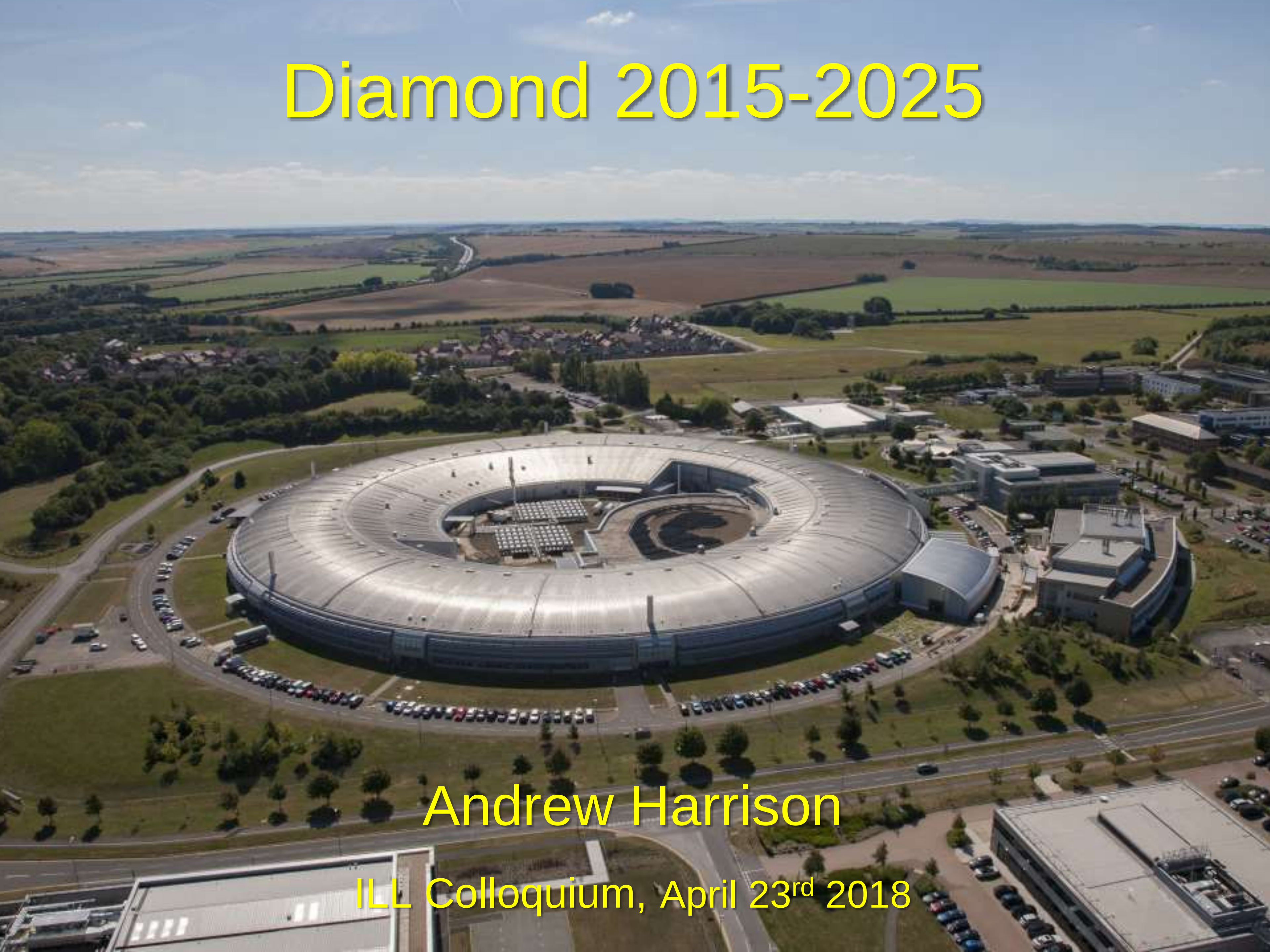


Diamond 2015-2025

Andrew Harrison

ILL Colloquium, April 23rd 2018


RÉSERVÉ DIRECTEUR
cannondale

From foundations to facility

Diamond Light Source Ltd created in 2002 as a Joint Venture between UK Gov't (STFC) – 86% - and the Wellcome Trust – 14 %

December 2003

May 2004

April 2006

May 2015

From foundations to facility

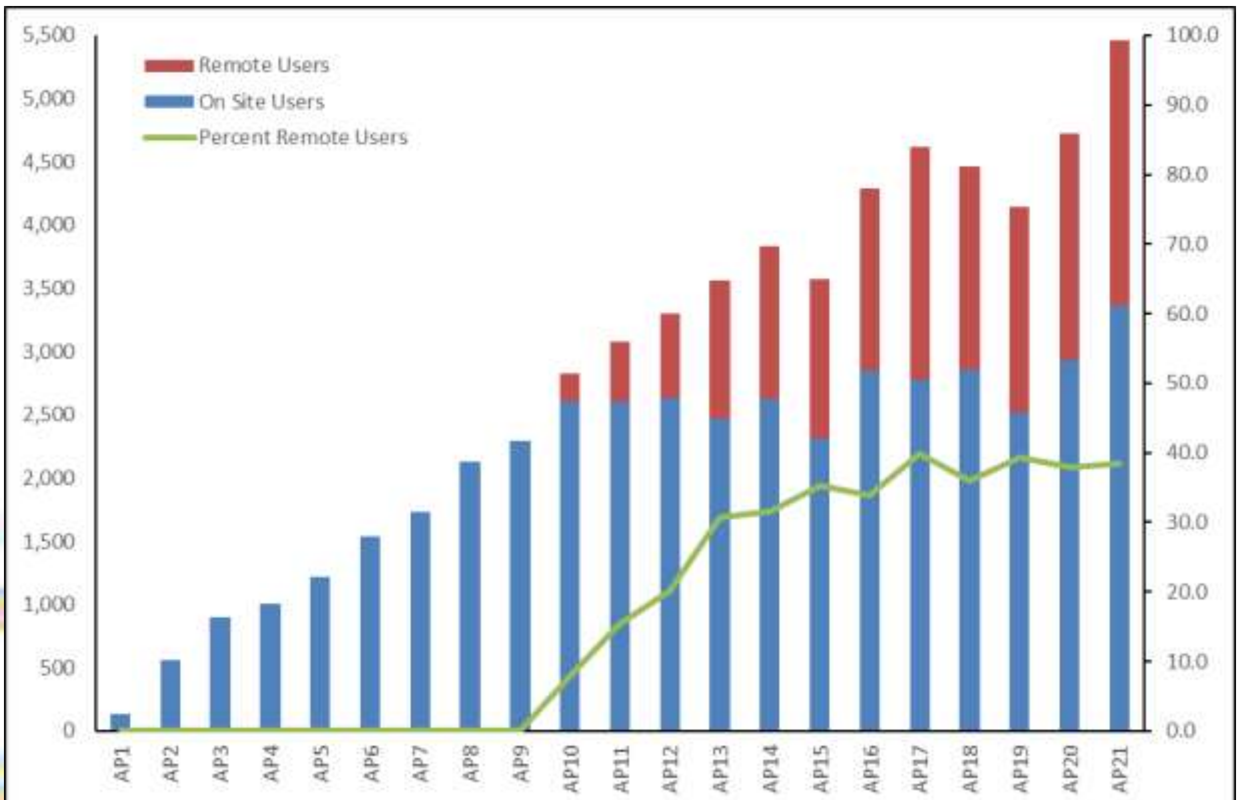
Diamond Light Source Ltd created in 2002 as a Joint Venture
between UK Gov't (STFC) – 86% - and the Wellcome Trust – 14 %

- Operational since 2007
- Particular emphasis from day 1 on:
  - Life Science – 45% of user base
  - Industrial engagement – dedicated Industrial Liaison team (now 11)
  - Public outreach

diamond

Building the community

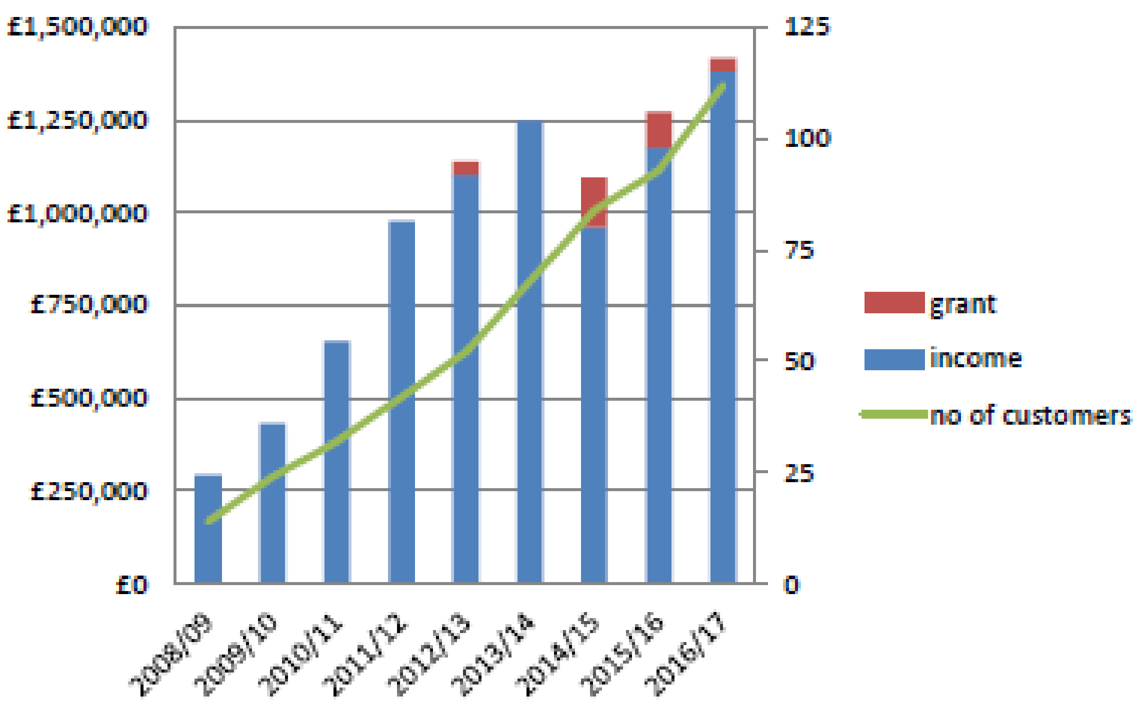
- Over 10,000 user ‘visits’ last year - 40% remote, 45 % life sciences



2017 Celebrating Diamond’s 15th anniversary and 10 years of research and innovation

Building the community

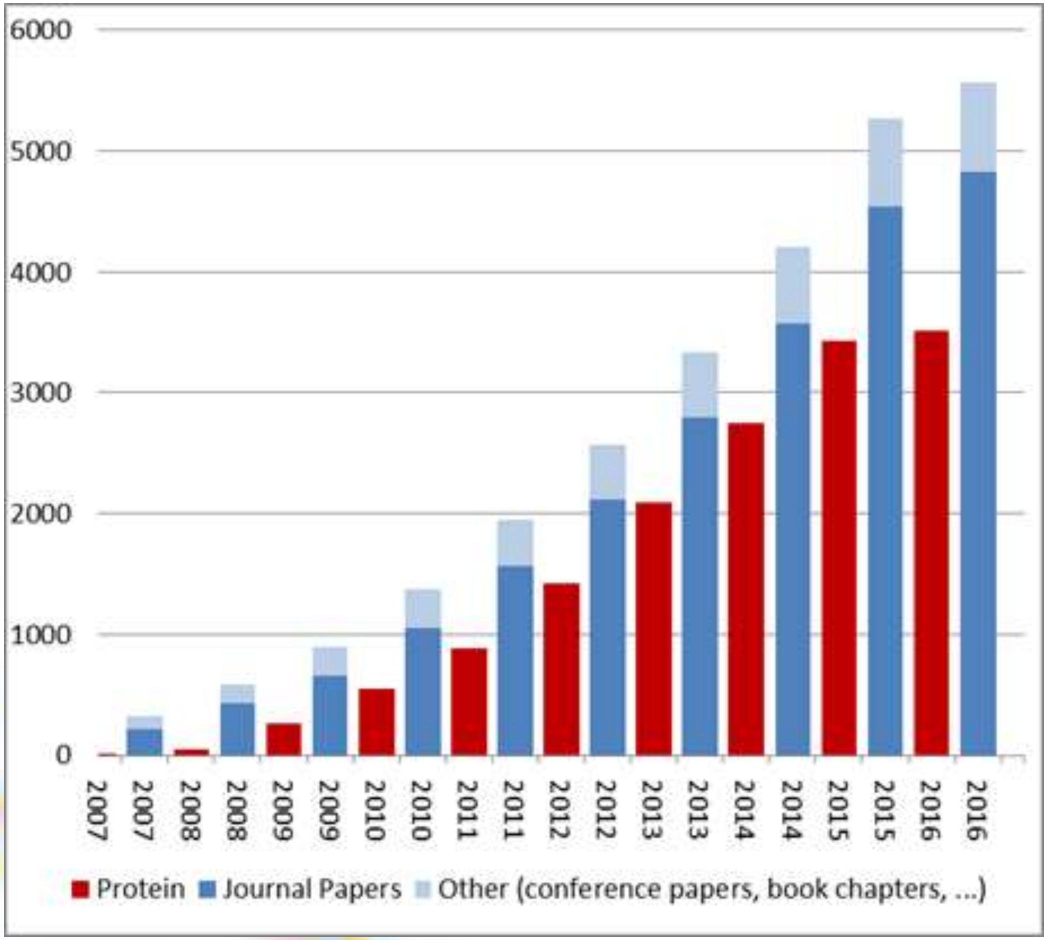
- Over 10,000 user 'visits' last year - 40% remote, 45 % life sciences
- 110 companies pay for access – 80% pharmaceutical and bio-tech
- Over 11,000 visits from the general public and schools last year



2017 Celebrating Diamond's 15th anniversary and 10 years of research and innovation

Delivering science

- Approaching 1000 papers per annum and set to rise further, and percentage with impact factor > 9 is greater than 25%



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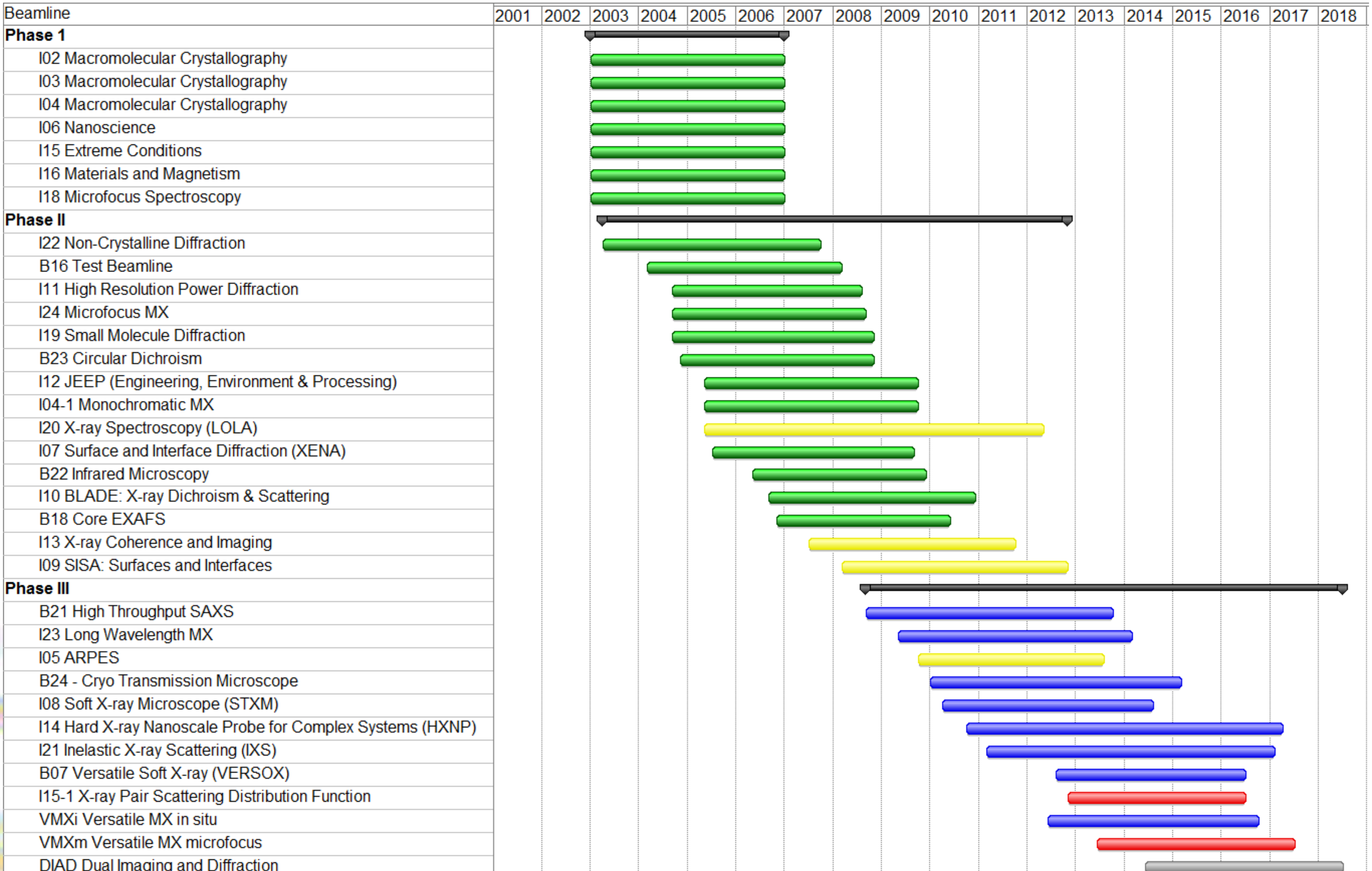
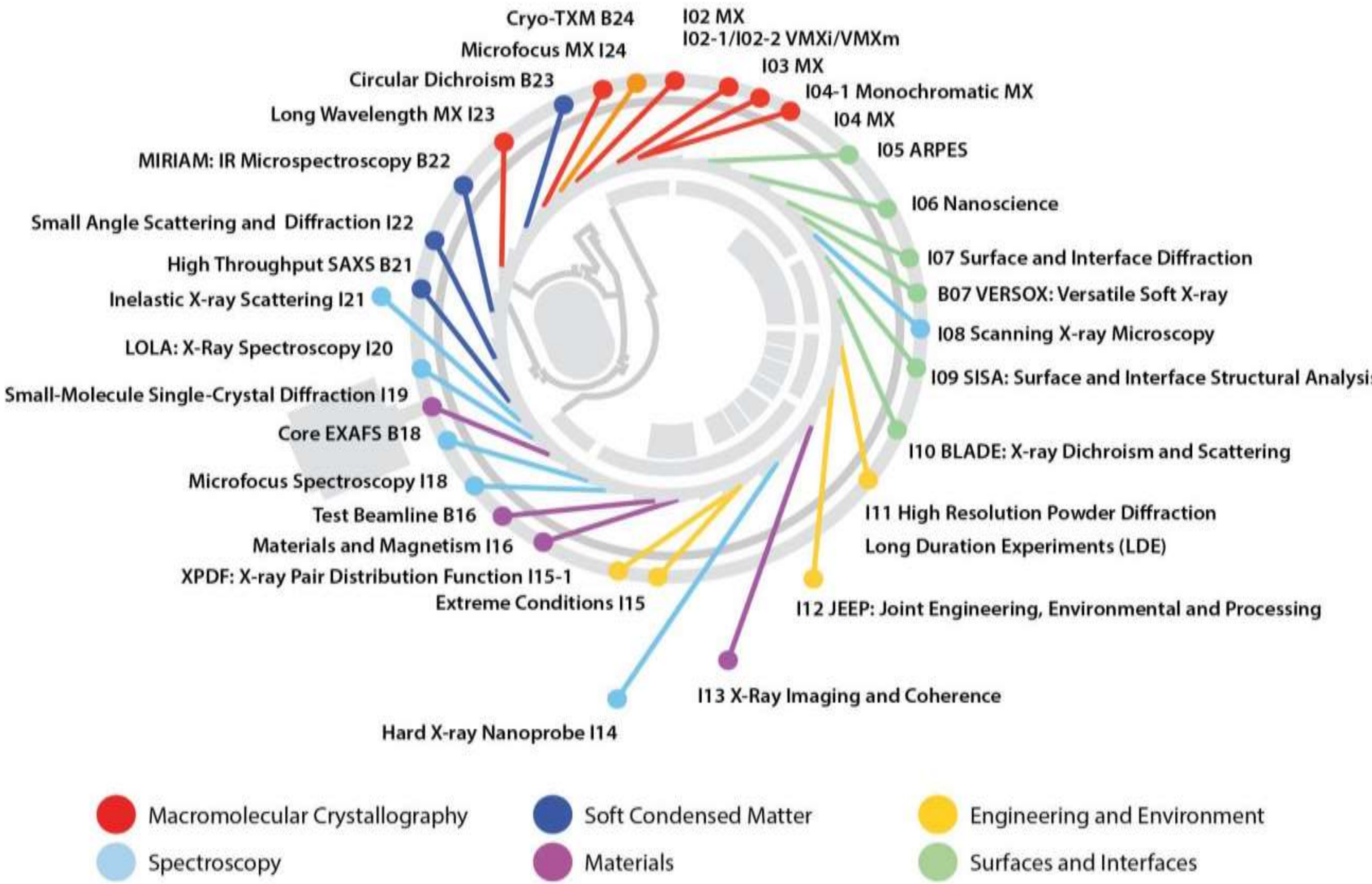
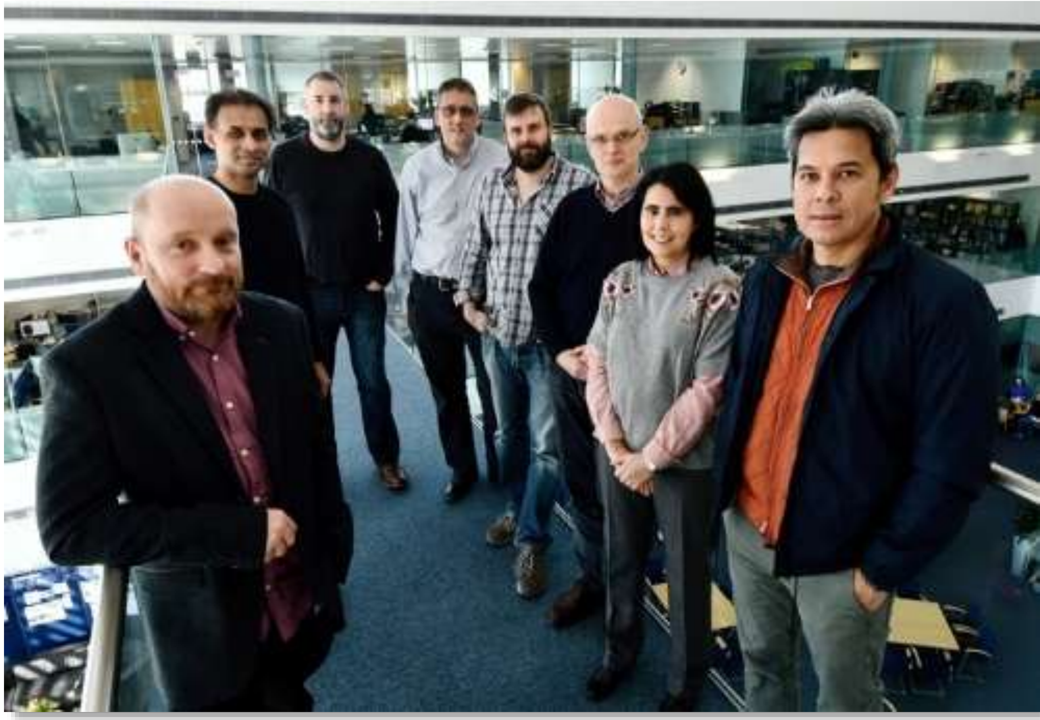
3-Phase Supply



