to very rare and/or unique museum palaeontological specimens, prevents these samples from being loaned for any 'destructive analysis'. This is also critical for meteoritic systems where it is essential that many analytical measurements are made on exactly the same areas, where it is known that 4.5 billion year old organic matter, amorphous iron silicates and key oxybarometer systems are all prone to beam damage within seconds on the current DLS spectroscopy beamlines^{25–27}.

3.2.4 Bioscience

Commodity and specialist enzymes are used in a wide range of applied settings. These range from the bulk use of cellulases in washing powders to specialist enzymes for organic synthesis. This is a multi-billion dollar international industry, spanning small companies to large corporations, e.g. *Novozymes*, a Danish-based company founded in 2000, the world's largest commodity enzyme corporation with an annual turnover of over \$1 billion.

Many, if not all, of the enzymes that are involved in the applications described above are metallo-enzymes (or metal-containing enzymes) which have active sites containing one or more metal ions. The study of the electronic and geometric structure of these metals thus becomes essential if these enzymes are ever to be used at maximum efficiency. There are several spectroscopies that can be used towards this goal, e.g. EPR, resonance Raman, and MCD; however, only XAS combined with theory has the interrogative power to provide detailed chemical information about these metal active sites. An example is the multiple XAS studies which have unravelled how nickel at the active site of Ni-Fe hydrogenase responds to the addition of H₂ gas, with the discovery that the Ni undergoes a significant shift in its coordination geometry at different stages of the enzyme's catalytic cycle.²⁸ More recently, Cu K-edge XANES from B18 was used to examine the copper active site in lytic polysaccharide monoxygenase (LPMOs). LPMOs were discovered in 2010 (with the help of XAS) and are Cu-containing oxygenases that find application in the production of cellulosic bioethanol (Fig. 5).²⁹

The enhanced time resolution provided by SWIFT will enable studies of these systems in real time, allowing the structural determination of reactive intermediates that cannot be isolated, but often hold the key to the operation of these enzymes, and ultimately, their catalytic power for bioconversion. Moreover, the availability of continuous scanning and fast acquisition times will reduce the effects of X-ray-induced damage in these systems. Therefore, the future of the study of these enzymes will be dependent on access to higher flux and fast detection timescales. This, coupled with the development of *in situ* cells, will permit the direct study of these enzymes at or near to their normal operating conditions.

Understanding the spatial and chemical relationships between elements with cellular and subcellular components of biological substrates is essential to address fundamental scientific questions regarding the role of endogenous and exogenous elements in health and disease. Metals are also essential

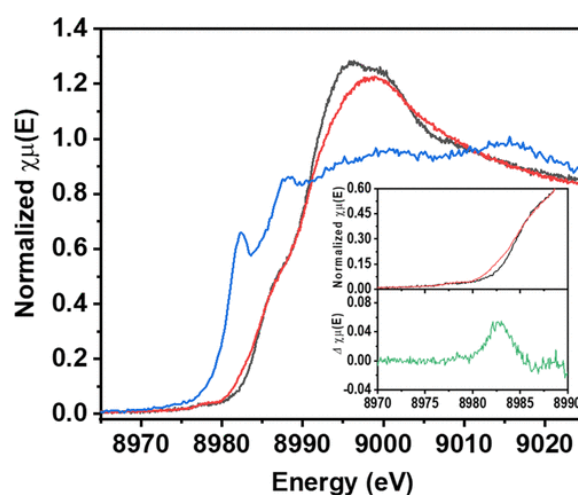


Figure 5. Normalized Cu K-edge XAS spectra (77 K) of an LPMO (LsAA9) at three oxidation levels, resting Cu(II)-LsAA9 (black), highly oxidised species LsAA9 (red) and reduced Cu(I)-LsAA9 (blue). Inset, difference spectrum (green) between highly oxidised and Cu(II) LsAA9, showing a 1s to protein transition, assigned as part of the enzyme's protective pathway.

for the conversion of electro-chemical energy into chemical energy, as well as the biosynthesis of DNA. The importance of endogenous metals such as Cu and Zn in neurodegenerative diseases such as Parkinson's,

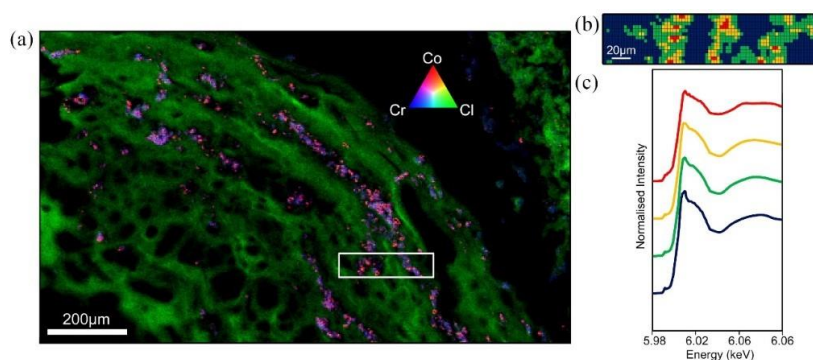


Figure 6. (a) XRF map of ex-vivo synovial sheath tissue taken from a failing total joint replacement, Cl (green) is a typical tissue marker and shows the geometry. A $3\ \mu\text{m}$ resolution beam was subsequently used to generate a $\sim 250 \times 50\ \mu\text{m}$ XANES map within the XRF map (white inset). The XANES map consisted of $\sim 1,400$ XANES spectra and took ~ 6 hrs to measure, which highlights the advantageous time efficiencies using a mapping approach. The resulting map is shown in (b) and their resulting XANES spectra are shown in (c) showing subtle changes in Cr speciation. The experiment was performed at I18 (DLS).

Alzheimer's and exogenous metals such as Cr and Ti in adverse responses to biomedical devices such as orthopaedic joint replacements has also been demonstrated. High flux X-ray probes are widely used to interrogate exogenous features within biological samples due to their detection limits and spatial resolution. However, a key challenge is the accurate characterisation of the full chemical variation within the sample. SWIFT's wide-field XAS mapping utilising the available $20\ \mu\text{m}$ spatial resolution will significantly enhance the current 2D XAS mapping studies (Fig. 6)³⁰.

In addition, the planned ability to change working energy range is essential for many 'on-tissue' biological measurements, particularly where exogenous and endogenous metal speciation is simultaneously of interest, as is the case in studies of anticancer metallodrugs.

3.3 Diamond-II portfolio

SWIFT will take advantage of the added capacity offered by Diamond-II, satisfying the increasing demand for *in situ* and *operando* measurements. SWIFT will be a high flux beamline able to follow processes on timescales of tenths of milliseconds, with the added potential to investigate sample heterogeneities at

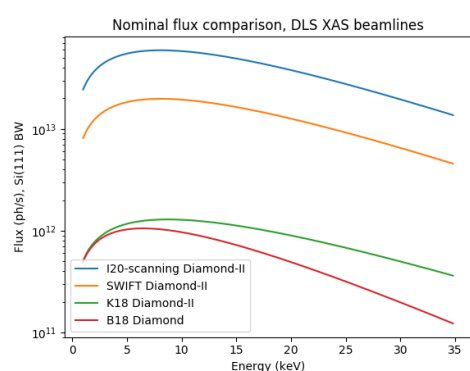


Figure 7. Flux comparison of the Diamond spectroscopy beamlines.

the $20\ \mu\text{m}$ scale. The beamline will exceed the capabilities of the other Diamond-II XAS beamlines for experiments that require an element of time resolution in dilute samples and will bridge the existing spatial resolution gap between I18 and B18. Furthermore, SWIFT will cover the scientific programme on time-resolved studies currently taking place in I20-EDE, due to close in the near future, expanding it by enabling the study of low concentration samples using fluorescence detection mode that is incompatible with the dispersive configuration. The new instrument will also improve data quality on heterogeneous samples, that are not particularly well suited to the energy dispersive setup, as changes in background compromise the normalization procedure.

SWIFT will thus bring new capability for fast scanning spectroscopy at Diamond-II beyond what will be offered at B18, while keeping a high level of complementarity. The higher flux delivered by SWIFT in comparison (Figure 7) will allow fluorescence mode QuickEXAFS in the energy range from 4 keV to 35 keV, which is currently limited by photon statistics at B18. Due to the unique characteristics of SWIFT, the combination of the new and the existing spectroscopy beamlines will allow a more efficient use of the

available beamtime across the whole instrument suite, by reducing the need to change between complex user configurations.

SWIFT's second end-station, providing a focal spot of around $20 \times 20 \mu\text{m}^2$, will be particularly complementary to I18, enabling the study of heterogenous samples with a larger field of view.

3.4 Academic user community and beneficiaries

The expected SWIFT user community will be an extension of the present, large user base of Diamond hard X-ray Spectroscopy beamlines. This community is very large (over 400 PIs over the last 5 years), and represents more than 140 Research Institutions, mostly located in the UK, but with a healthy proportion of international research.

More than 60% of experiments performed in the spectroscopy group beamlines at Diamond on chemistry and catalysis and energy materials require the study of systems under *operando* conditions. The strong demand for XAS *operando* experiments can be exemplified by the recent trend of proposals in the energy research area at B18. In AP17, when the Energy BAG came into operation and started providing access for static experiments, we saw a progressive reduction of beamtime requests in this area, although the number of high impact publications grew substantially as access to beamtime was more straightforward (Figure 8). However, new Government initiatives like the Faraday Institution and the call for clean transport and industrial processes, have dramatically driven an increasing demand for experiments for which time resolution is essential. The same trend can be seen in chemistry and catalysis, the largest user community of core-level spectroscopy. SWIFT will be able to provide the UK user communities of these two large science areas with an instrument optimized for studies under *operando* conditions on faster timescales than currently offered at DLS.