31 beamlines, 2 more to come

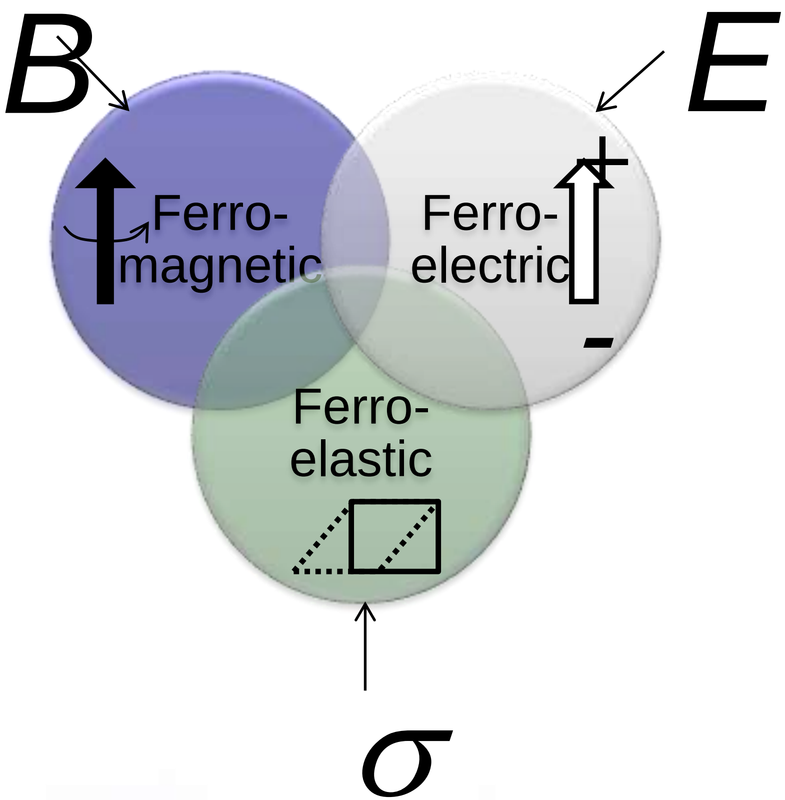


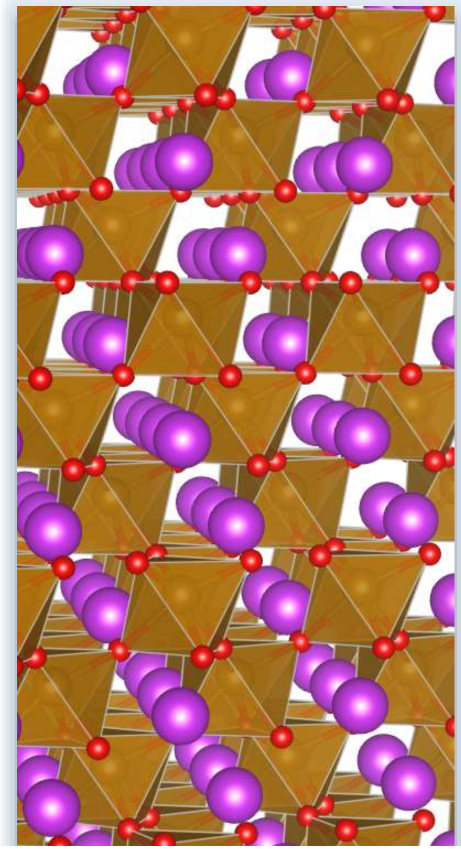
SGLs and IGLs

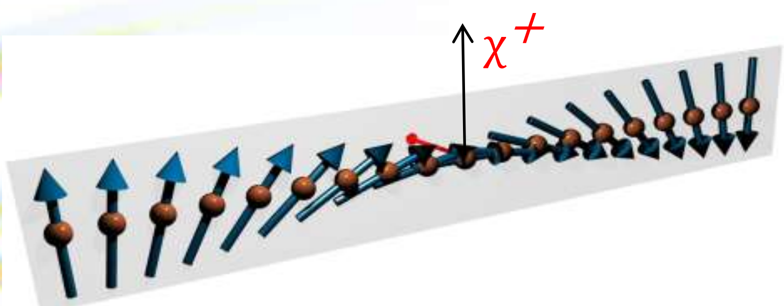


- New *Scientific Group Leaders* appointed in 2018 to provide strategic lead in science delivery and collaboration, and form new integrated teams with engineering, software, controls.

Multiferroics : from bulk to nano



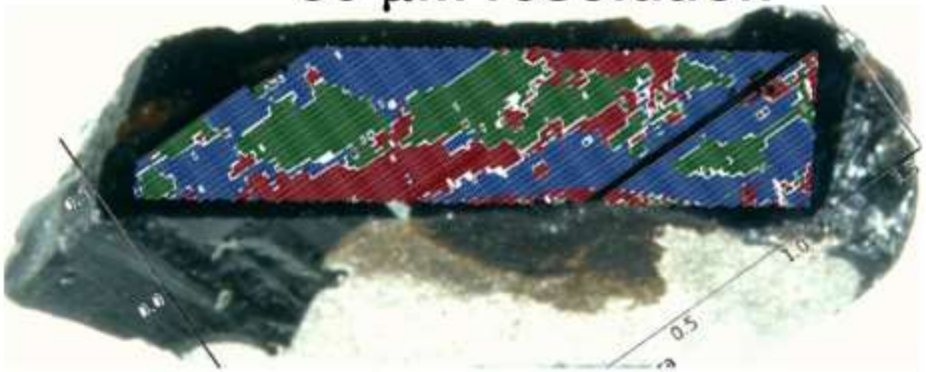


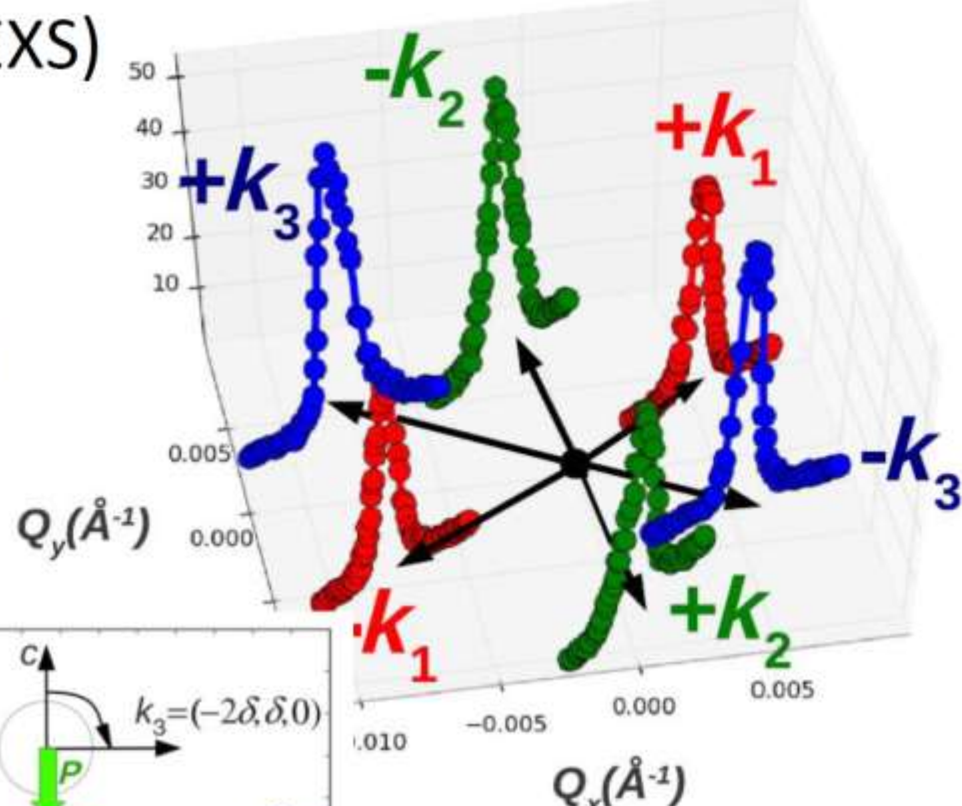


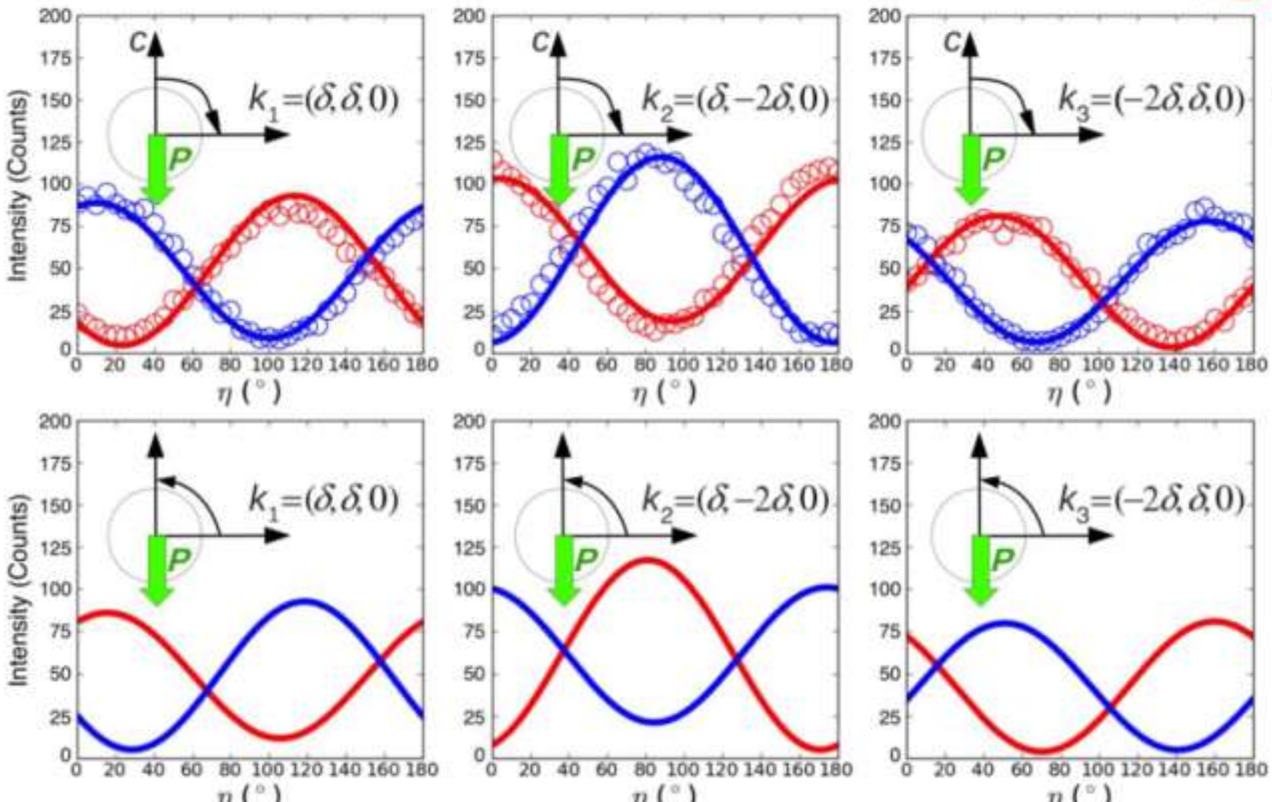
May contain cycloidal magnetic
states – polar objects that can b
manipulated with a magnetic fie

Bulk $BiFeO_3$ (I16 hard X-ray REXS)

50 μm resolution



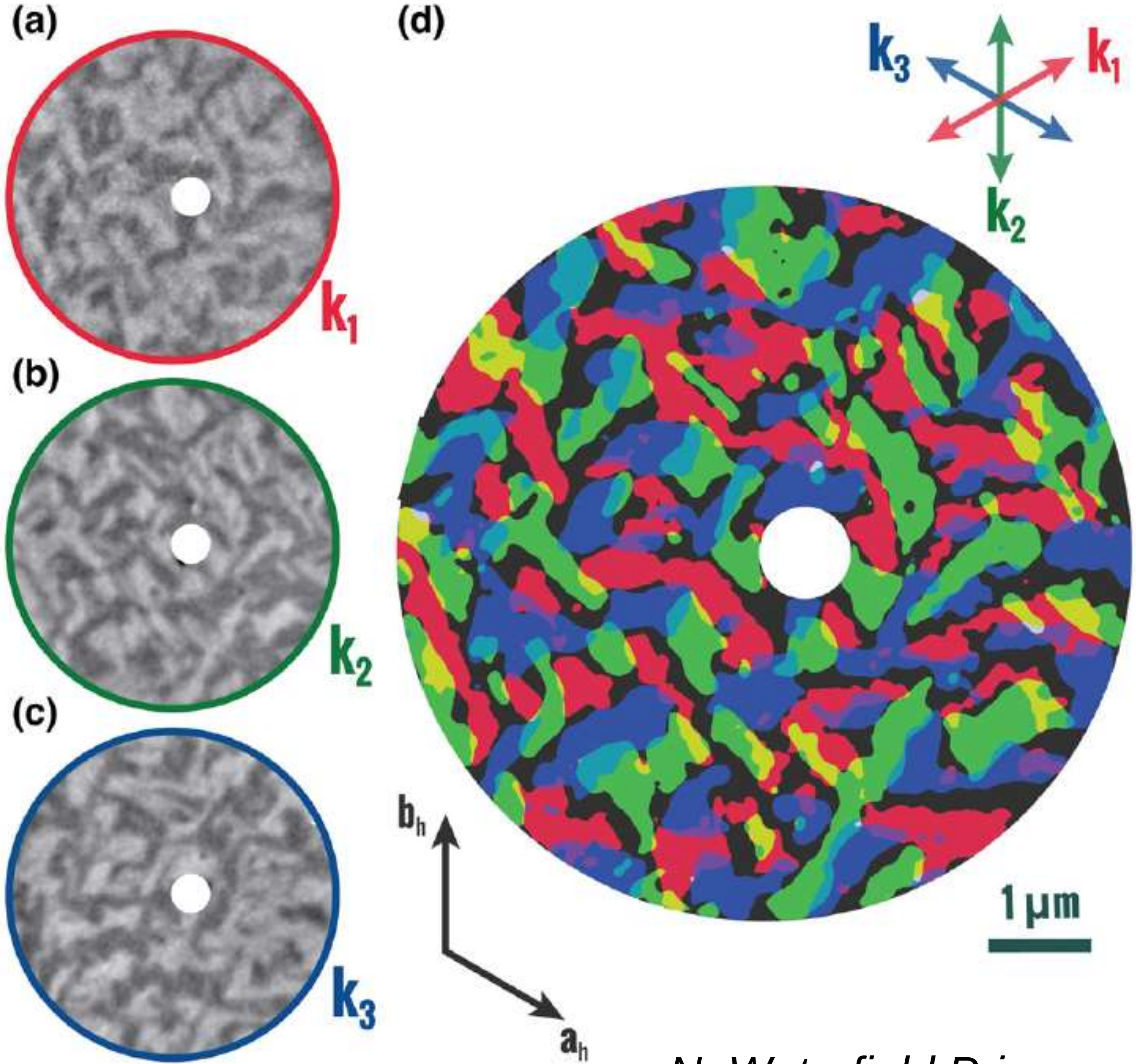




BFO – multiferroic properties at RT. Single crystal study of single P electric domain – observe 3 cycloidal magnetic domains, study each with left and right circular polarisation to show rotation direction same – coupled to same P

R. Johnson et al., PRL 110, 217206 (2013)

Epitaxial $BiFeO_3$ (I06 XMLD-PEEM)



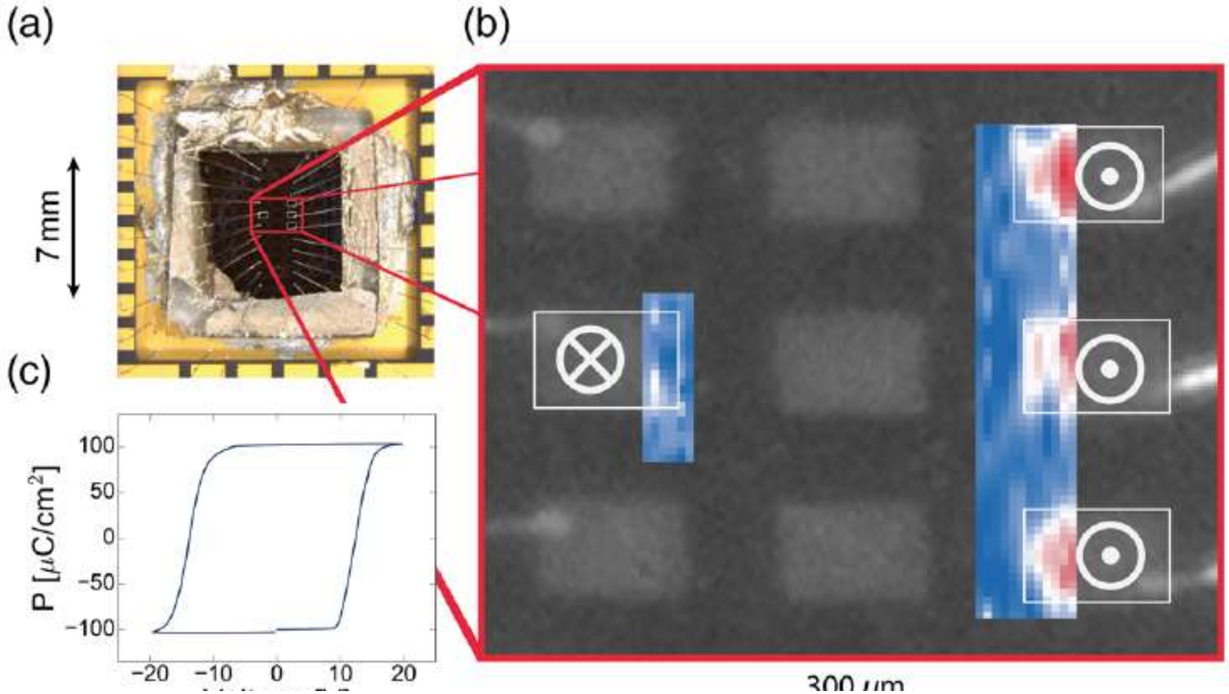
Bulk material characterised by single crystal neutron and X-ray studies

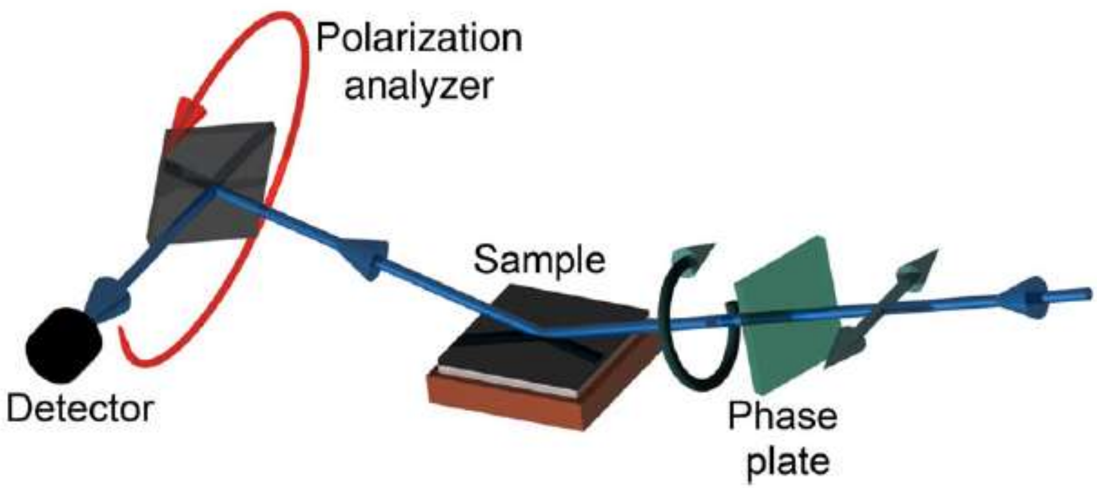
$BiFeO_3$ as epitaxial film
Vector map of domain magnetisation at ~1 µm resolution

N. Waterfield Price
PRL 117, 177601 (2016)

diamond

Epitaxial relaxed $BiFeO_3$ (I16)





Direct imaging of reversible electrical switching of cycloidal rotation direction (magnetic polarity) in micro device by non-resonant X-ray scattering

Against expectation the rotation of domains changes significantly – of the order of 90° - between cycles