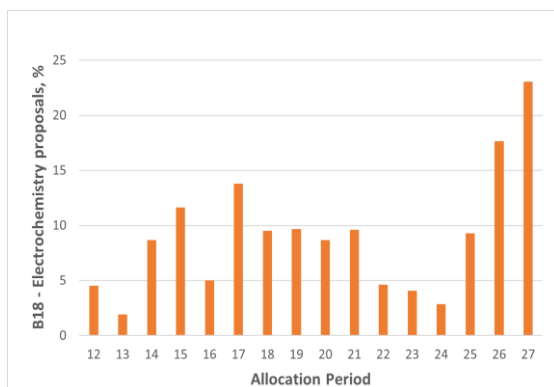


Figure 8. Time evolution of proposal submissions for electrochemistry on B18 in the last 8 years.

allow mapping with unprecedented detail of devices under operational conditions, as well as artefact microstructures.

Currently DLS has limited capacity to probe sub-second reactions and processes with high sensitivity. SWIFT will significantly expand this capability, by providing a world-leading instrument of high flexibility, and integrating and combining multiple time-resolved characterisation techniques. SWIFT is needed for the UK XAS community to stay competitive, especially now that other fast scanning facilities in Europe are looking to upgrade, and new sources (ESRF-EBS) and instruments (Quati and Q-XAS) are ramping up their operations (see section 3.6 for details).

3.5 Industrial user community and beneficiaries - impact on UK PLC

X-ray absorption spectroscopy applied under *in situ* and *operando* conditions, both combined with other techniques or standalone has become a go to technique for studying structure-activity relationships in

functional materials research. To date, XAS has underpinned activities in the fields of environmental catalysis, fine chemical catalysis, energy storage etc. However, there are still gaps in our understanding which can be tackled using a beamline that can obtain data with a higher time and spatial resolution. This will be particularly beneficial for companies such as Johnson Matthey with an interest in understanding how their technologies can be improved and will typically be realised through the development of new products and/or exploitable IP. Many industries appreciate that engaging with facilities like DLS could be very beneficial for their research and subsequently for business but are often unsure of how best to realise this. There are typically two mechanisms to do this; through the Diamond Industrial Liaison group and increasingly through companies specialised in bridging academic and industrial research (e.g. Finden Ltd, a UK SME specialising in providing advanced characterisation and expert analysis, deriving structure-activity relationships in functional materials under operating conditions to clients). For companies like Finden Ltd., this new beamline will provide an opportunity to exploit/train new data processing capabilities for large volume data screening. The development of novel beamlines like SWIFT have in the past proven a big draw for international companies to exploit and consequently, leads to revenue generation for the facilities and for companies/researchers offering technical and analytical support. It is expected then that through industrial engagement SWIFT will enable companies to expand their products and services, gaining access to new clients and increasing their market share. This in turn drives further investment in the application of such techniques and jobs as increasing numbers of highly-skilled people are needed to exploit these new capabilities. Importantly a number of leading companies not only purchase beamtime but also regularly publish their findings which will contribute to the academic output of SWIFT.

Coupled with the opening of the new National Nuclear User Facility Active Materials Building, SWIFT opens exciting new possibilities for advanced nuclear science and engineering research, particularly in the fields of radio-materials, environmental radio-science and fundamental actinide radiochemistry. The developments enabled in these areas, which are traditionally funded by research councils (UKRI, Euratom H2020, US NSF), Government sources (e.g. UK Nuclear Decommissioning Authority) or directly from the nuclear industry itself (e.g. Sellafield Limited), have far-reaching impacts, which include: (i) developing soil /water remediation and decommissioning technologies to clean-up the 60-year legacy of radioactively contaminated materials and land arising from nuclear power; (ii) developing new materials, chemicals and processes for future nuclear fission and fusion reactors and the associated fuel-cycle technology; (iii) influencing policy decisions on the development and application of new nuclear fission and fusion power sources, thus supporting UK and global commitments to reduce CO₂ emissions; and (iv) influencing policy and implementation of safe radioactive waste disposal options, for example geological disposal facilities.

3.6 Comparison to other synchrotron facilities, current and planned

X-ray Absorption Spectroscopy on fast time scales is available at most synchrotron sources. These beamlines support an ever-growing demand for *in situ* and *operando* spectroscopy studies, and in particular cater for the needs of many research communities (see section 3.2). Some of these beamlines can also provide small focal spot sizes, relevant for studies where the heterogeneity of the sample determines its function. In this section the leading international beamlines have been chosen for comparison.