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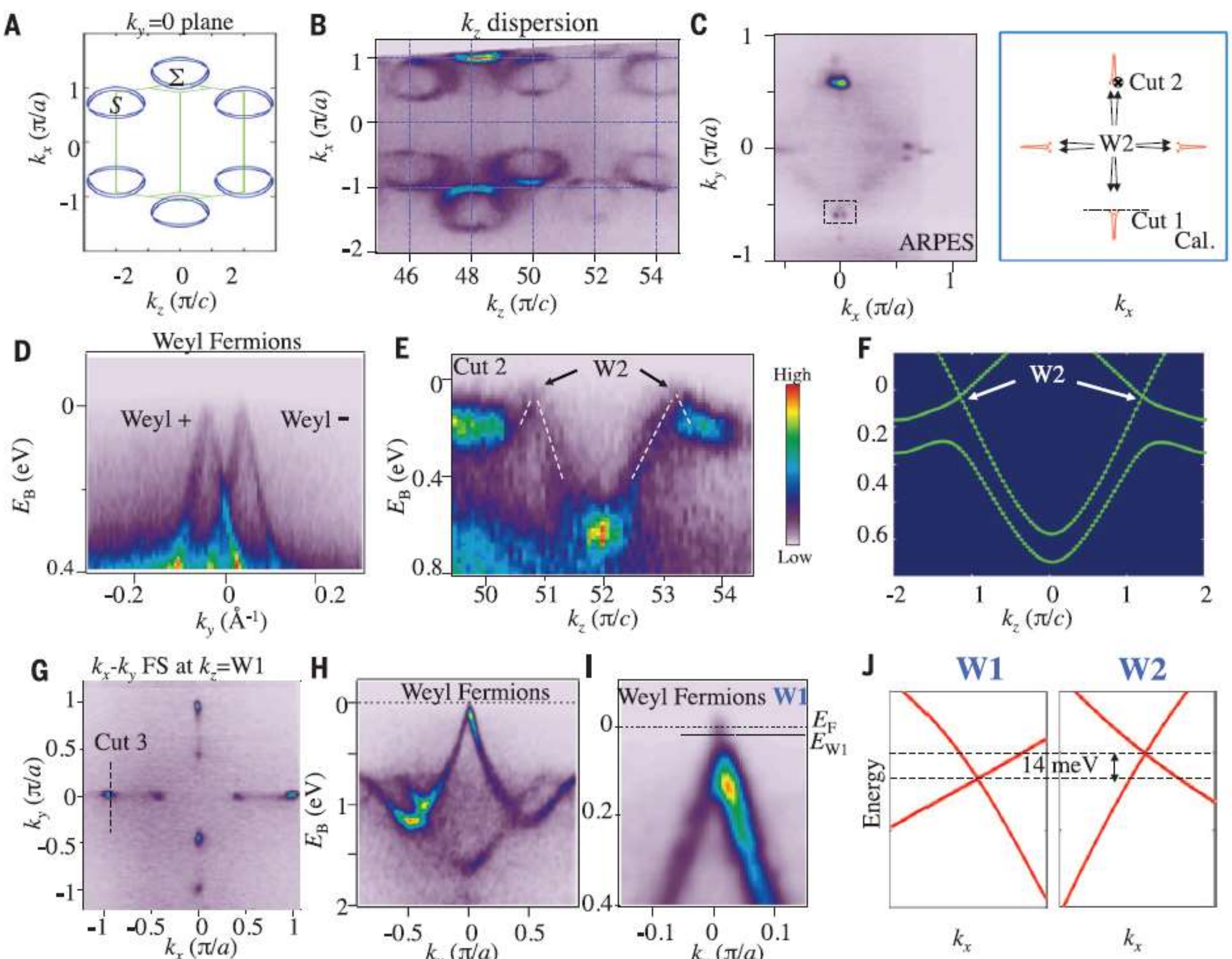
PRL 8, 014033 (2017

TOPOLOGICAL MATTER

Discovery of a Weyl fermion semimetal and topological Fermi arcs

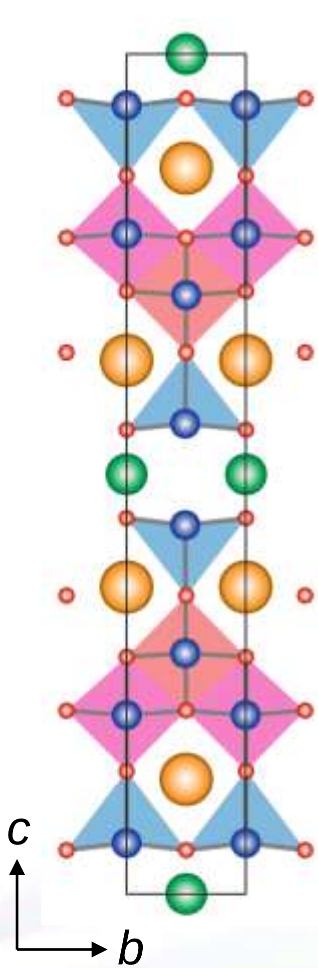


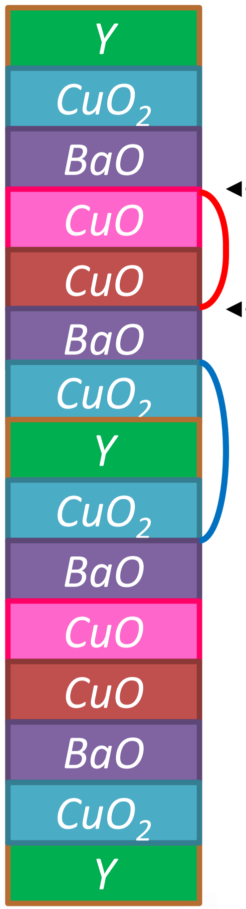
ARPES on I05 has produced over 100 papers in 4 years of operations, including most highly cited (>800)

First observation of Weyl modes/particles - 90 years after prediction – solution of Dirac equation for massless particles, appearing as quasiparticles (low E excitations of many-body system)

Seen here in topological material TaAs

Plane and chain domains in bilayer $YBa_2Cu_4O_8$





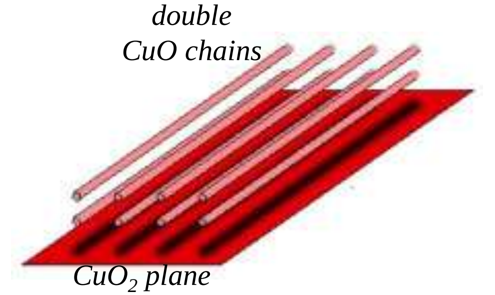
Cleave

Termination (1) : CuO

Chain bilayer

Termination (2) : BaO = CuO_2

Plane bilayer



Kondo, PRL **105**, 267003 (201

YBCO archetypal superconductor, T_c = 83K

Properties depend on interplay between superconducting CuO2 planes and planes of CuO chains planes

Cleavage normally at interface CuO and BaO leaving surface termination of either CuO chains or CuO2 planes

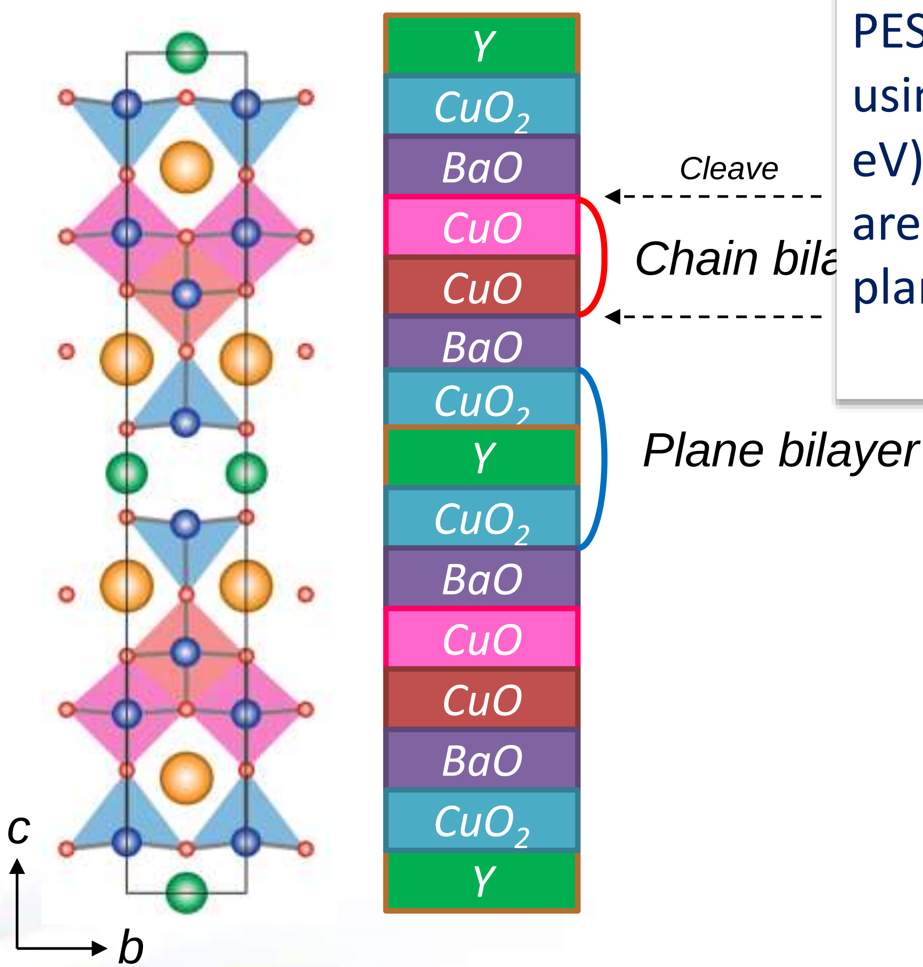
Explore electronic structure in each by nano-ARPES

$YBa_2Cu_4O_8$: Y124 (T_c ~ 82 K)

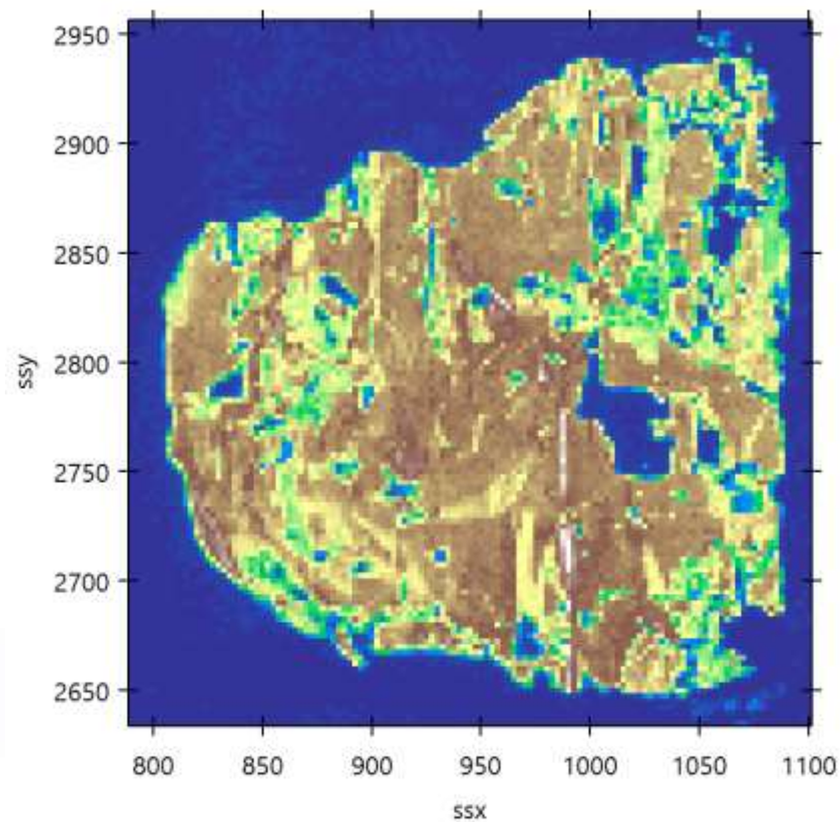
- *Bilayer – CuO chain*
- *Bilayer – CuO_2 plane*

diamond

Plane and chain domains in bilayer $YBa_2Cu_4O_8$



PES total intensity mapping measured on I05 using a Zone Plate to focus the XUV beam (60 eV) down to 700 nm spot size, for ~300x300μ area - clear presence of chain (brown) and plane (green) domains is detected.

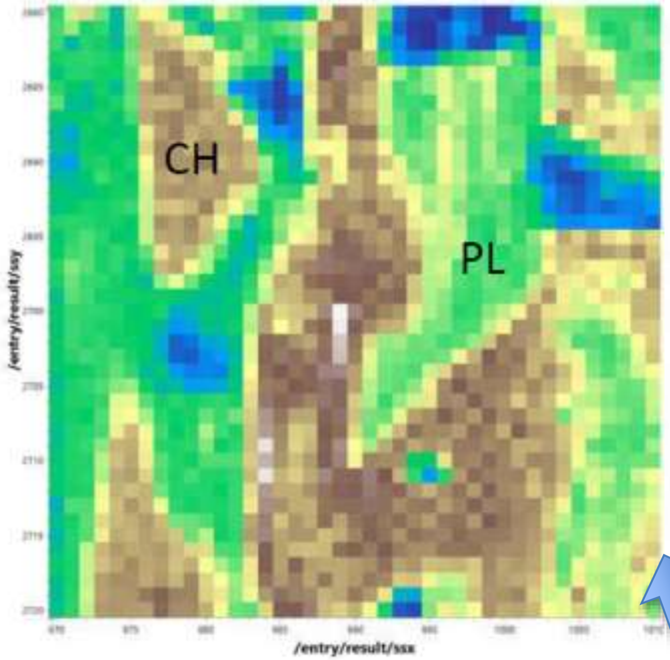


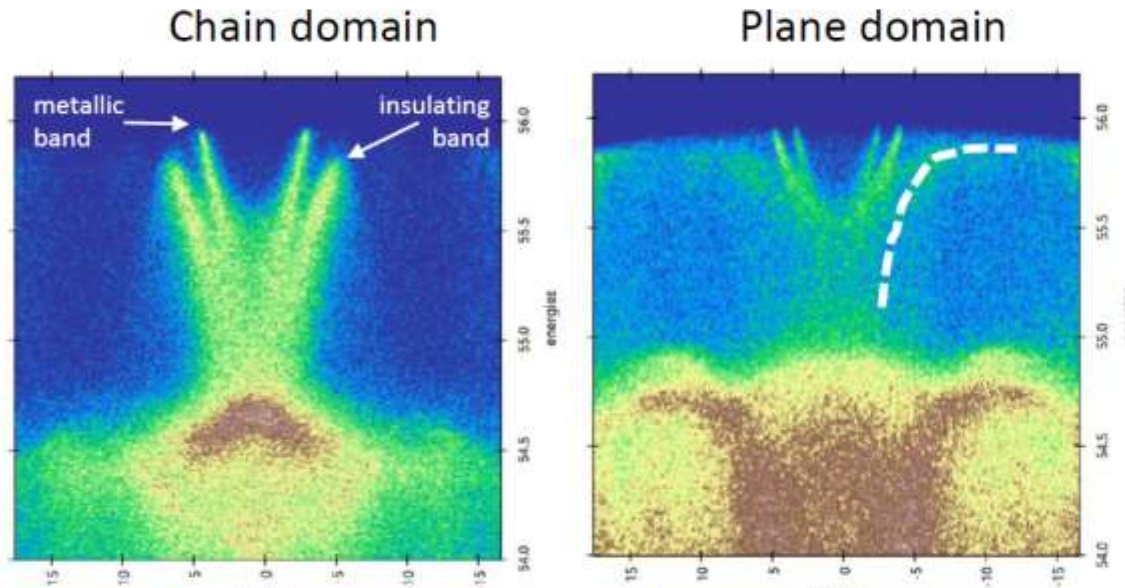
$YBa_2Cu_4O_8$: Y124 (T_c ~ 82 K)

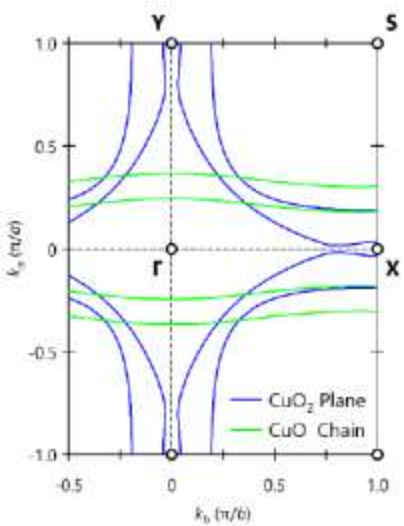
- *Bilayer – CuO chain*
- *Bilayer – CuO_2 plane*

Probing the embedded CuO chain in $YBa_2Cu_4O_8$

Courtesy of H. Iwasawa (Diamond Light Source)
H. Iwasawa, …, et al. (2018)







40 x 40 μm photoemission map in < 2hr reveals regions where CuO2 planes exposed (PL), and regions with CuO chains (CH)

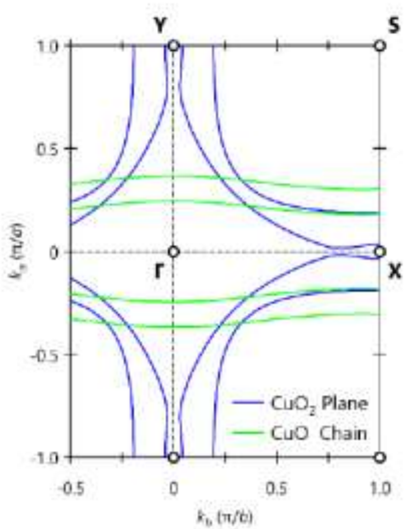
High-symmetry ARPES cuts for each domain – 10 mins, 30 meV resolution at 60 eV photon energy

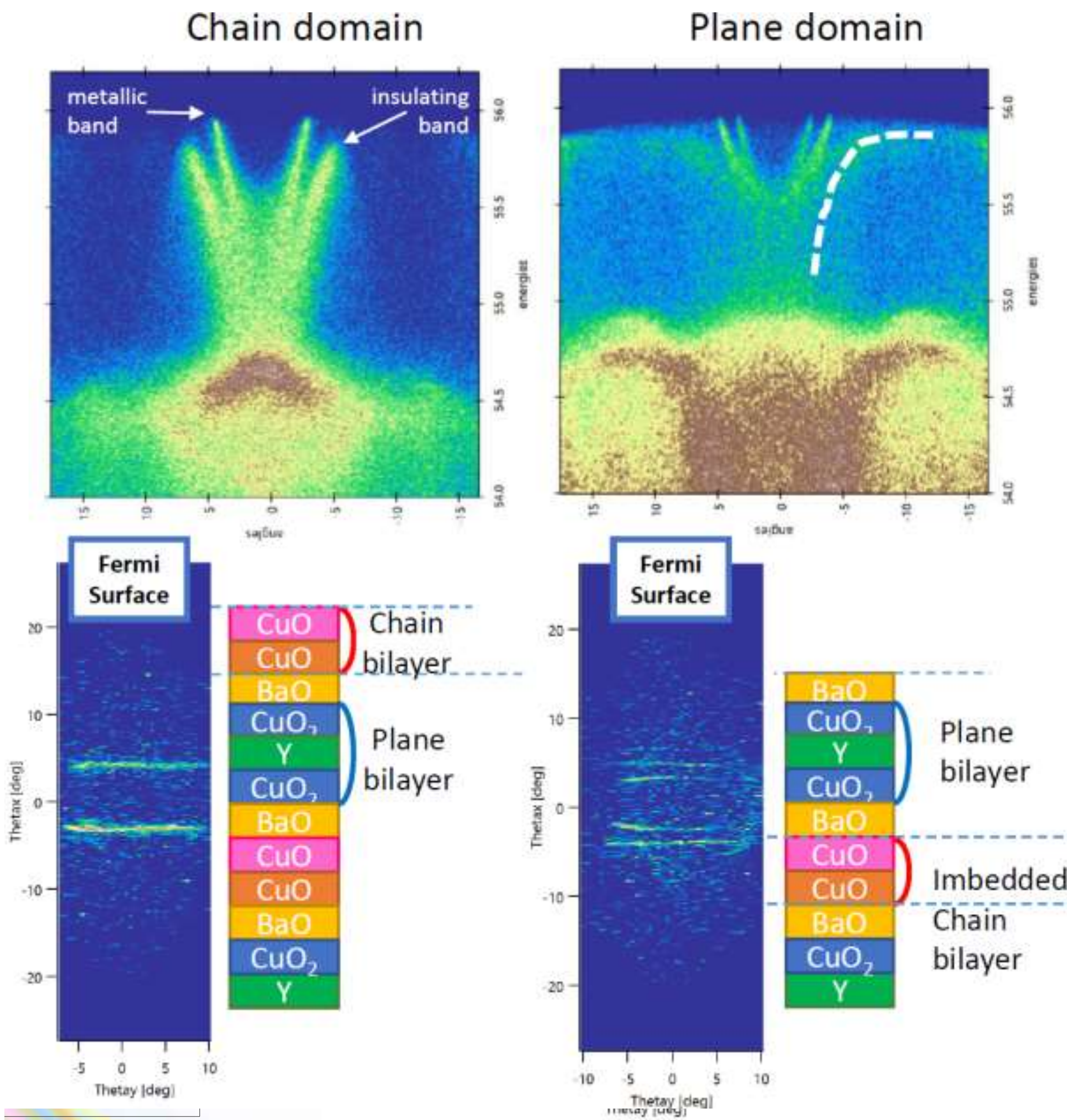
Probing the embedded CuO chain in $YBa_2Cu_4O_8$

ARPES cuts in 10 mins

CH: 2 strong bands – one insulating and one metallic with linear dispersion on Fermi surface characteristic of 1D CuO Chain

For CuO2 plane expect bulk Cu band (dashed white line) – but also observe two weak metallic bands from underlying CuO chains -