Recently built beamlines such as Quati³¹ at Sirius, and 7-BM (QAS)³² at the NSLS-II, as well as more mature instruments such as SuperXAS³³ at the SLS, and ROCK³⁴ at Soleil, use fast scanning monochromators to achieve sub-second time resolution using an optical design similar to the one proposed for SWIFT. As a high photon flux is required to facilitate high time resolution, these beamlines are based on high field super-bends or three pole wigglers. SWIFT will build on this trend by adopting a multipole wiggler as its source, and this will deliver considerably higher flux and consequently higher performance. SWIFT will in fact benefit from similar flux levels to undulator based beamlines such as P64³⁵ at Petra III, and the TOYOTA beamline³⁶, BL33XU, at Spring-8. Even in comparison to these beamlines, the multipole wiggler selected for SWIFT offers advantages over the undulator sources, as those need to be tapered to broaden the energy range that is

required for QuickEXAFS operation. In the case of SuperXAS and ROCK, the current flux is almost one order of magnitude smaller, as shown in Figure 9. With the planned upgrade of both sources, higher field super-bends for the XAS beamlines will be used, increasing the available flux and benefiting mostly the performance of the instruments at intermediate to high energies. In the case of the CRG beamlines at the ESRF-EBS, the short wiggler or high field bend sources deliver an almost constant flux across the hard X-ray energy range. SWIFT's higher flux and fast scanning capabilities will not only be internationally competitive but will surpass the current beamlines optimized for the study of fast kinetics, especially for fluorescence mode experiments that are limited by photon statistics.

Many of the existing XAS beamlines deliver focal spot sizes on the hundreds of microns (ROCK, SuperXAS and P64) or in the micron range (BM23³⁷ at the ESRF and BL33XU when using the focusing capabilities). SWIFT's second end-station, providing a focal spot of around 20x20 μm^2 , will bring intermediate beam size capability, an uncommon feature for fast scanning beamlines.

The user consultation carried out in 2018, clearly highlighted a need for Diamond to develop experimental facilities that can satisfy the increasing demand for *in situ* and *operando* measurements. The proposed beamline will ease the demand on B18, that is currently oversubscribed by more than a factor of 3, and SWIFT will also provide access to faster kinetics and lower concentrations, that are important for matching industrially relevant conditions. This combination of factors will consequently resolve many of the present limitations that are faced by studies that are currently proposed, and performed, at B18.

Without the development of SWIFT, Diamond and its user community risk falling behind their international competitors. In particular, the lack of competitive fast scanning spectroscopy will have a detrimental effect on academic and industrial research in critical areas such as catalyst and energy materials development.

3.7 Combined impact of project and added value in relation to activities on the Harwell Campus and beyond.

There is increasing interaction between the activities on the Harwell Campus including Diamond, CLF, ISIS and the Research Complex at Harwell (RCaH). SWIFT will enhance these interactions by enabling complementary measurements to be undertaken to enable, for example, the liquid structure and diffusion characteristics using NIMROD and IRIS at ISIS with structural measurements of metal centres on SWIFT. In addition, SWIFT has a strength in developing catalytic and materials science and engineering which is focus of the research being undertaken within the research complex. The major research themes in RCaH are advanced manufacturing, catalysis, cross cutting imaging, energy materials and structural & molecular biology, which are all areas where SWIFT will have significant impact. The high temporal resolution of SWIFT will also enable complementary time resolved data to be obtained within the CLF, for example in the areas of chemical reaction mechanisms including in the fields of catalysis and electrochemistry as well as in studying biochemical and biophysical processes.

The importance of SWIFT in the areas of catalysis, biological systems, energy materials and materials in general, including nuclear, as noted in the case above, places SWIFT critically at the interface between Diamond and major research initiatives including the UK Catalysis Hub, the Sir Henry Royce Institute, the Faraday Institute and the Rosalind Franklin Institute as well as exploiting to the full the capability of the new National Nuclear User Facility Active Materials Building. These research centres' raison

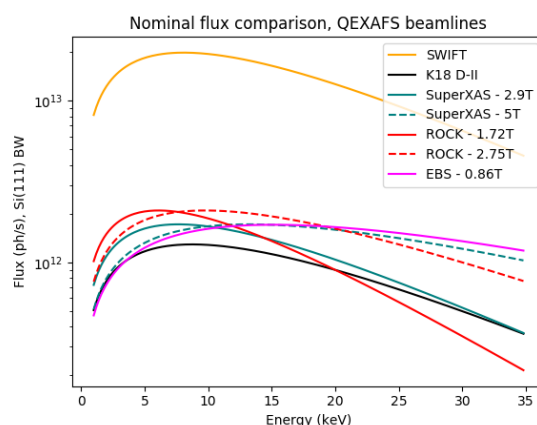


Figure 9. Flux comparison of some of the fast scanning beamlines in Europe and their future upgrades.

d'être is to provide an understanding of the fundamental science and engineering in order to develop new products and processes and SWIFT will be critical to this goal. It will provide the necessary spatial and time resolved information at relevant conditions including investigating low concentration species to develop and optimise the materials involved.