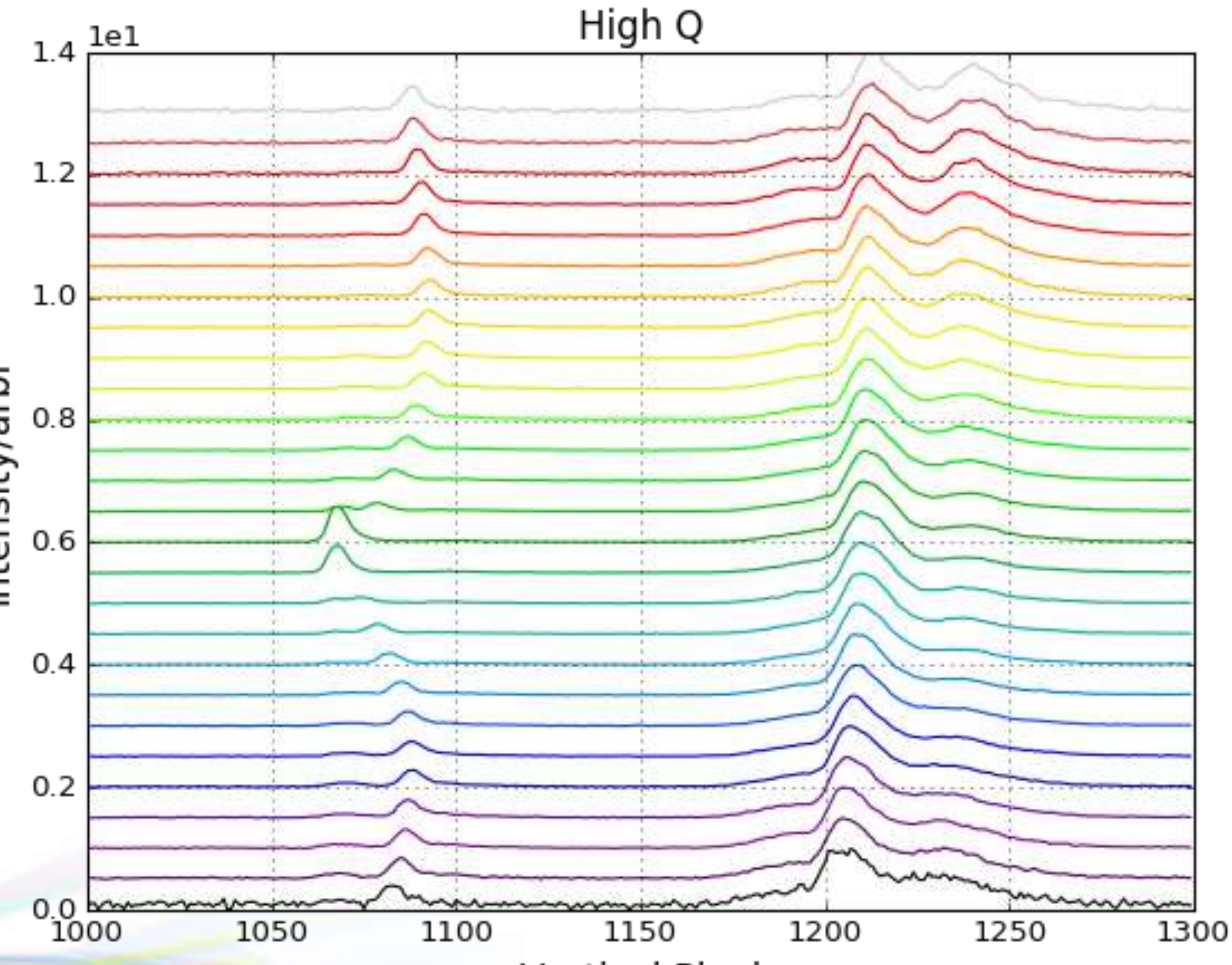


I21 –RIXS- First users (22-9-17)

- ***Currently in commissioning: Oct 2017 – Mar 2018***

- ***Open for proposals: deadline 1st October 2017***
  for the period of Apr – Sept 2018

I21 : First measurements



First I21 measurement was performed on LCO

Dispersion of single magnon mode followed with scans 2 min per spectra – data shown here done in 1.5 hour

Currently, best resolution is 35meV at Cu-edge and 15 meV at O-edge

- *Sample - La2CuO4 single crystal, (p,p)*
- *Temp – 36 K*
- *total energy resolution – 72 meV @ 930 eV (VPG2 + SVLS1)*
- *Acquisition time – 120 secs / spectrum*

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Dispersion in nanolayers

Superlattices: $[(LaTiO_3)_1/(LaNiO_3)_1/(LaAlO_3)_3]_3$

The combined RIXS energy resolution of ~ 33 meV is achieved at Ni L_3-edge (854 eV)

The effective thickness of the $LaNiO_3$ is 3 unit cells and acquisition time for each Q ~ 1 hr

For each Q-dependent RIXS spectrum shown right, acquisition time is 1 hour

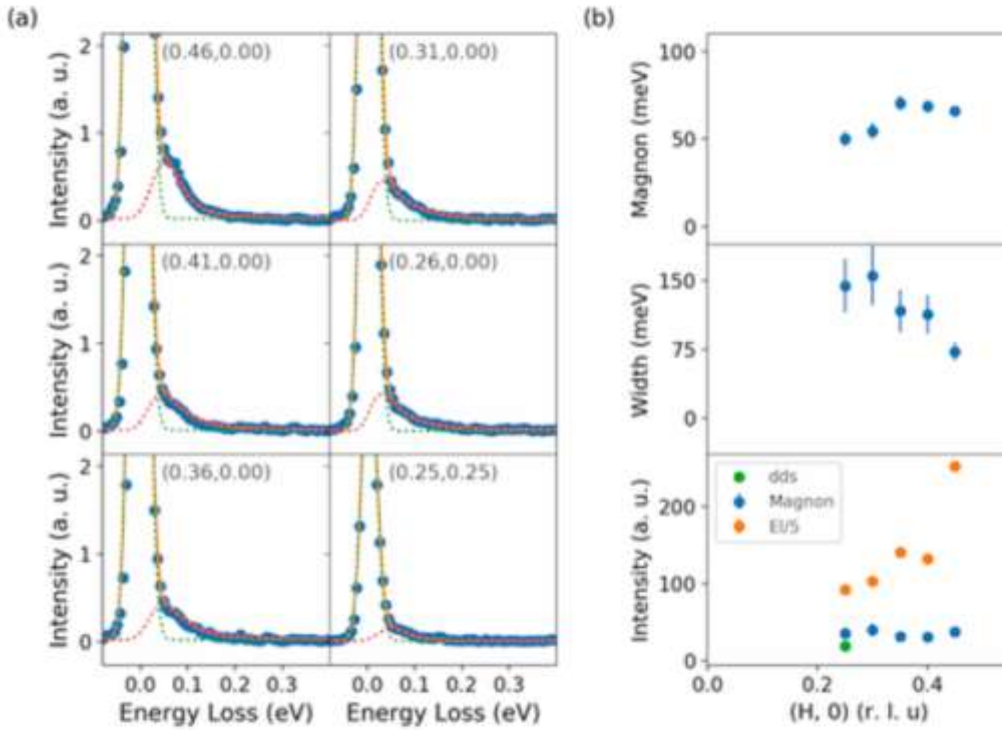
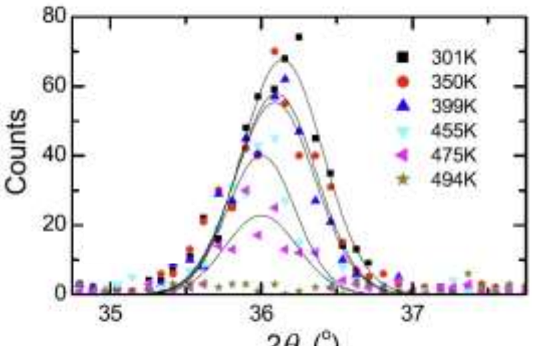


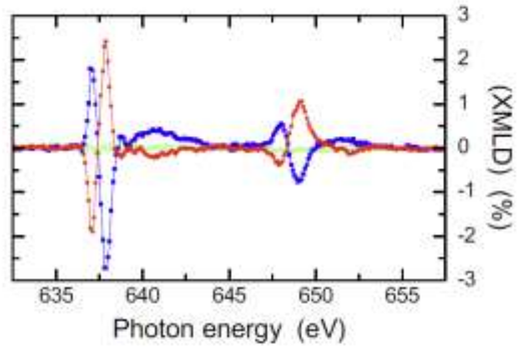
Fig. 1: (a) Raw spectra at multiple Q along (H, 0) direction. (b) Dispersion, width, and intensity of magnetic excitations.

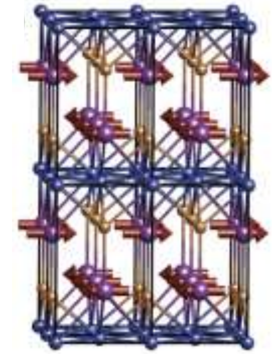
Experiment Report of SP18492 at I21
Date of Experiment: Feb 9^{th}, 2018

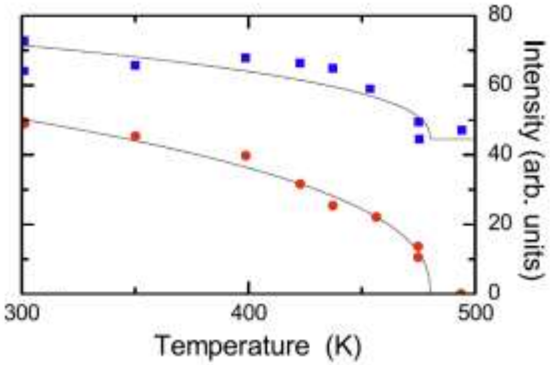
Increasingly multiprobe measurements

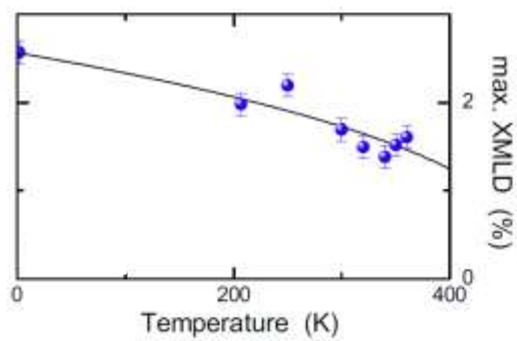
Potential spintronic material CuMnAs studied in 500 nm film on GaP by ND (D10 – ILL - and WISH – ISIS) and 10 nm film by XMLD (I06 – DLS)

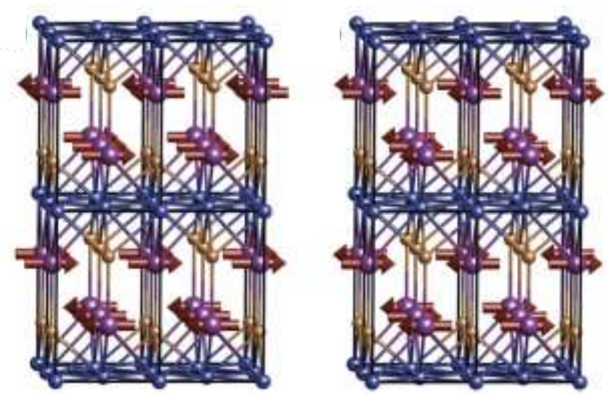












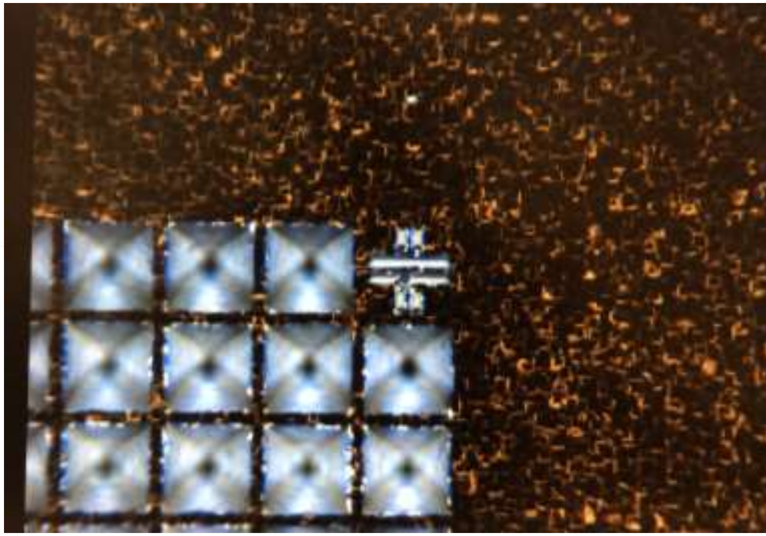
SCIENTIFIC REPORTS

P. Wadley[1], V. Hills[1], M. R. Shahedkhah[1], K. W. Edmonds[1], R. P. Campion[1], V. Novák[2], B. Ouladdiaf[3], D. Khalyavin[4], S. Langridge[4], V. Saidl[5], P. Nemec[5], A. W. Rushforth[1], B. L. Gallagher[1], S. S. Dhesi[6], F. Maccherozzi[6], J. Železný[2,5] & T. Jungwirth[1,2]

SCIENTIFIC REPORTS | 5:17079 | DOI: 10.1038/srep17079

MX

- Day 1: 3 ‘traditional’ beamlines now expanded and developed
  - Early exploitation of next-generation detectors: low-noise, huge pixel array with fast frame capture
  - Robotic systems for fast, automatic sample change, *in-situ* measurements, remote access 24/7 (>>50% of all samples) with integrated data management (ISPyB with ESRF).
  - New, portable sample delivery systems for 2,500 crystals/minute (D.A. Sherrell, R.L. Owen et al, J, Sync. Rad (2015) 22)
  - Support laboratories for membrane protein crystallisation; level 3 containment



Replacing Phase I beamlines: I02 → VMXi

Last Light I02 - August 5th

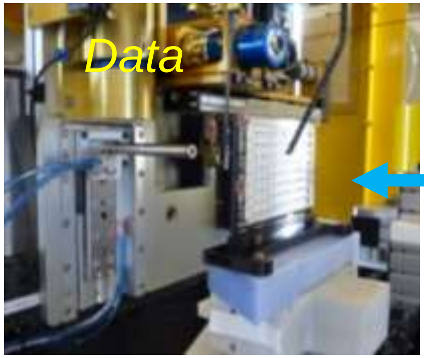
First Light VMXi - October 5th

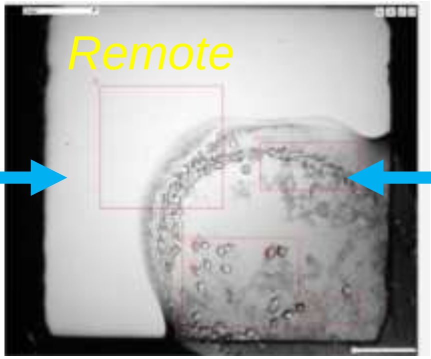
First data collection VMXi – December 2016

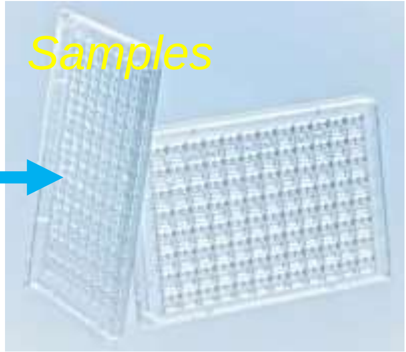
VMXi – automated in situ beamline

Why VMXi?

- *Data-based crystallisation*
- *Difficult samples*







VMXm – micro/nanocrystallography

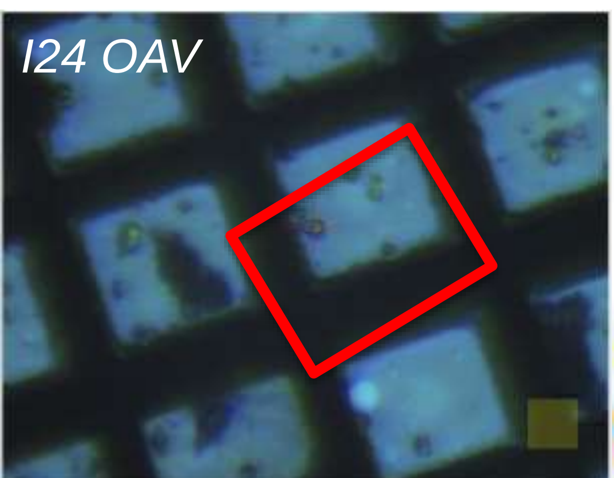
"… push physical limit of MX using SR…"

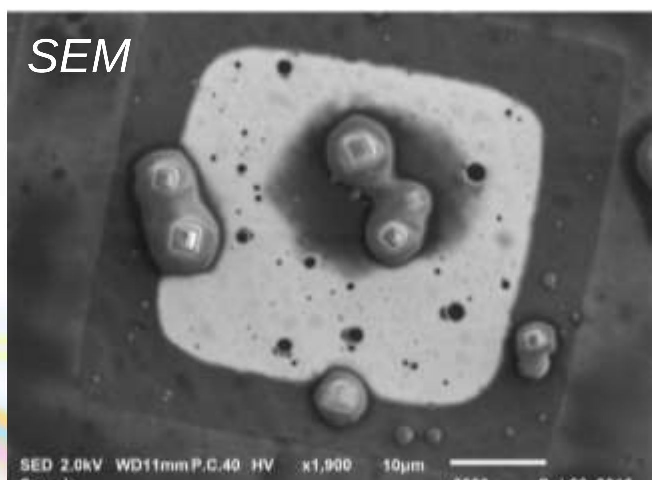
grid holders – machined prototypes (above) and moulded final (right)

Target crystals between 0.5 and 10 microns deposited on Cryo-EM grid to give multicrystal data sets recorded using rotation method

- SEM used to image and record crystal locations
- Crystals aligned in turn to X-ray beam and exposed

Aim to use minimal protein material for structure determination





Samples prepared using cryoEM blotting methods rapid plunge cooling. Life-time gains due to photoelectron escape from (small) crystals

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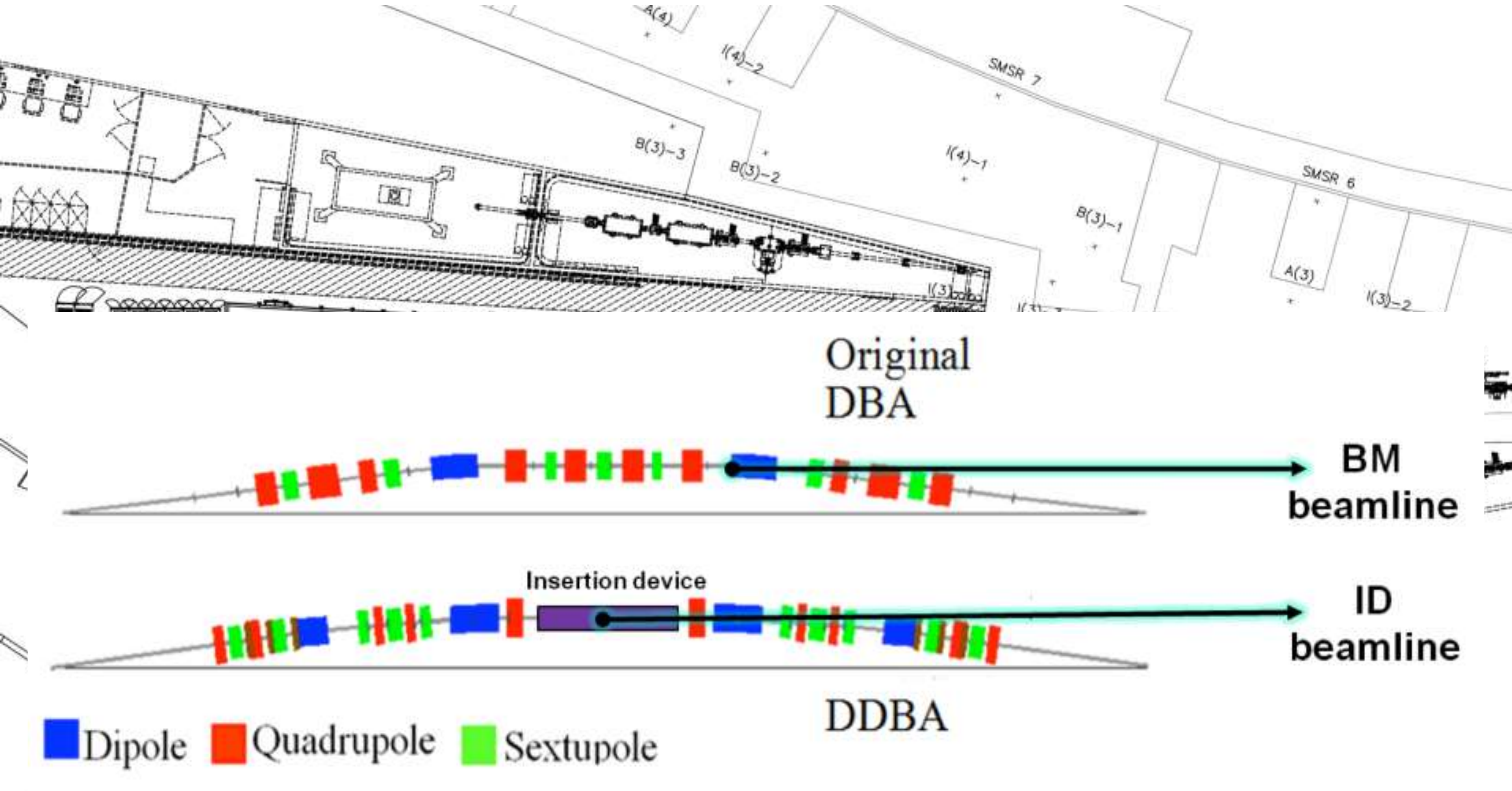
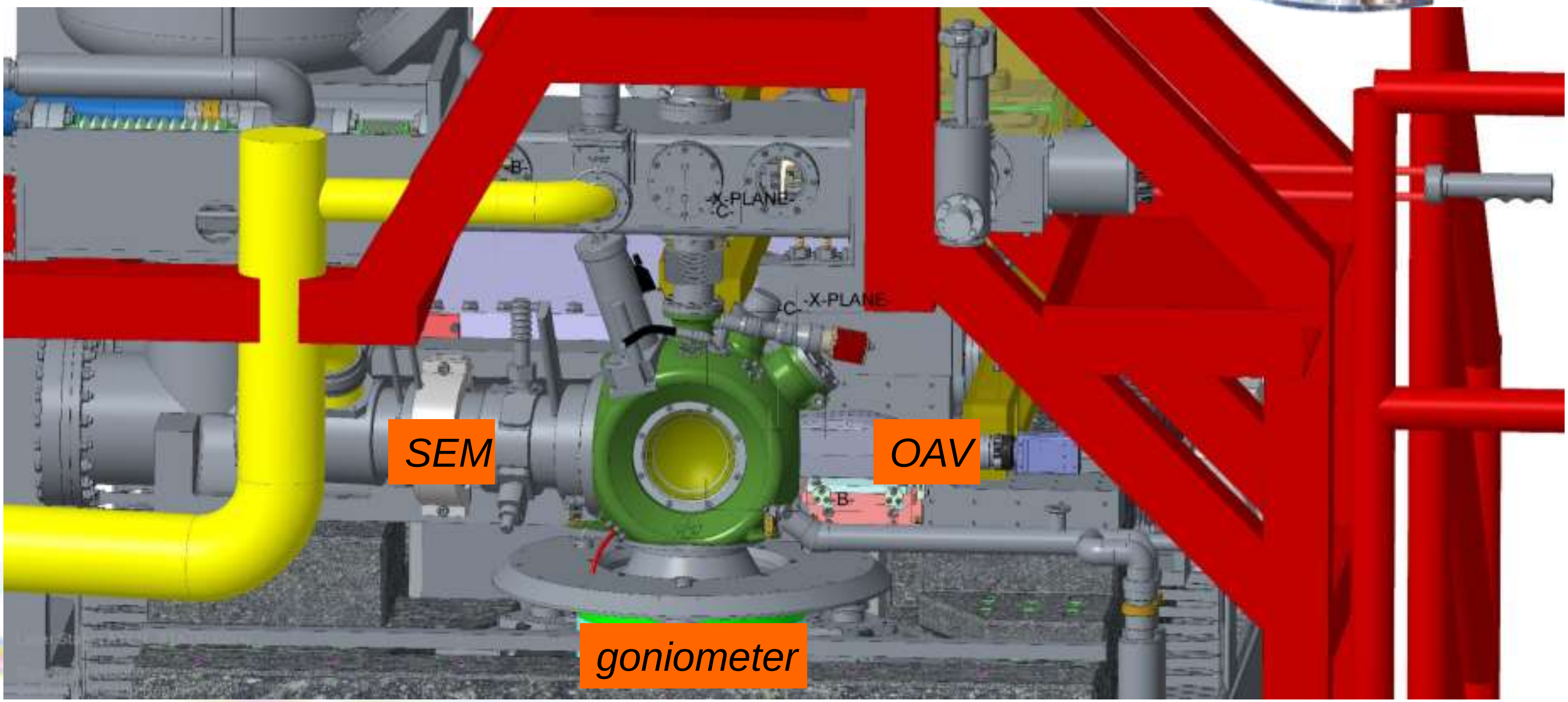
VMXm optical scheme using DDBA



SEM incorporated into evacuated sample chamber

3D printed vacuum chamber

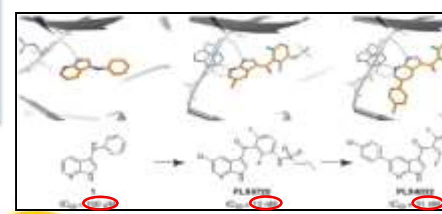


First light on sample 6-3-18; first users in June 2018

Fragment screening on I04-1 - XChem

Conventionally		Now @ Diamond
	Crystal generation	
weeks	Adding compounds to crystals	30 min
1 week	Crystal harvesting and logistics	1 days
3 weeks	Automated data collection	1.6 days
1 month	Finding hits	(days)
	Hit optimization	
900 crystals 3 months		1000 crystals 1 week

Spurlino, Meth Enz, 2011



Murray et al. (2012) Trends in Pharmacological Sciences

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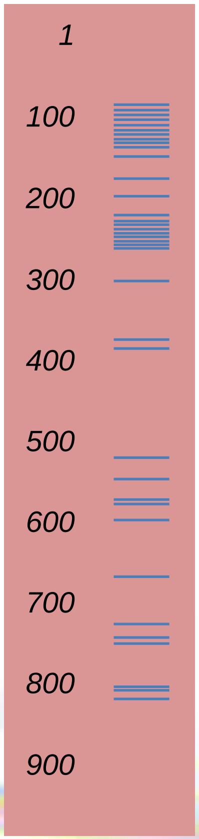
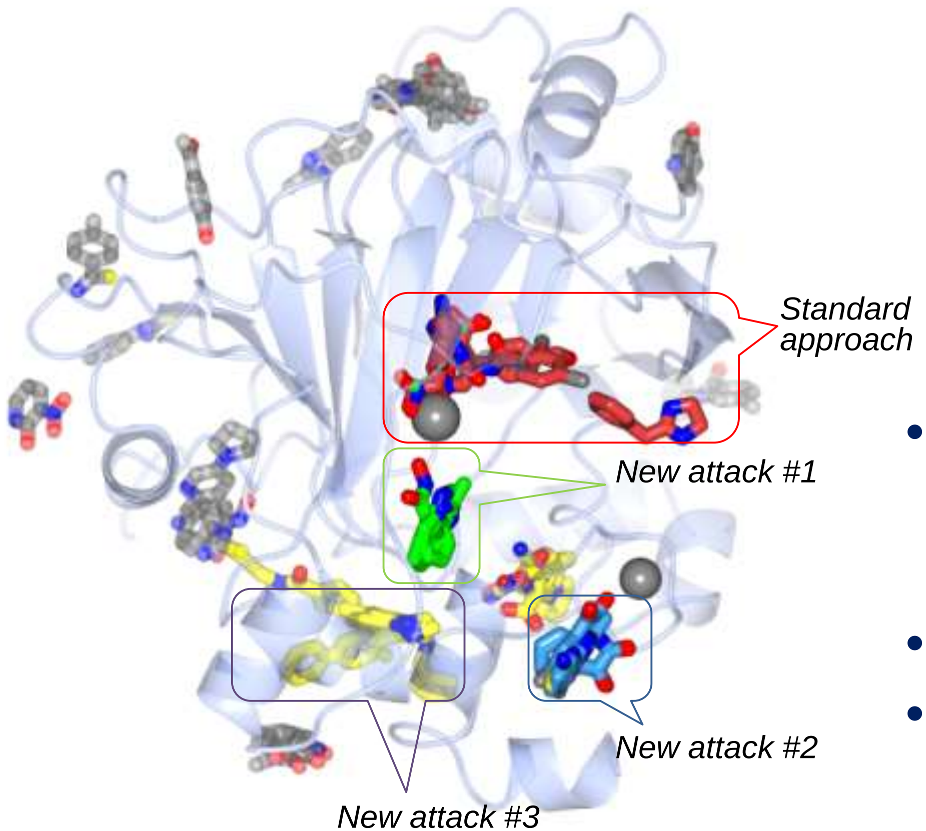
Finding needles in haystacks





- High throughput, semi-automated fragment screening
- ~1000 structures in 48h
- This is driving pipelines for automated analysis,

Frank von Delft
Tobias Krojer
Anthony Bradley
Oakley Cox
Romain Talon

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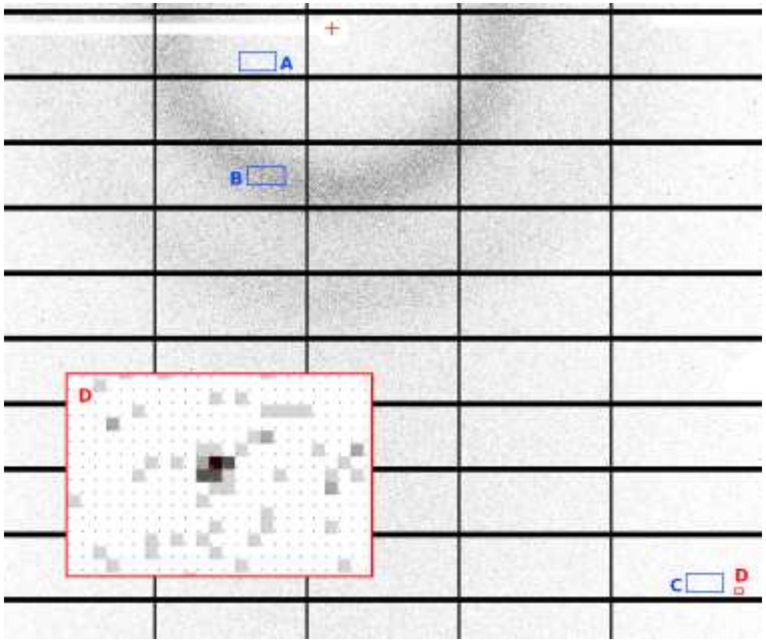
Protein Data Bank depositions

Edgier instrumentation



- I23: first large area detector in a vacuum allows diffraction with softer X-rays to be used because background (air scattering) is greatly reduced, offering access to S edge and opening up natural biomolecules

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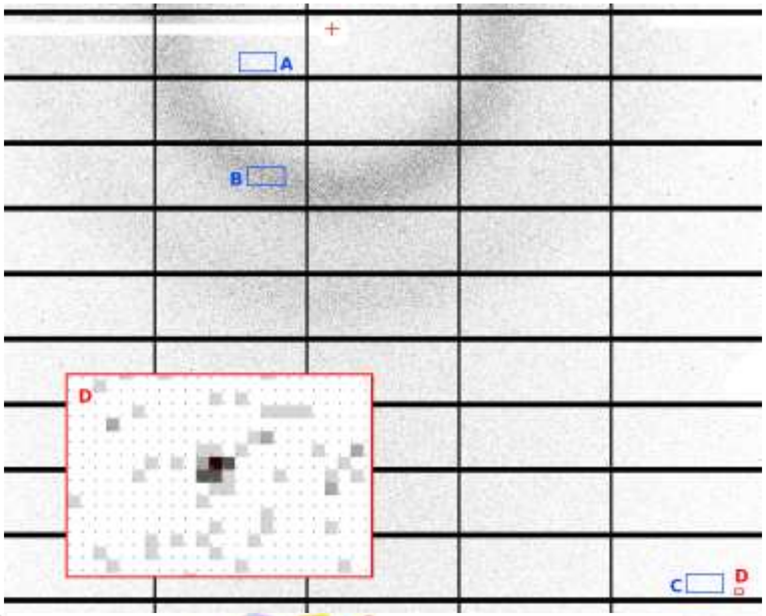
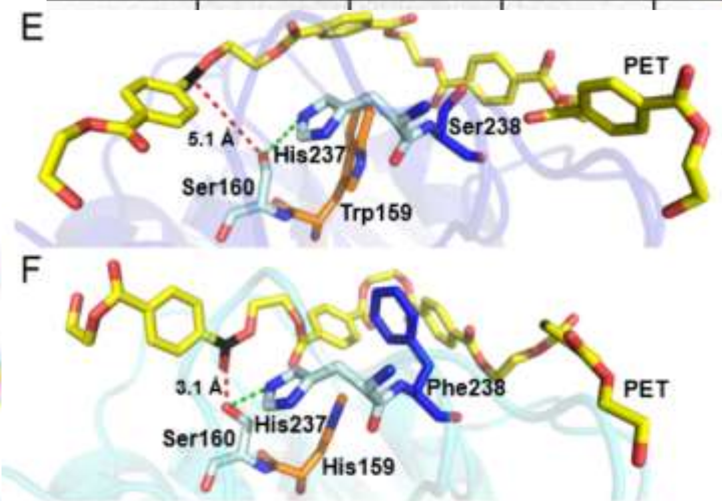
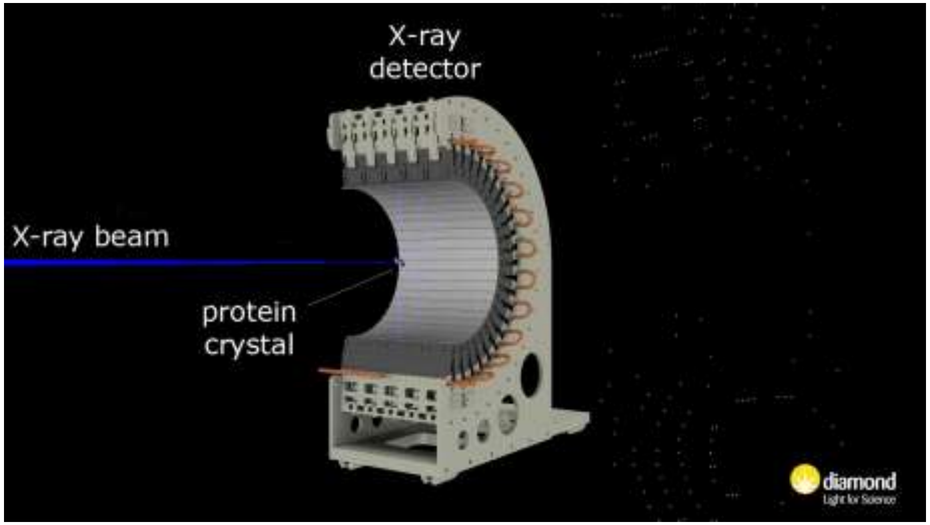
Engineering PET-eating enzymes



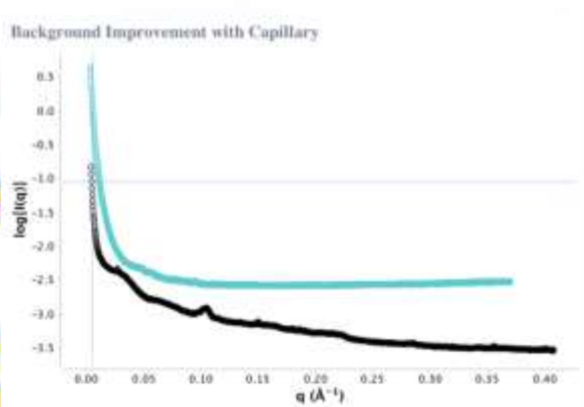




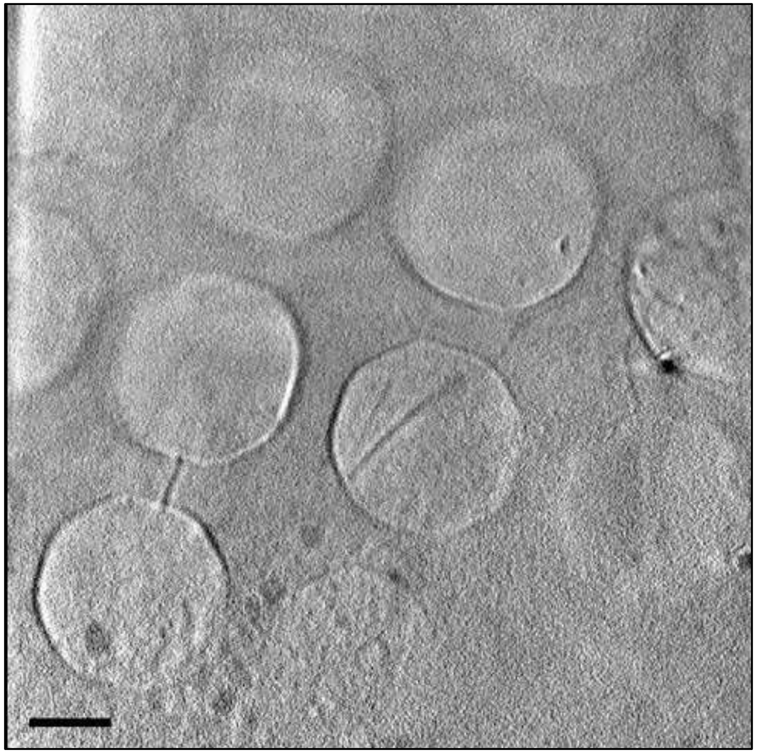
Characterization and engineering of a plastic-degrading aromatic polyesterase, PNAS (2018), *Harry P. Austina,1, Mark D. Allena,1, Bryon S. Donohoeb,1, Nicholas Rorrerc,1, Fiona Kearnsd,1, Rodrigo L. Silveirab,e, Benjamin Pollardd, Graham, Dominickc, Ramona Dumanf, Kamel El Omarif, Vitaliy Mykhaylykf, Armin Wagnerf, William E. Michenerc, Antonella Amoreb, Munir S. Skafe, Michael F. Crowleyb, Alan W. Thornea, Christopher W. Johnsonc, H. Lee Woodcockd*, John E. McGeehana*, and Gregg T. Beckham*

bioSAXS on B21

- Optics upgrade (2017) and background reduction (Eiger 2M Oct 2018)
  - Includes installation DMM (0.8% bandwidth) and toroidal focussing mirror – 20x reduction in high-q sample background
- Integrated multi-angle light scattering into SEC-SAXS
  - In-line purification of particles during SAXS (SEC)
  - Independent assessment particle mass and low-q info (USAS)
  - Develop SIN flow cell with 0.5 mm window to minimise scattering (>100x)
- Bespoke sample cells
  - Compatible with BioSAXS robot, 5 min switching (equilibration) time
  - Lowest possible background (ultrathin windows)
  - Prototyping with 3D printing

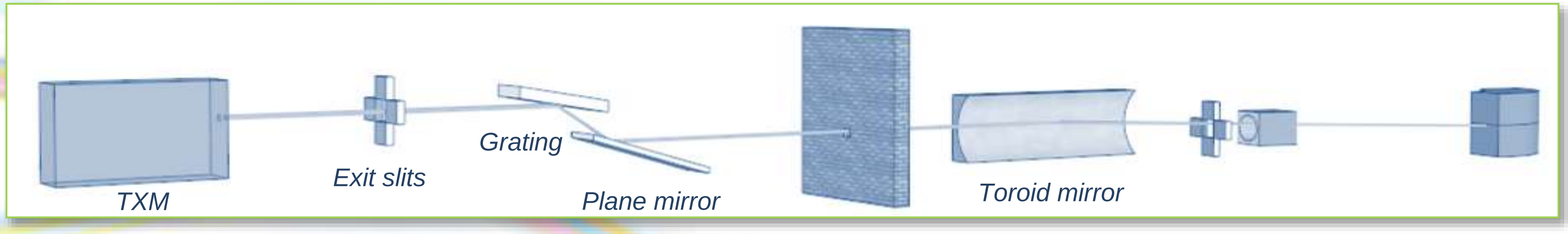


B24 - Full field cryo soft x-ray microscope



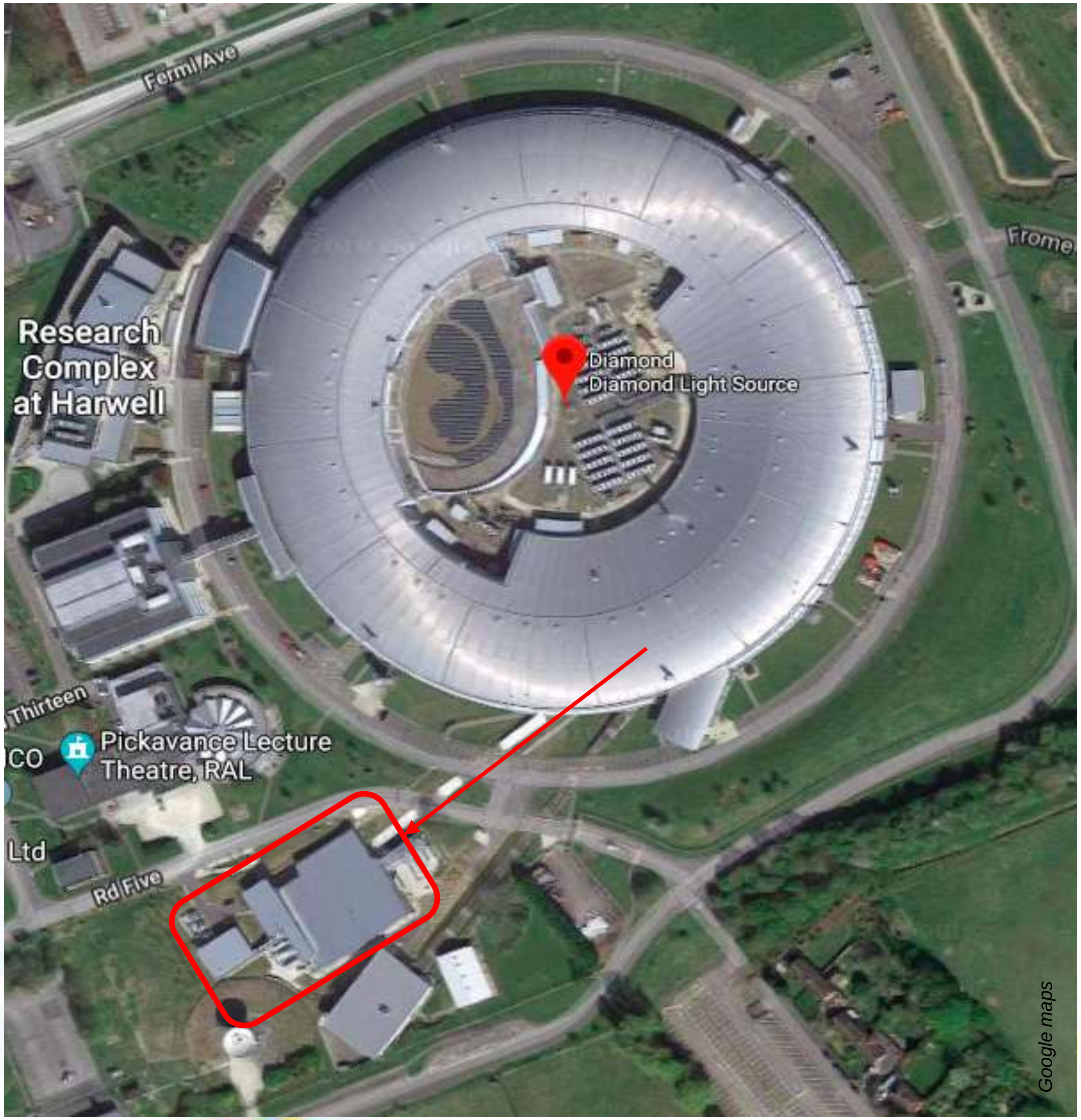
- *Currently operating at 500eV (water window)*
- *Zeiss/Xradia microscope end station (in-vacuum)*

Tomogram of dsRed expressing Toxoplasma gondii parasites in host cells (Ota, Sabil et al (2015), FOV 15 x 15 mm²)



B24 Full-field microscopy; energy range: 0.2-2.6 keV; spot size/resolution 30 nm

EM at Diamond



diamond

EM at Diamond

I14 beamline & Electron Imaging Centre

A national centre for nanoscale imaging for the life and physical sciences

eBIC

electron Bio-Imaging Centre

A collaboration between Birkbeck College, Diamond and Oxford University

wellcome trust | MRC Medical Research Council | BBSRC bioscience for the future

diamond Electrons for Science

I14

Hard X-ray nanoprobe

A nanoscale X-ray beam for advanced imaging applications

Science & Technology Facilities Council | wellcome trust

diamond Light for Science

ePSIC

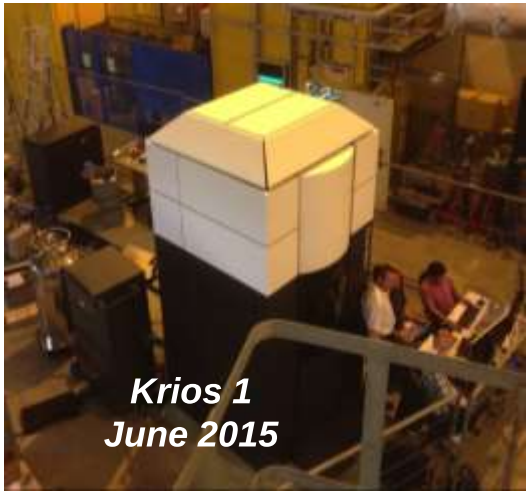
electron Physical Sciences Imaging Centre