4. Beamline performance specification and requirements

SWIFT will provide fast scanning spectroscopy capabilities in the energy range from 4keV to 34keV. Two end-stations will be available. The bulk-XAS end-station will provide over an order of magnitude improvement in flux in comparison to the core EXAFS beamline, B18 ($\sim 10^{13}$ ph/s). The moderate focal spot size (100 μ m) is ideal for the study of fast processes when a large beam will help to provide good quality data. The micron-XAS end-station will provide over 10^{12} ph/s in a round focal spot of around 20 μ m. This is optimized for performing spatially-resolved studies on these length scales. Although the flux available is lower than in the bulk-XAS end-station, it will still provide a 5-fold improvement with respect to B18.

The SWIFT QEXAFS monochromator will enable the study of faster processes by up to two orders of magnitude, moving us from the current minutes scale capabilities to sub-second timescales. SWIFT will also enable full structural studies of processes by following the entire EXAFS region of the absorption spectrum, where currently only XANES can be undertaken. The higher flux of the beamline can also be used for the study of more dilute samples with time resolution using fluorescence detection mode, reducing the concentration limit ≤ 1 %wt in solids and breaking the current millimolar concentration limit. The SWIFT micron-XAS end-station will enable the investigation of spatial heterogeneities at the 20 μ m scale with time resolution.

An important aspect of SWIFT will be the use of complementary techniques (see section below) to provide an experimental facility highly optimised for holistic *operando* studies. With these additional capabilities, SWIFT will allow the chemical mapping of fast evolving systems across different investigative directions: spatial, temporal and cross-technique (e.g. obtaining local and long-range structure information).

4.1 Additional developments required

SWIFT will be optimized for the study of samples under *operando* conditions in a great variety of scientific disciplines. It is thus essential that it is equipped with a broad range of sample environment equipment for low and high temperature and/or using reactive gas mixtures experiments. We will ensure that this equipment is compatible with the other beamlines in the group where possible, so it can be shared. As part of the infrastructure of the beamline, we will supply the most common gases used in catalysis experiments to both end-stations. It is important that this is part of the design of the beamline during the design phase, so experiments can be performed under conditions (gas type, flow rate and pressures) that are as close as possible to realistic situations. This will reduce the time needed to set up experiments making the use of beamtime more efficient.

Combining multiple time-resolved X-ray characterisation techniques or X-ray with optical spectroscopic techniques on synchrotron beamlines is a research approach that is well-known to offer advantages for understanding structure-activity relationships in advanced materials, and where the UK and UK synchrotron facilities have traditionally led the way. Many of the additional X-ray facilities (i.e. XRD) and peripheral techniques (DRIFTS instruments/Raman and UV-Vis fibre optic probes) are sufficiently compact and comparatively simple to integrate into the beamline experimental setups and data acquisition network. Furthermore, they offer data acquisition rates comparable with the speeds offered by the new SWIFT beamline (i.e. \sim sub-s). A full integration will be required so co-refinement of data can be achieved, combining the information provided by the different techniques.

SWIFT will generate a significant amount of data (see sec. 5.5), so a robust pipeline for advanced data-reduction and analysis to aid real-time data acquisition is essential. Decisions about accumulations

needed to reach desired signal to noise ratios will need to be supported with on-the-fly processing. Modulation excitation with phase sensitive detection analysis will be one of the advanced data analysis methods that will be integrated in SWIFT. The codes will be developed primarily for XAS ME data, but it will be applicable for other complementary techniques such as UV-vis or IR spectroscopies. It is expected that by the time SWIFT will be operational, automatic pattern recognition systems, driven by machine learning algorithms, will reach maturity. Pattern recognition could be used to identify outliers and clustering in hyperspectral XAS maps, provide preliminary identification of species when used in conjunction with reference databases and detect transients in time-resolved acquisitions. Adapting those algorithms to the analysis of XAS data and optimising the performance to provide live feedback during experiments will require dedicated coding effort. It is envisaged that the codes developed and integrated within SWIFT will be made available as open source developments that can be freely used for analysis in the home institutions of interested users.

5. Schematic outline of beamline or project

We are proposing to build SWIFT on one of the newly available mid-straight sections. The layout of the beamline is shown in Figure 10. The beamline consists of an optics hutch (OH) that houses most of the optical components, a component and instrumentation area (CIA) housing the electronic racks, and two experimental hutches. The first (EH1) will operate with a beam size of around $100\ \mu\text{m} \times 100\ \mu\text{m}$ FWHM (VxH), while a $20\ \mu\text{m} \times 20\ \mu\text{m}$ FWHM (VxH) focal spot will be available in the second end-station placed in EH2. A large control cabin for controlling the experiments will complete the layout of the beamline.

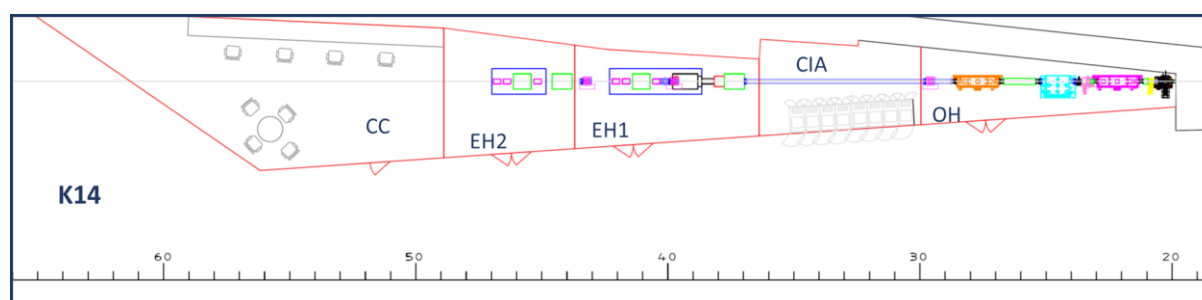


Figure 9. Outline layout of SWIFT on to the experimental floor space for K14 port.

5.1 Source

SWIFT will be based on a conventional out of vacuum multipole wiggler, operating at 1.3 T. The wiggler source has been selected to provide a continuum energy spectrum over the beamline working energy range. The following considerations are based on the I20-EDE source (0.7 m, 15 poles for a total power of 2.4 kW @300 mA and peak power $4.7\ \text{kW}/\text{mrad}^2$), which was designed to offer a good compromise between high flux, power load and critical energy to cover the whole energy range between 4 and 35 keV.

5.2 Optics

The optical configuration is a well-established scheme that is widely used on modern XAS beamlines. The first optical element will be a 1.2 m upward reflecting vertical collimating mirror to achieve good energy resolution and reduce the heat load impinging on the next optical element. The mirror will operate at 2.3 mrad incidence angle and it will be coated with Rh and a Pt stripes to give options for harmonic suppression.

Two Double Crystal Monochromators (DCM) will be installed on the beamline. Both instruments will be equipped with Si(111) and Si(311) crystals to cover the entire energy range. The main DCM will be a fixed-gap, channel-cut system, with fast oscillation mechanics to provide full EXAFS capabilities at high repetition rate, up to 50 Hz. This type of DCM provides a monochromatic beam with very high stability. In

this configuration, the monochromatic beam is allowed to travel along the second crystal, causing a small vertical displacement which is compensated by the following focusing optics. Fast oscillatory mechanics are already operating at other facilities (SLS, ROCK and Petra), but heat management developments will be necessary to deal with the higher power load delivered by the SWIFT wiggler source.

A second, conventional fixed-exit monochromator will also be installed to perform those experiments that do not require fast scanning, providing step-scanning with high energy stability and beam positional accuracy.

The monochromatic beam will be focused on the first experimental station using a 1.2 m long toroidal mirror. The mirror will operate in a 2:1 focusing geometry, delivering an almost aberration free focal spot. A double mirror will be used to ensure that both, Pt and Rh coating, are available.

The primary focus simulations show a focal spot to be of the order of $100 \times 50 \mu\text{m}^2$ FWHM (VxH), including slope errors in the range of $1 \mu\text{rad}$ and $4 \mu\text{rad}$ RMS in the meridional and sagittal directions, respectively. The monochromatic beam flux at the primary focus using the Si(111) crystal pair will be of the order of 10^{13} ph/s at 10 keV.

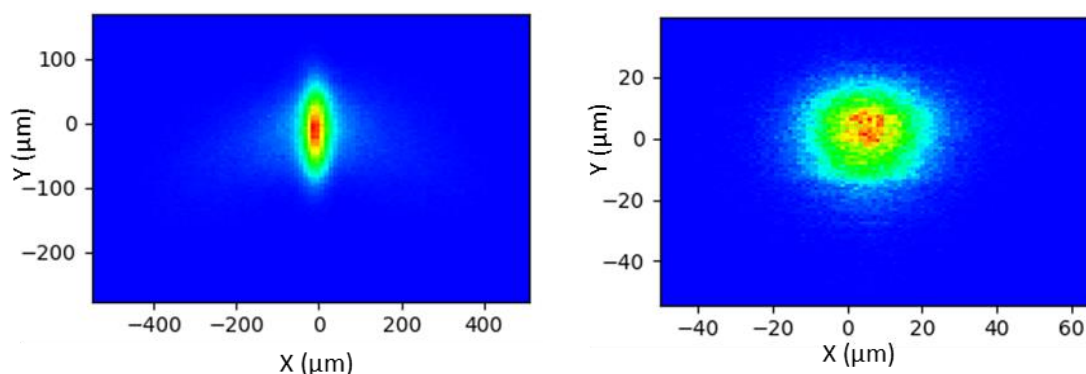


Figure 10. Shadow simulation of the focal spot obtained on the first end-station (left) and after refocussing the beam for the second end-station (right). Simulations do include shape errors. Image scales are in microns.