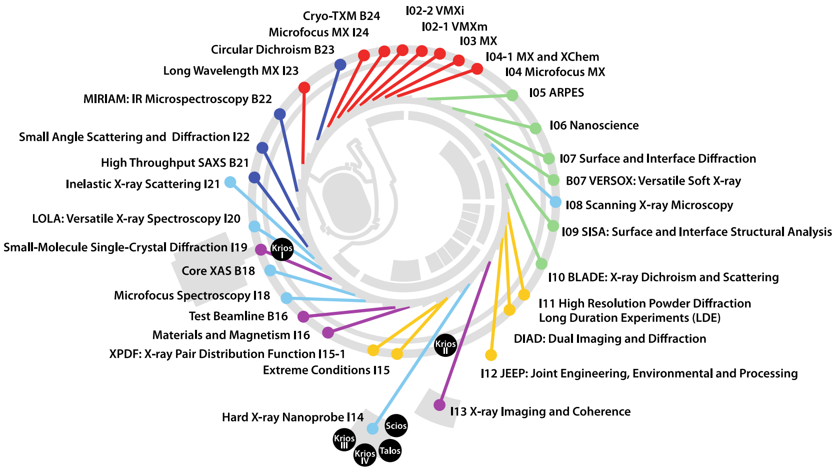
A collaboration between Diamond, Johnson Matthey and Oxford University

JM Johnson Matthey | UNIVERSITY OF OXFORD

diamond Electrons for Science

eBIC: UK National CryoEM centre



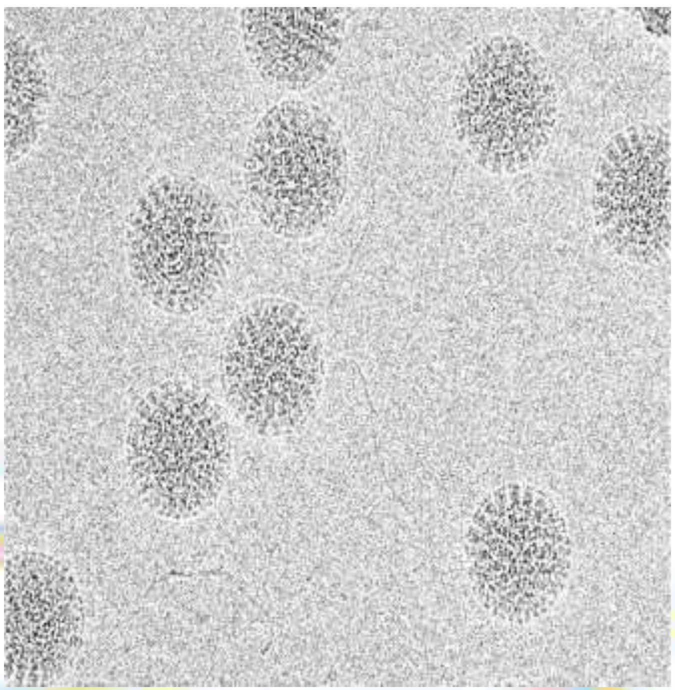


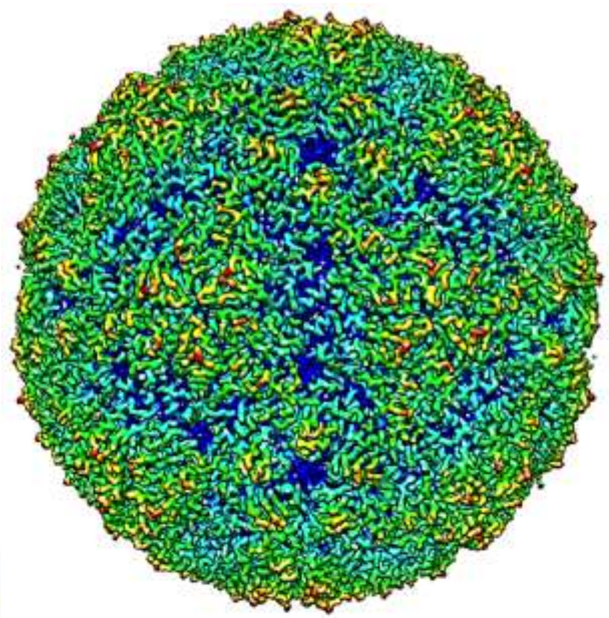
diamond

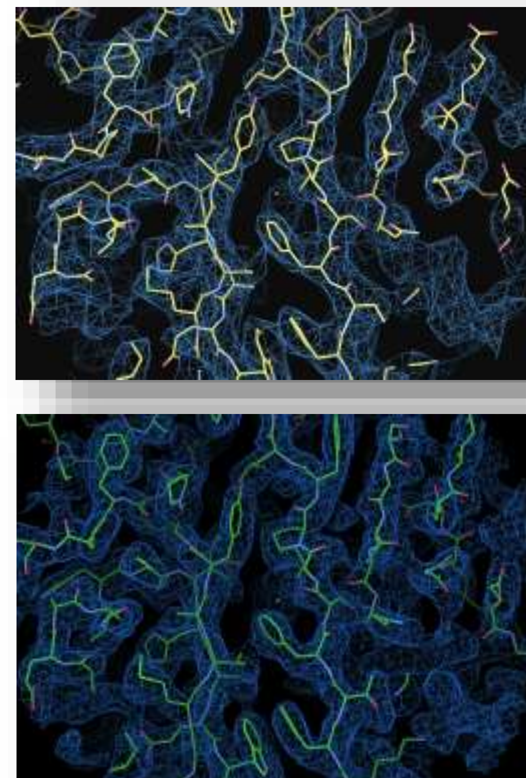
More on the way, with industrial access, technical development and training centre, 12x oversubscribed

Complementarity of Cryo-EM and MX

- New detector technology allows ‘movies’ to be made of large molecule frozen in ice, enabling correction for motion of the objects being image and thus a revolutionary leap in spatial resolution for systems that are very challenging or practically impossible to crystallise
- Does not yet have the resolution or throughput of MX…



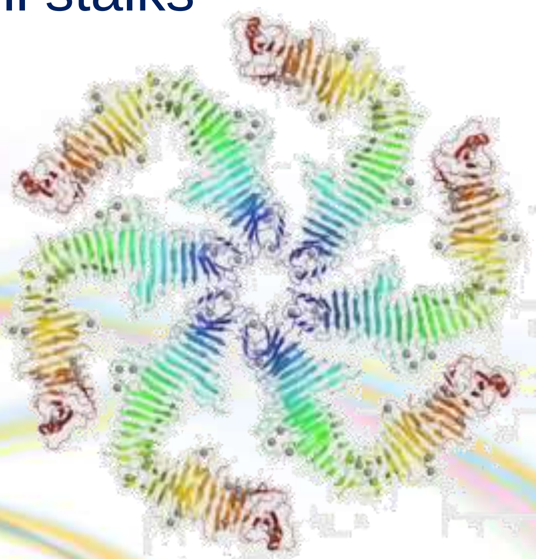




Combining MX and Cryo-EM

Structure of *Caulobacter crescentus* hexagonal surface layer – I04

- 2.3 Å X-ray structure showed hexameric S-layer lattice
  - Solved by Ho SAD
- 7.4Å structure of S-layer by electron cryotomography and sub-tomogram averaging of cell stalks

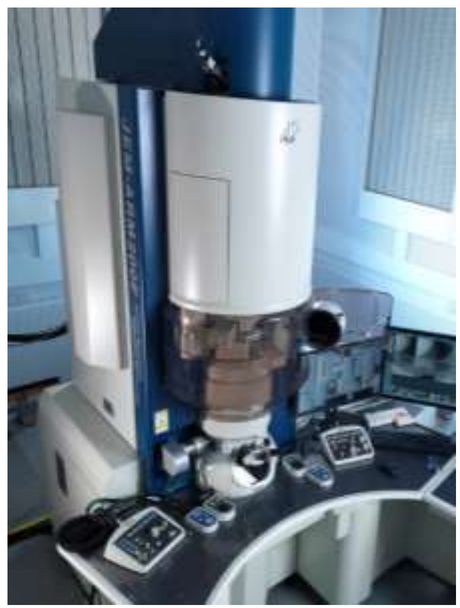


Bharat … Lowe, MRC-LMB, Nature Microbiology ***2*** *1705*

Electron Physical Sciences Imaging Centre

ePSIC
electron Physical Sciences Imaging Centre

- Ultra-high resolution EM centre for the Physical Sciences set up with Oxford University, Johnson Matthey and JEOL, also providing beam-time for peer-reviewed UK-wide access. Opened September 2016
  - *JEOL ARM 300 CF ultra high (< 50 pm) resolution*
  - *JEOL ARM 200 CF for chemical analysis with environmental cells < 100 pm*
  - *Integrated with I14 hard X-ray nanoprobe beamline, transferable sample env…*



Commission call completed 30/09/2017

Total number of User shifts offered during commissioning call	57
Total number of group leaders (PI's)	18
Total number of Universities	10
Total number of proposals with industrial involvement	7

14 Publications from the commissioning call and first full user run, including 4 in Nature group journals.

UNIVERSITY OF OXFORD

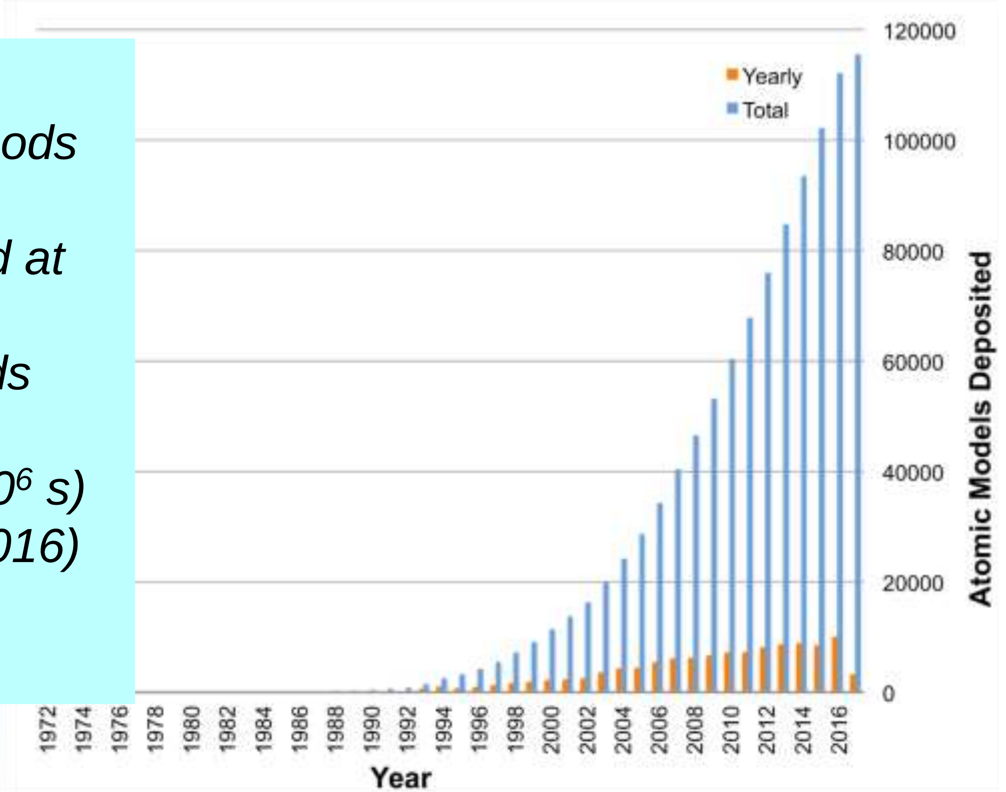
JM Johnson Matthey
Inspiring science, enhancing life

The XFEL Hub at Diamond

- X-Ray Free Electron Lasers (FELs) offer prospect of measuring structure much faster (1000x) than synchrotrons – and make movies of chemical reactions
- WT, MRC and BBSRC funded the XFEL Hub at Diamond to develop methods in sample delivery and data analysis – led by Allen Orville – and applied to FELs around the world (heavily involved in EU-XFEL commissioning)

PDB to April 2017

- ***115,487*** *atomic models with x-ray methods*
  - ***95,834*** *from* ***synchrotron*** *sources*
    - *typically < 10 big crystals, held at 100 K*
  - ***189*** *with "****time-resolved****" key words*
    - *Various incubation times*
    - *0.1 ps to 15 weeks (9.072 x 10^6 s)*
  - ***148*** *from* ***XFEL*** *sources (2011 – 2016)*
    - *typically 10,000s μ-crystals*
    - *~ 50% time-resolved (fs – s)*



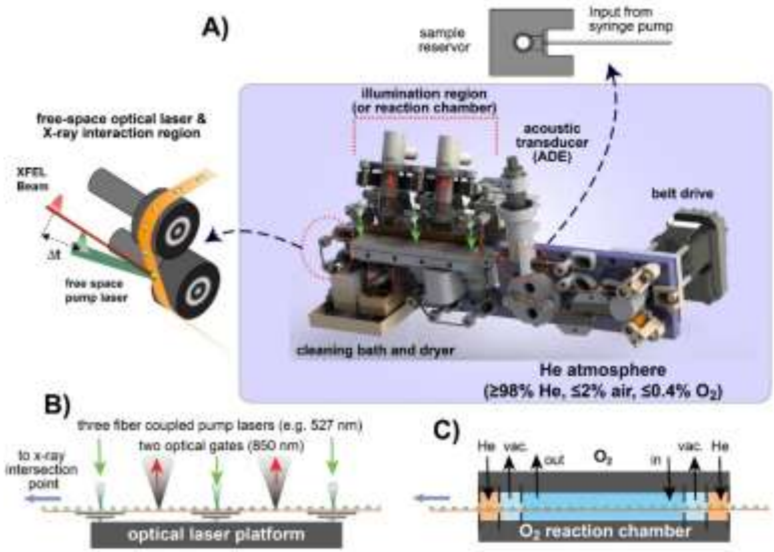
≥ 50% of all life-science proposals at SACLA (2017A) and LCLS (run 15) related to time-resolved studies (pump-probe, mix-inject, temp-jump, EF-X)

The XFEL Hub at Diamond

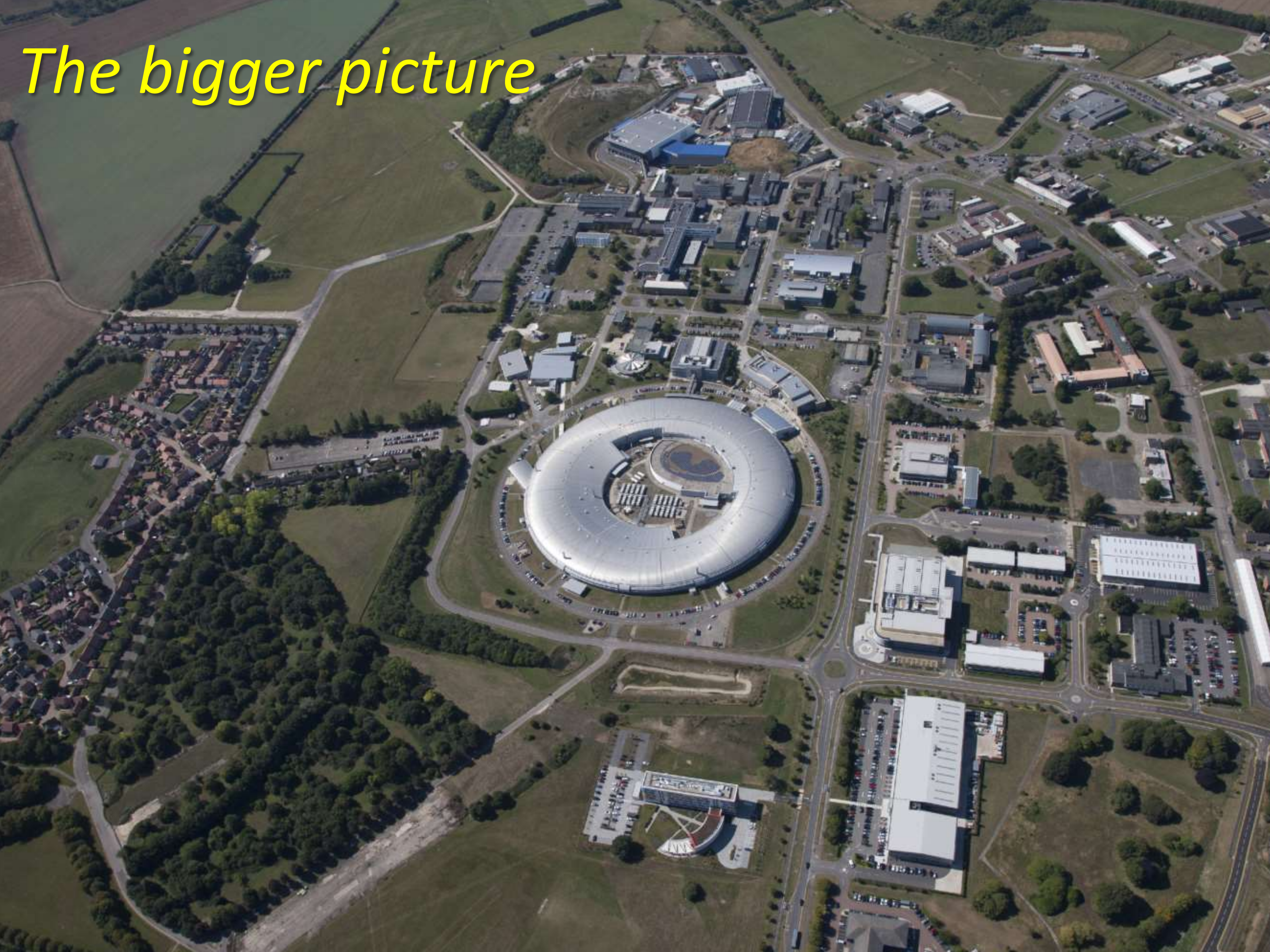
allen.orville@diamond.ac.uk

- Will facilitate:
  - (Time-resolved) serial structural biology experiments via sample preparation, deliver data collection, and processing
  - Transfer of methods between XFEL, synchrotron, and/or cryo-EM sources
  - Access to, and data collection from complementary facilities (DLS, CLF, eBIC)
- Support for a new BAG – Dynamic Structural Biology at Diamond and XFELs
  - 18 members from UK, EU and USA
  - µ-crystals, serial MX strategies, room T & P; I04, I24, & VMXi.
  - Fixed targets, LCP / viscous injector, on-demand acoustic injector(s) at VMXi

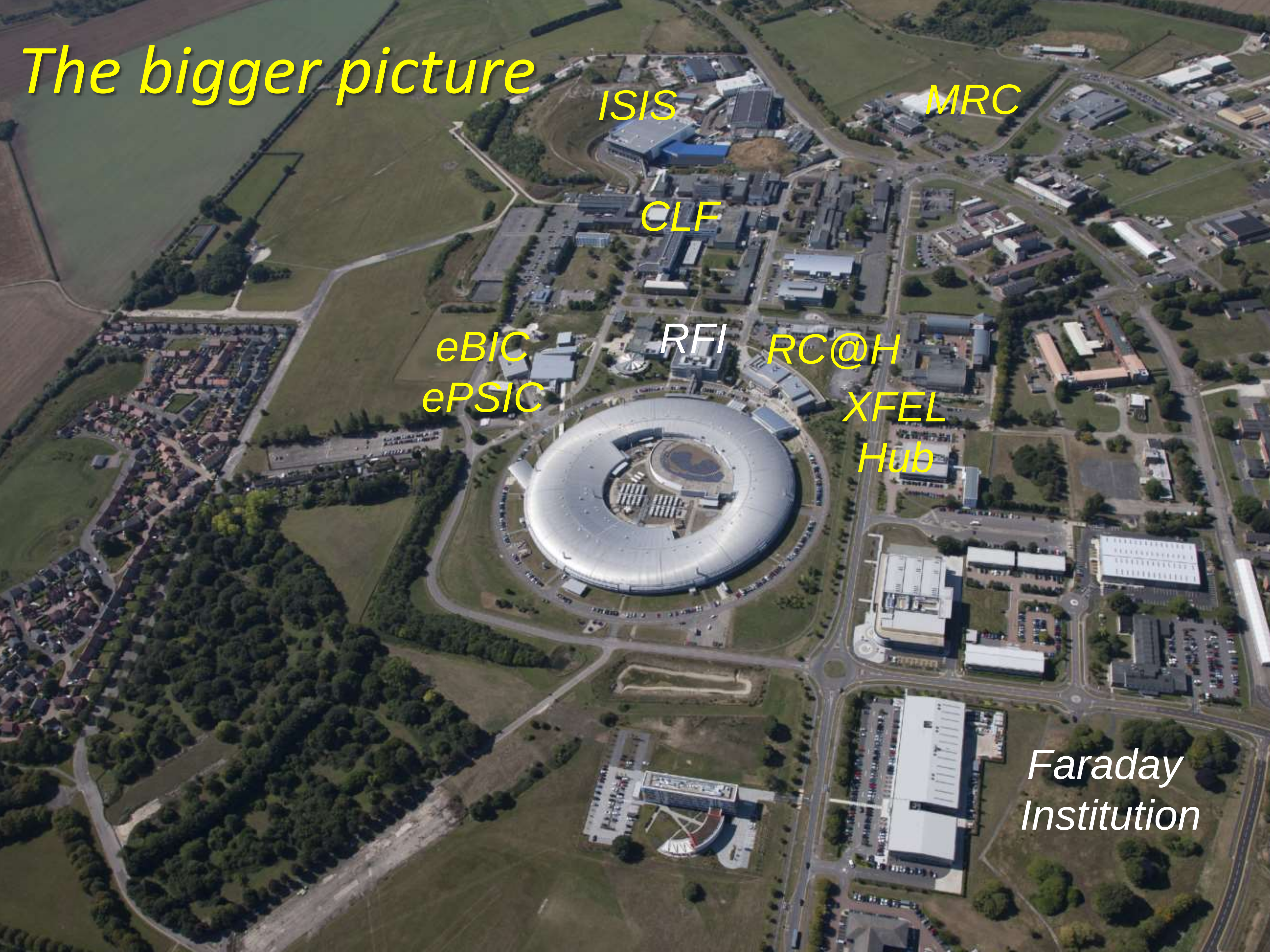
PolyPico on-demand droplet injector at VMXi, sample crosses beam ~100 µs, Eiger at 500 Hz (2 ms) 30 pL drop in calibration view