The beam will be focussed further by using a pair of focusing mirrors in Kirkpatrick-Baez configuration. The KB mirrors will image the primary focus, using it as a secondary source, delivering a focal spot of $20 \times 20 \mu\text{m}^2$. A long working distance for the KB mirrors (W.D. ~ 40 cm) has been included in the design to ensure that the second experimental station will have ample space to house complex sample environments. This will reduce the total flux delivered at the sample position to about 3×10^{12} ph/s, mostly limited by the horizontal beam acceptance aperture of the short KBs coupled with the larger beam divergence in the horizontal direction.

In both cases, higher order beam harmonics will be removed by inserting a pair of short harmonic rejection mirrors close to the experimental point for low energy operations in EH1.

5.3 End-station(s)

The beamline is formed by two end-stations, providing access to both 'large' focus and microfocus configurations. We are proposing to house the two end-stations in two independent hutches, allowing experiments to be setup in EH2 while EH1 is in operation. This will account for the longer times that the preparation of experiments in EH2 will take, due to the need for more precise sample alignment. The availability of a small beam will also encourage combined spatial/temporal experiments that often require significant time for setting up.

Detectors

SWIFT will be equipped with detectors to work both in transmission and fluorescence detection mode compatible with high count rates, as they will need to match the flux and speed delivered by the beamline.

Gridded ionisation chambers will be used as transmission detectors, allowing for the fast detection of transient phenomena. Multielement germanium detectors and silicon drift diodes, coupled with XSPRESS-4 and XSPRESS-3 signal processing systems respectively, will be used for fluorescence measurements. This will allow us to cover the broad energy range of the beamline. It is expected that by the time that SWIFT becomes operational, the evolution of the XSPRESS signal processing will work at >50 kHz, high energy resolution, synchronised frame rates, enabling the use in SWIFT.

An X-ray emission spectrometer will also be used on the microfocus end-station to complement the XAS measurements. HERFD-XAS and XES are rapidly evolving techniques that will enhance the capabilities of SWIFT, and they are increasingly available on scanning XAS beamlines. The XES spectrometer available on SWIFT will enable measurements that require scanning of the incident energy (resonant XES and HERFD-XAS) to be performed in a time resolved manner.

The beamline will also be equipped with a large area XRD detector that will be able to make use of the high flux delivered by SWIFT. The detector should be able to acquire hardware-synchronised frames, so time-resolved experiments can be performed.

5.4 Sample preparation facilities

Our experience has shown that access to off-line sample preparation and characterization facilities are often key for the success of spectroscopy experiments. This is especially critical in the case of experiments requiring *operando* conditions, where a well-equipped chemistry laboratory is often needed for the preparation and characterization of the samples. Activities span tasks ranging from simple assembly of instruments such as a microfluidic cells, all the way to the construction of large equipment, such as the SPACI-MS, or the pre-treatment of catalytic samples before studying them in the beamlines.

Due to the high turnaround of user groups that are expected for SWIFT and the complexity of the sample environments foreseen, a dedicated laboratory will be needed. This will enable more than one user group to use the laboratory simultaneously, allowing the overlap of user groups preparing for experiments in advance of their beamtime, with those performing experiments. This will also facilitate the commissioning and setup of sample environments for the two end-stations of the beamline. It is important to highlight that the user community specifically requested access to a laboratory, so as to ensure that samples can be setup and prepared at Diamond.

The small focal spot available in EH2 will also enable experiments under HP conditions, so access to a HP laboratory will be necessary to prepare and load samples into Diamond Anvil Cells. In addition, the Active Material Laboratory that is currently being built at Diamond will provide state of the art facilities for the handling of radioactive materials, facilitating the experiments that will take place in SWIFT in this area of research.

5.5 Computing infrastructure and support

Data throughput will be significant due to the high acquisition rate. Simply scaling the present data storage structure used for XAS on the group beamlines, we could expect to generate 200 MB/s minimal data for XAS only, without considering raw detector output. Fluorescence data only for a 36-element detector, with the present EPICS strategy on B18 would require storing/retrieving 500 Gbit/s which could be reduced to 5 Gbps in event-list mode but requiring intense downstream postprocessing to present meaningful results. XRD will be potentially even more demanding if full rate acquisition is considered and would require I18-like infrastructure.

On-line visualisation, pre-analysis and data reduction of Quick-EXAFS plus ancillary methods (XRD, XRF, Raman/FTIR) and their integration will need to be considered for sizing of the computing. For data analysis (see section 4.1) automatic pattern recognition systems, driven by machine learning and advanced XANES simulations will require guaranteed access to computing clusters.