The bigger picture



The bigger picture

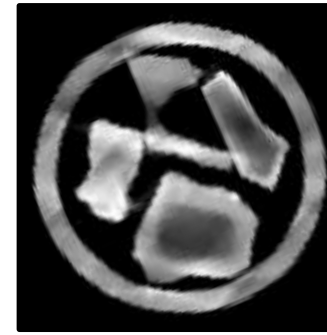


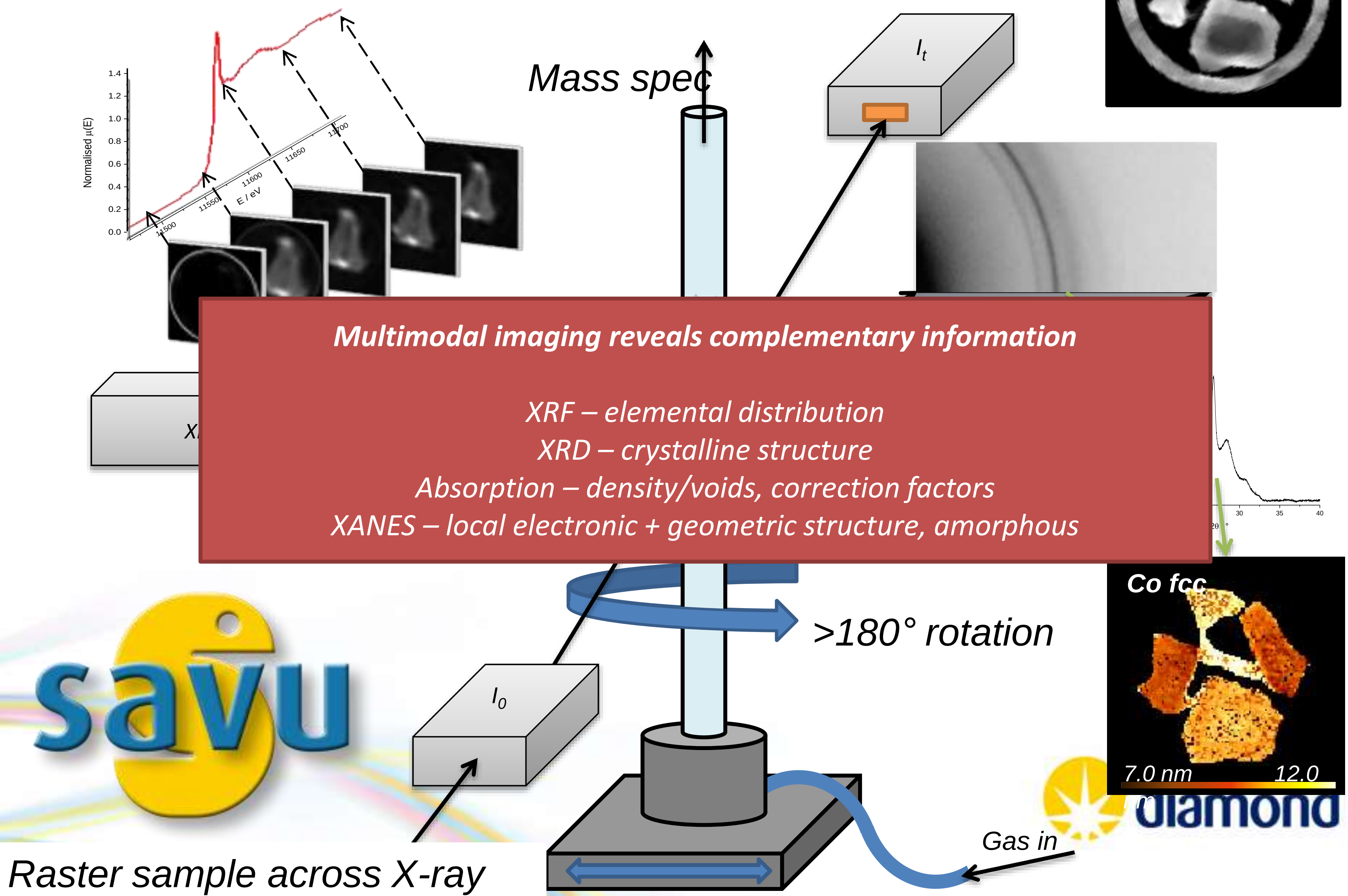
The Research Complex at Harwell

- Inspired by the PSB/CIBB
- RCUK-Diamond venture to exploit and develop Diamond, ISIS and CLF - 5000 m^2 to host research groups with funded projects from industry and univs.
  - Imaging for materials, biology and nanotechnology (Manchester)
  - Structural biology: protein crystallography and cell imaging (IC)
  - Materials: extreme conditions, hydrogen storage, engineering (Edinburgh, Oxford)
  - Ultra fast laser technology applied to chemistry and biology (Notts)
  - The UK (EPSRC) catalysis hub (UCL,Bath, Cardiff, QB)

- Over 150 visiting or resident scientists in any year and 14 core staff
- Over 220 publications *per annum*
- Citation levels greater than facility-only

In situ/operando multimodal

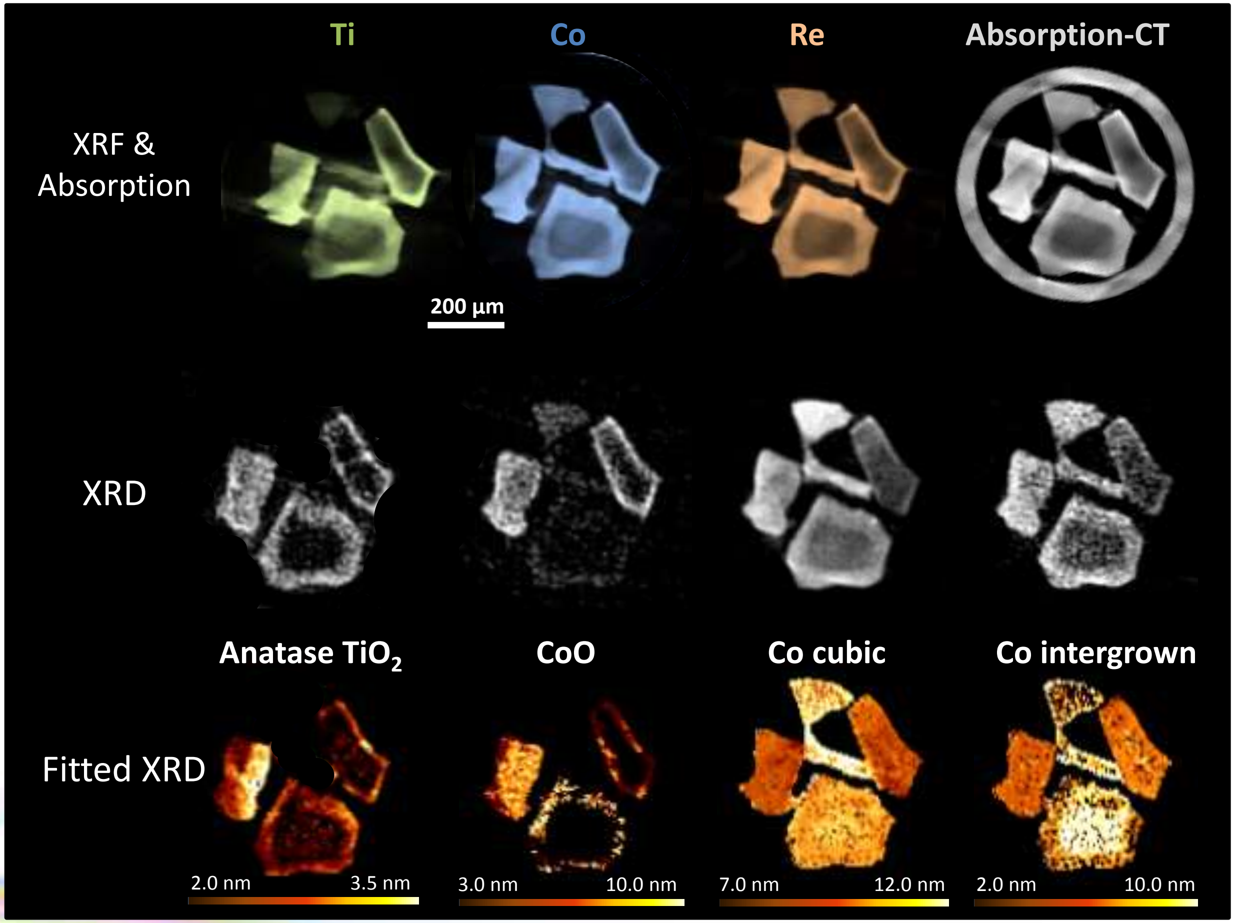




Multimodal imaging reveals complementary information

XRF – elemental distribution
XRD – crystalline structure
Absorption – density/voids, correction factors
XANES – local electronic + geometric structure, amorphous

In situ/operando multimodal



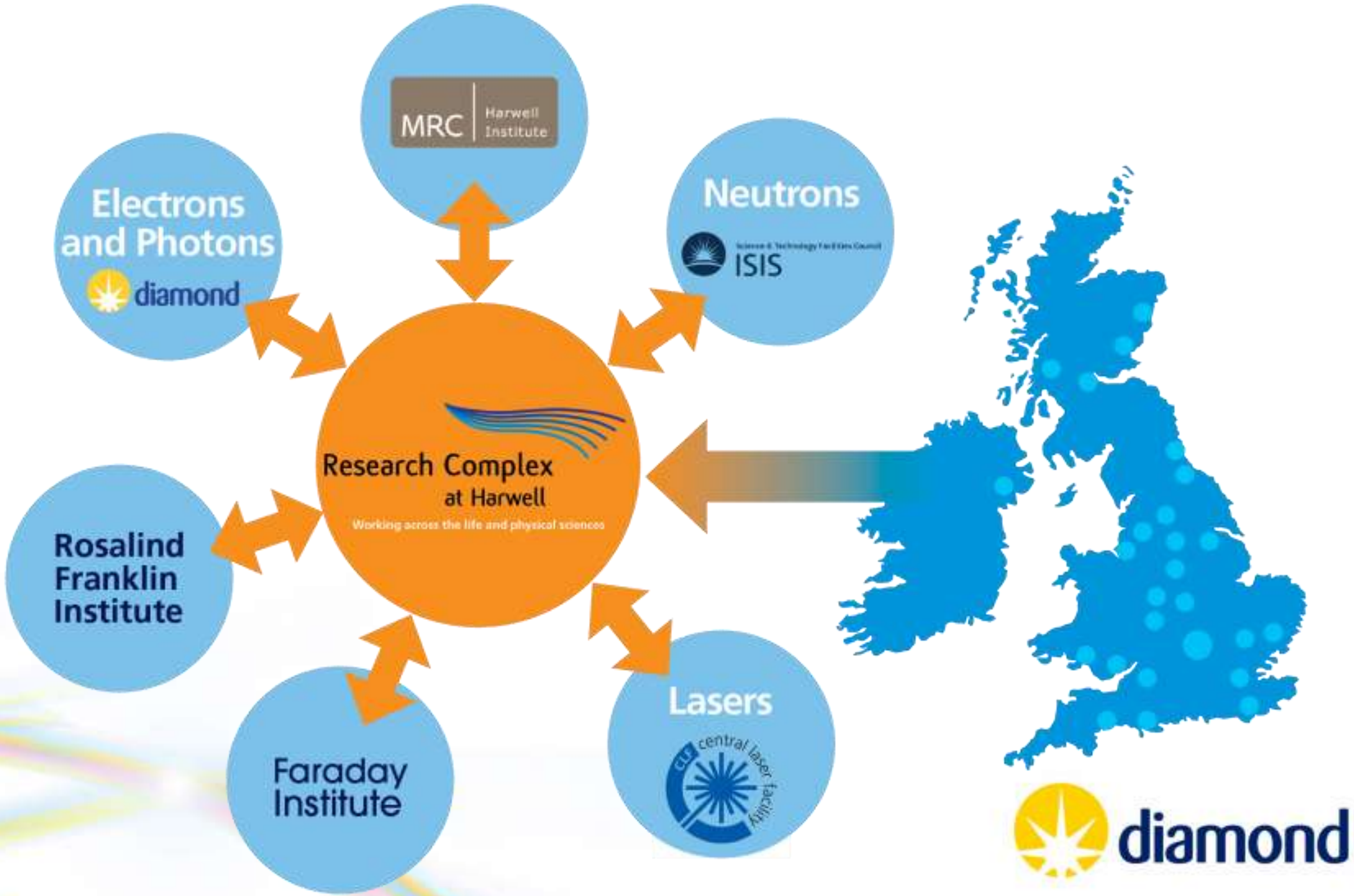
Revealing structure and elemental distribution of an important catalyst simultaneously on B18

Fischer-Tropsch synthesis (production of hydrocarbons from 'syngas' - $CO + H_2$) at 2 bar on TiO_2/CoO catalyst

Stephen W. T. Price,[1]* David J. Martin,[2,3] Aaron D. Parsons,[1] Wojciech A. Sławiński,[4] Antonios Vamvakeros,[2,3] Stephen J. Keylock,[1] Andrew M. Beale,[2,3,5]* J. Frederick W. Mosselmans[1,6]

Price *et al.*, *Sci. Adv.* 2017; **3** : e1602838   17 March 2017

The Research Complex at Harwell



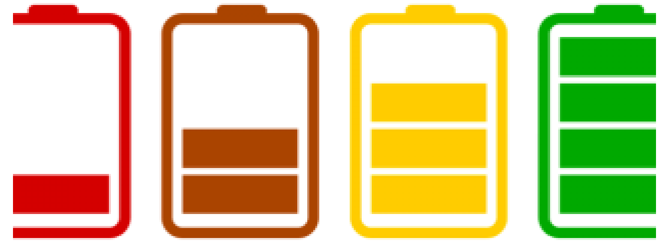
Rosalind Franklin Institute

- £100M initiative to develop new physical methods for biomedical science and engineering
- Hub at Harwell with spokes to10 partner universities in 5 areas
  - Structural Biology (focused on next-general X-ray techniques)
  - Biological mass spectrometry
  - Next generation chemistry for medicine
  - Imaging with Sound and Light
  - Correlated imaging (X-rays, lasers and EM including unique ps EM)



Oxford, B'ham,Cambridge, Edinburgh, Leeds, London (Imperial, Kings, UCL), Manchester, S'ton

Business Secretary to establish UK as world leader in battery technology as part of modern Industrial Strategy



EPSRC
Engineering and Physical Sciences Research Council

Calls for Batteries Research Institute and research projects open

Issue date 24 July 2017

Research into batteries

Separate to these competitions, the Faraday Challenge will support activities across research, innovation and scale up. This includes a call by the Engineering and Physical Sciences Research Council (EPSRC) to establish a virtual research institute, plus associated research into battery development.

ISCF Faraday Challenge - Batteries for Britain
ISCF Faraday Challenge - Call for Establishment of a Batteries Research Institute

Innovate UK

Funding competition

Faraday Challenge: Innovation - research and development

UK businesses can apply for a share of up to £30 million to work on innovation projects to design, develop and manufacture batteries for the electrification of vehicles.

Competition opens: Tuesday 25 July 2017
Competition closes: Thursday 14 September 2017 12:00pm

Battery innovation for the electrification of vehicles

- the Department for Business, Energy and Industrial Strategy (BEIS) and Innovate UK have up to £30 million available for collaborative research and development projects for new battery technologies, and up to a further £10 million for feasibility studies
- the competitions open on 25 July 2017, and the deadline for applications is at midday on 14 September 2017
- we expect research and development projects to range in size from £1 million to £15 million and last up to 3 years
- we expect feasibility studies to range in size from £150,000 to £1 million and last between 3 and 12 months
- businesses could attract up to 70% of their project costs

ADVANCED PROPULSION CENTRE UK

Funding competition

Faraday Challenge: Scale up - National Battery Manufacturing Development Facility

UK businesses and research organisations can apply for funding. This will establish a National Battery Manufacturing Development Facility as part of the Faraday Challenge Industrial Strategy Challenge Fund.

Competition opens: Tuesday 25 July 2017
Registration closes: Thursday 7 September 2017 12:00pm

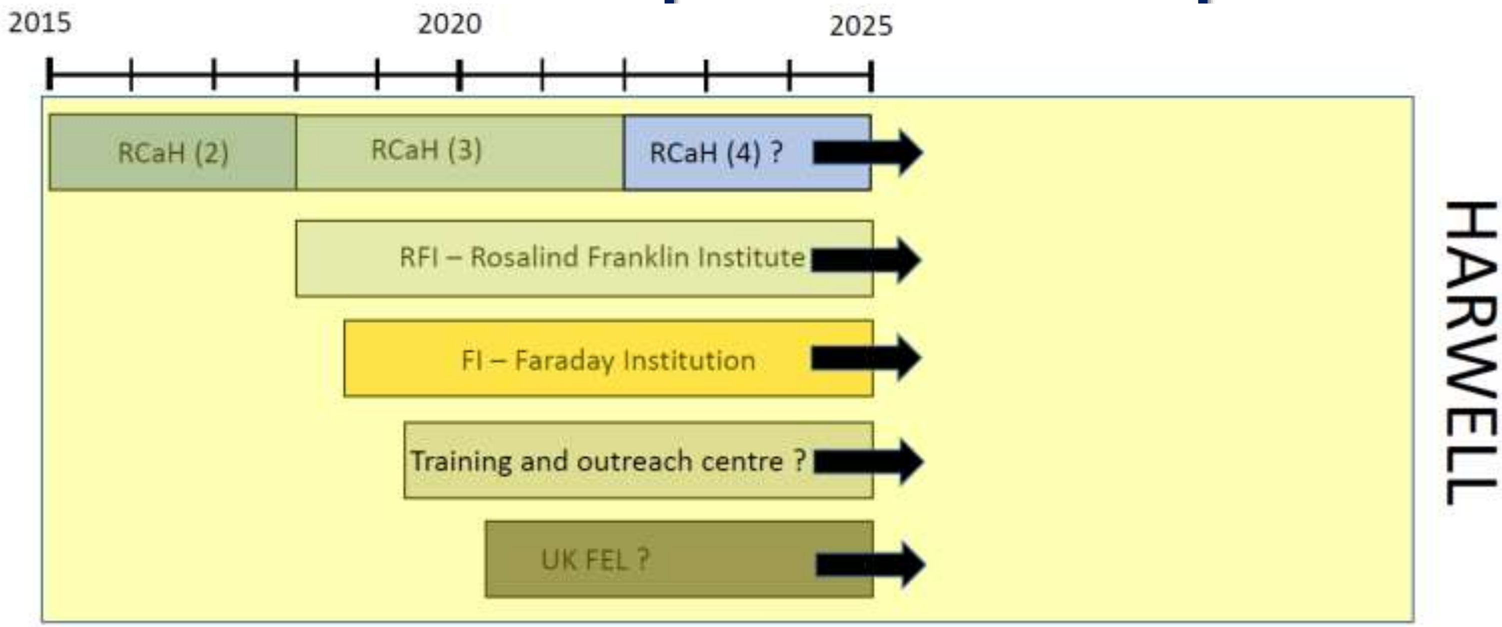
National battery manufacturing development facility

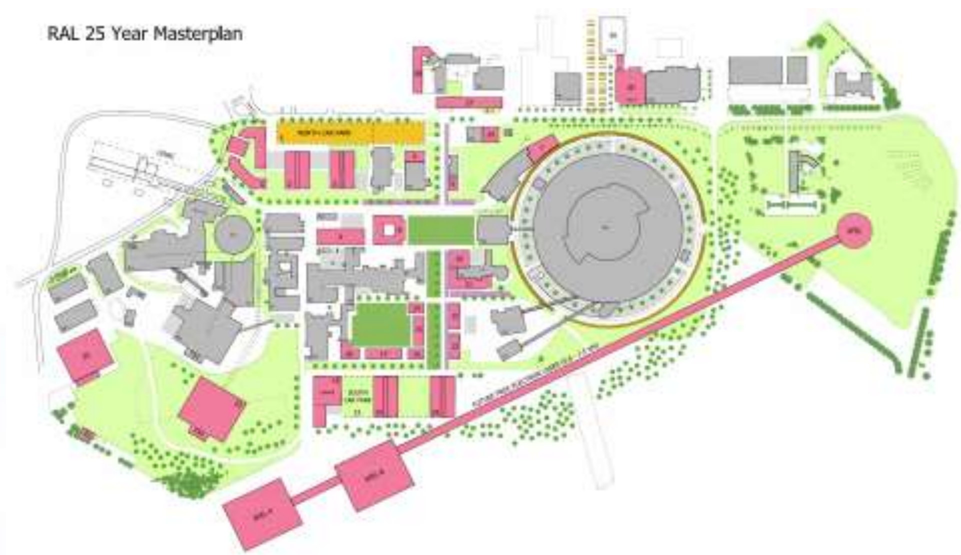
- the APC will fund one project for a new state-of-the-art battery manufacturing development facility
- projects are anticipated to be in excess of £40 million
- the competition opens on 25 July, and the registration deadline is midday on 13 September 2017
- work must be carried out in the UK
- project build is expected to last a maximum of 24 months, with the construction complete and the facility operational by early 2020
- you may be eligible for up to 100% of your project costs if you or the delivery organisation is a non-profit research organisation

Faraday Institution Headquarters to be located on the Harwell Research and Innovation Campus 04 Oct 2017

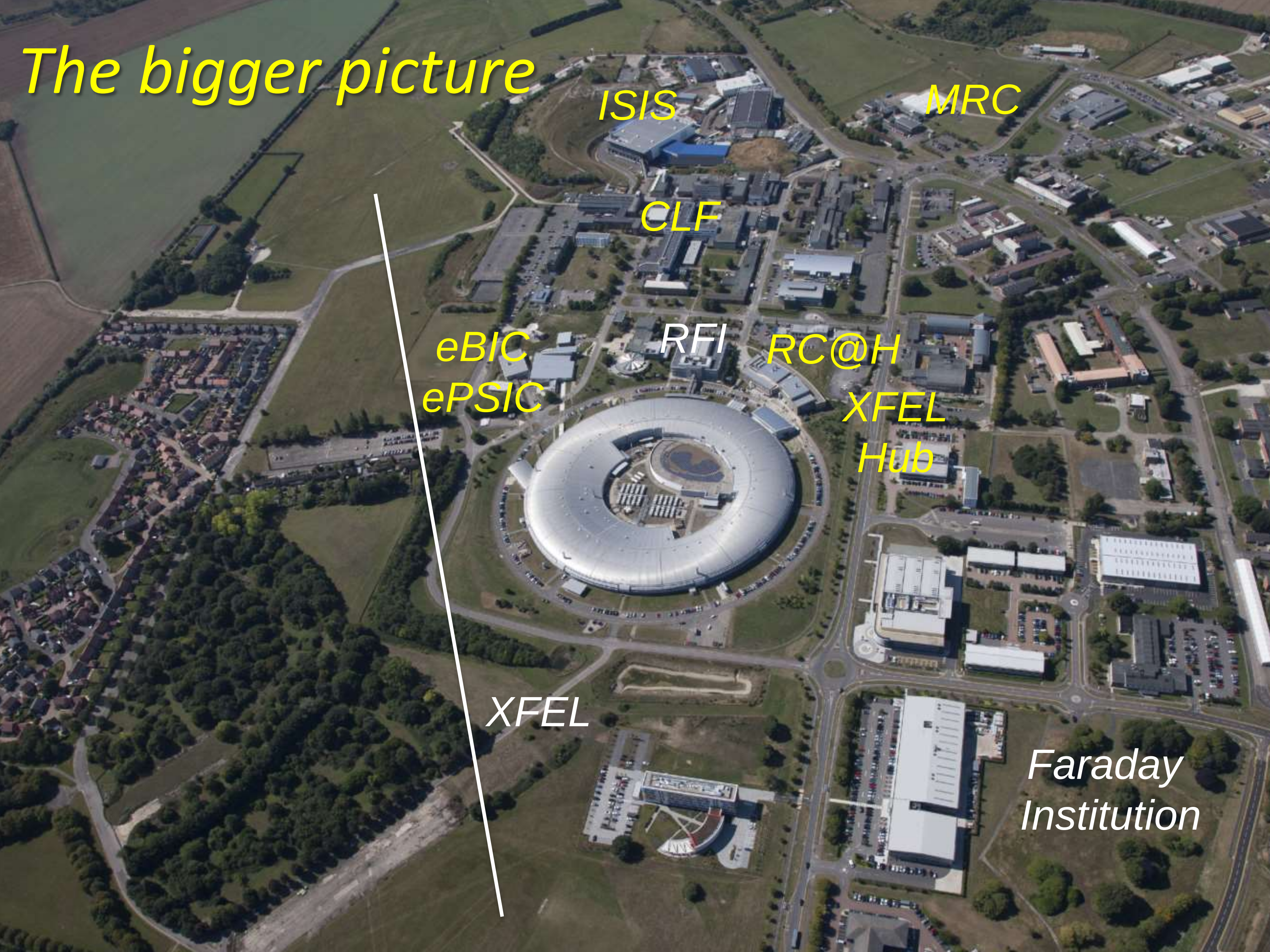
A major new initiative for energy storage research, the Faraday Institution (FI), has been announced by the Department for Business, Energy and Industrial Strategy.