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7. Expressions of interest & support from the community

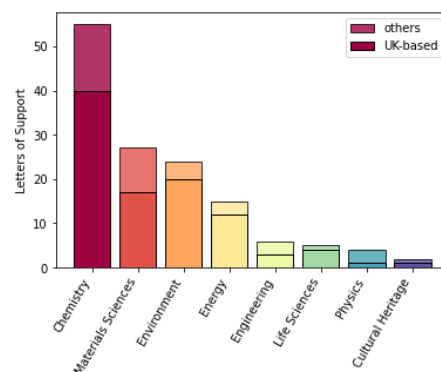
SWIFT received 137 statements of support, reflecting the strong Diamond XAS user community as well as interest from a number of investigators that are not currently Diamond users (10%). The distribution among disciplines reflects the UK tradition of XAS applications in Chemistry and Catalysis, Materials Science, Earth and Environmental Sciences and Energy. The support is predominantly UK-based (Fig.1), although with a healthy proportion of international interest (24%) demonstrating the high appeal and novelty of the SWIFT proposal in Europe and further afield.

Beyond the individual researchers' statements, 30% of the expressions of support received by SWIFT have been submitted on behalf of research groups, institutions or industries, indicating the potential contribution and impact of SWIFT on strategic UK research investment programs.

In the Energy sector, SWIFT received support from **The Faraday Institution** and two of its nine projects (**NEXGENNA** and the **Battery Degradation**). The **STFC Global Challenge Network in Batteries** and the **UCL Electrochemical Innovation Lab (EIL)** have also submitted their support, while for the **Electrochemical Materials Division of the WMG (Warwick University)** stated that "Fast high-quality data acquisition is critical for high through-put operando studies. [...] We support this proposal without reservation". Both the **Dalton Nuclear Institute**, and the **National Nuclear Laboratory (NNL)** have expressed their interest in SWIFT, the latter stating: "In nuclear science the potential applications are broad covering historic challenges [...], decommissioning activities [...], safe disposal of radioactive materials [...] and supporting the development of the next generation of nuclear reactors". From the industrial sector, F. Coomer from **Johnson Matthey Battery Materials** says: "SWIFT will allow in operando measurements to be made on a battery cell cycled at rates much more representative of real usage scenarios".

In Chemistry and Catalysis, the **UK catalysis Hub**, the **Inorganic section at UCL Chemistry**, **The Henry Royce Institute for Advanced Materials** and the **Manchester Faculty of Science and Engineering** strongly support SWIFT. Industrial support is also very compelling with statements received from **Shell** ("SWIFT would [...] offer improved capability for combined time and spatial resolution, which is especially relevant for industrial catalysts, where spatial inhomogeneity is typically present"), **BP** ("In bp, we see catalyst development in combination with catalyst analysis under realistic process conditions and using advanced characterization techniques as the crucial intermediate step between fundamental science and process applications.[...] It is only with capability like this that the next generation of catalyst processes will be developed, where catalysts are measured under realistic gas conditions, temperatures and fast time scales to understand the catalyst and innovate with new opportunities."), **Infineum UK** and **Finden Ltd.**

SWIFT has also received strong support from the Earth, Environment and Cultural Heritage communities. According to the **National History Museum**: "The SWIFT beamline is a crucial capability that directly fits within our strategic priorities written into our new Science Plan - The timing of SWIFT (2027) coincides excellently with the imminent NHM £180 million investment into a Science and Digitisation Centre on the Harwell Campus[...] Within the NHM Science Group we anticipate that several areas of our science will be able to utilise SWIFT to substantially enhance our in house research activities". Prof. Roy Wogelius, from the **Centre for Ancient Life (ICAL)** highlighted SWIFT's potential for this research area ("It would be completely reasonable to state that the breadth of results such an investment would yield will be far beyond what the proposers envision-the concept will allow new areas to be explored in ways that are simply not possible with the current beamlines at DLS"). The scientific department at **The National Gallery** has also expressed its support "SWIFT will also enable fast processing of more dilute systems than B18 or I18, which is vital if we are to detect and identify species of interest which are present in very small amounts within a dominant matrix in our samples".



Statements of support summary

Total number of submissions: 137

Key for statements in Appendix A	Respondent's primary field of research	Percentage of respondents
	Chemistry	39.4%
	Materials Sciences	19.7%
	Earth Sciences & Environment	17.5%
	Energy	10.9%
	Engineering & Technology	4.4%
	Life Sciences & Biotech	3.6%
	Physics	2.9%
	Humanities (Cultural Heritage)	1.5%

Respondent location	Percentage of respondents
UK	75.9%
International	24.1%

Type of organisation supporting	Percentage of respondents
Academic	85.4%
Industry	5.8%
Government	2.2%
Charity	0.7%
Non-Governmental Organisation (NGO)	0.7%
Other	5.2%

Diamond user status	Percentage of respondents
Not currently a user at Diamond	10.2%
Currently a user at Diamond	89.8%

About 30% of the 137 statements of support received for SWIFT have been submitted on behalf of institutions, large research groups or industries. The remaining 70% represent individual support statements from researchers from academia, industry or government institutions.

The two webinars organized were very well attended, and the discussions helped shape the science case, and ensure that the needs of the community were covered.

Engagement webinar summary

Date of webinar/s: Thursday 17th September and Wednesday 4th November

Total number of attendees: 183

Attendee location	Percentage of attendees
UK	76.5%
International	23.5%