Campus Development

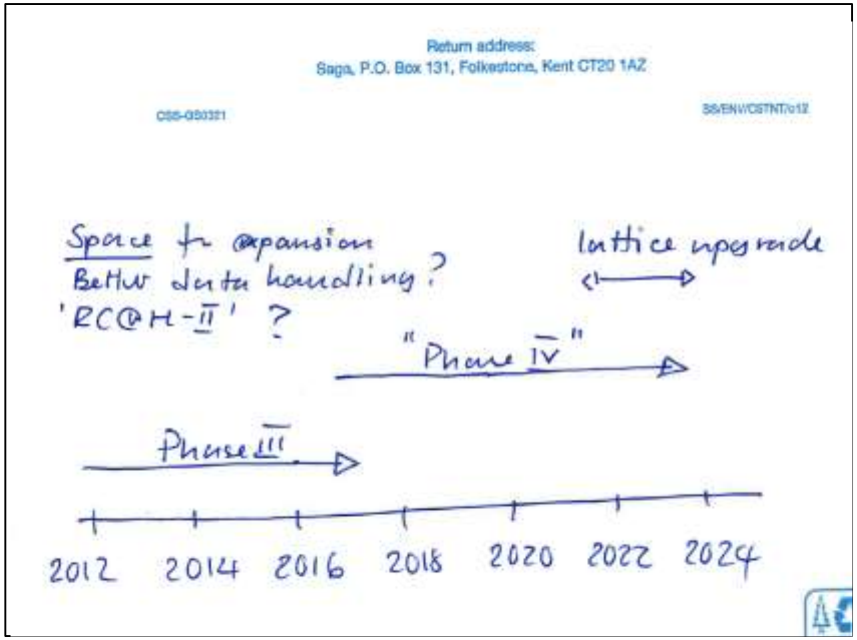




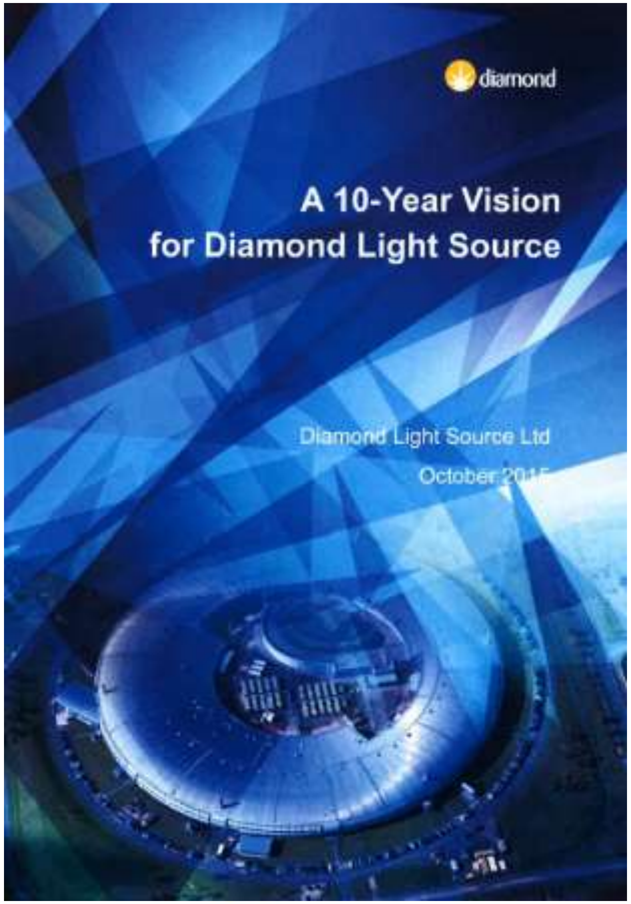
The bigger picture



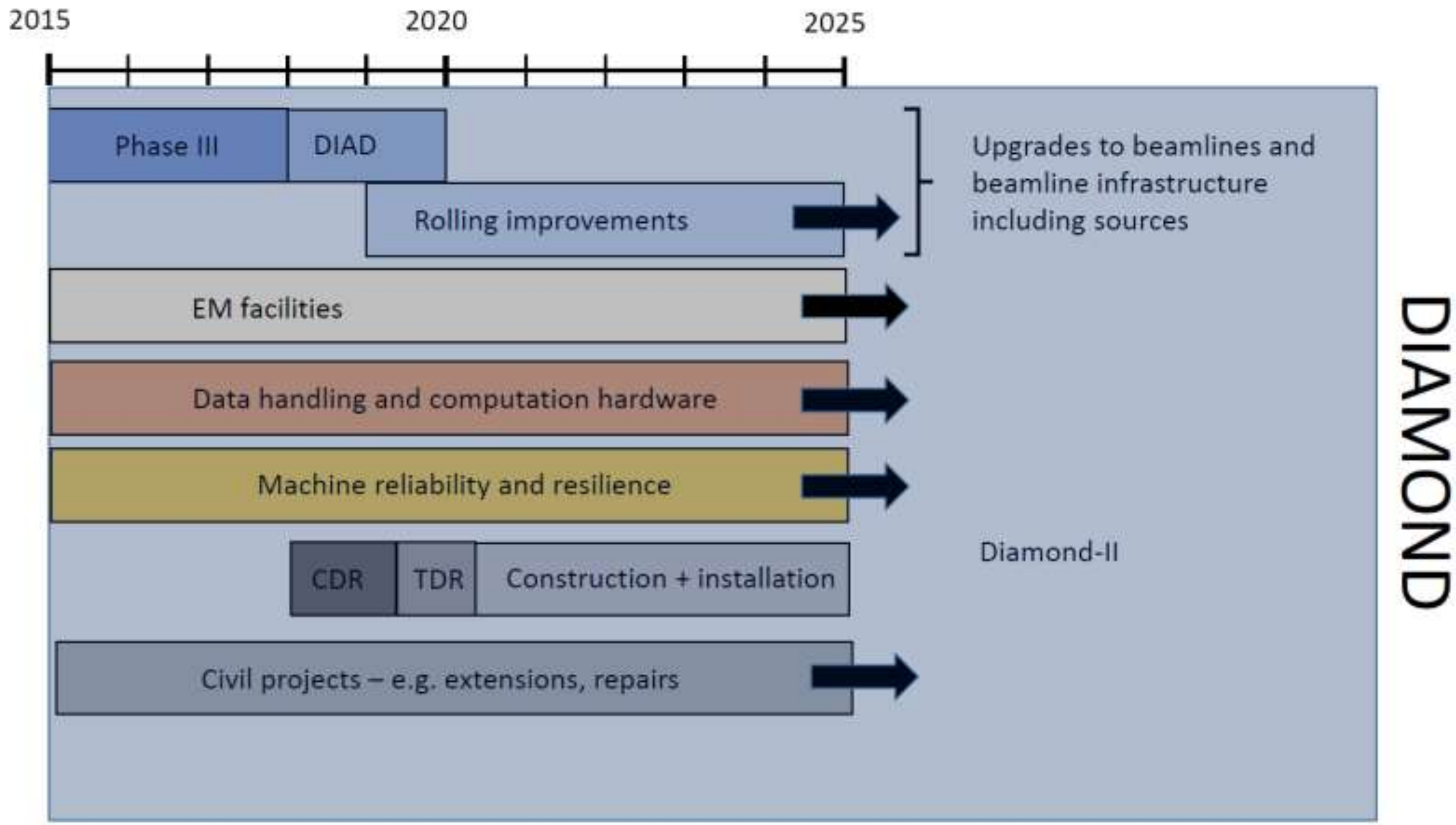
What next ?



http://www.diamond.ac.uk/Home/Corporate-Literature/newsletter/Spring2016/News/10-year-vision.html



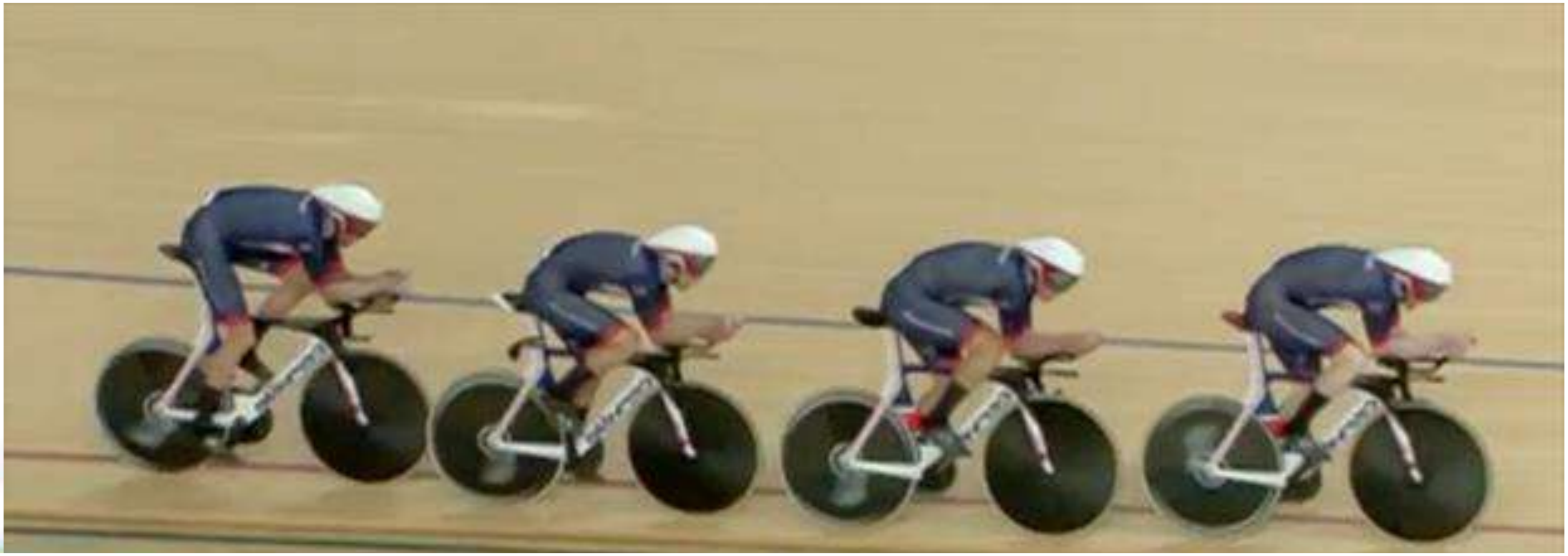
What next ?



Major uplift in capital based on ESRF model to fund rolling upgrades to beamlines

Upgrades

- Diamond Vision presents scientific opportunities provided through upgraded technology from source to data analysis



Upgrades

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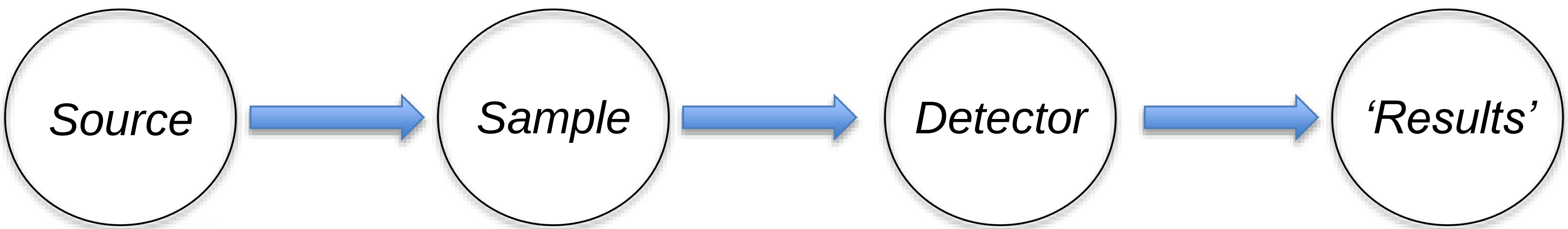

Upgrades

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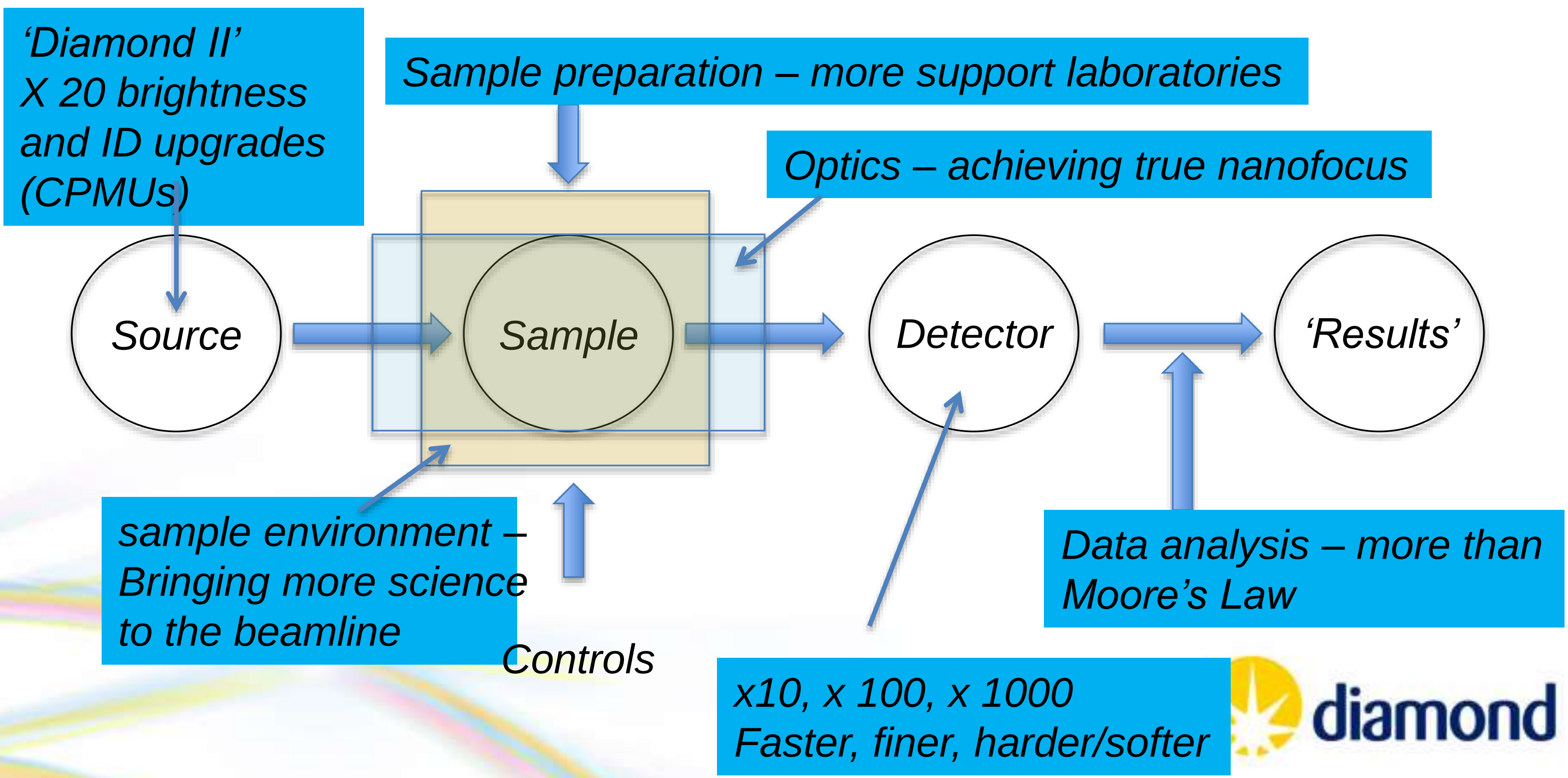


diamond

Physical Sciences

Number		SAC Grade	DISCO Grade	Start	Comments
	PHYSICAL SCIENCES				
1	XPDF-ARC Detector. 15-1	2	1.8	FY18/19	
5	Soft X-ray ARPES + momentum microscope	1	3.2	FY18/19	
10	I11 new diffractometer and high energy detection	2	2.2	FY18/19	
8	I21 RIXS updates	1	3.3	FY17/18	(detector only in FY17/18)
9	High throughput XPS/NEXAFS for B07	2	2.6	FY19/20	
3	State of art spot size, electron spectrometer HR ARPES	1	3.9	FY18/19	
13	Low temperature aberration corrected XPEEM	2	2.9	FY18/19 or 19/20	
11	Thermomechanical test rig for tomography and diffraction	3	2.0	FY18/19	
6	I19 detector upgrade	3	2.8		
4	Sample environment I07	4	3.2		Ongoing programme of smaller upgrades, once refined and reviewed by UWG
12	PILATUS3 2M for XRD on I15	4	3.5		
2	FIB for material science	5	2.7		
7	Thin film sample preparation facilities	5	2.9		
14	Super conducting undulator for high energy imaging	5	2.9		

Go ahead in next 2 years

to be reconsidered alongside new projects

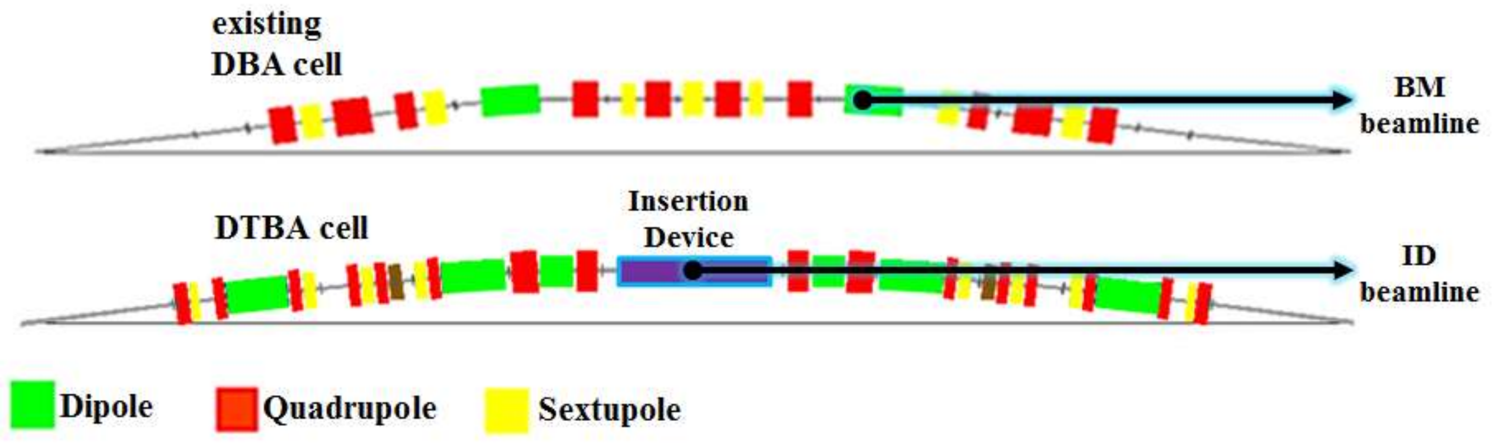
Life Sciences

Number		SAC Grade	DISCO Grade	Start	Comments
15	Optimised handling of cryosamples (including Smart pucks)	1	1.4	FY18/19	Activate ASAP when smart puck technology mature
18	VMXm CdTe Eiger	2	1.6	FY19/20	Still technical issues to be resolved
16	I23 end station upgrades (Day 3 goniometer + new vacuum transfer/sample changer)	1	3.2	FY18/19	Dependent on engineering resource, will be prioritised
17	I24 new detector	3	1.3	TBD	Accelerate if possible, Si sensor
24	Extending XChem Fragment screening via ID upgrade	4	2.3	TBD	Dependent on ID schedule. Timing at risk
19	Development of a system to locate protein crystals in-situ	4	3.0	hold	On hold. Explore through collaboration.
20	Automated Crystal Harvesting	4	3.8	hold	On hold. Explore proof of principle through collaboration
21	TEM upgrade of VMXm end-station	5	2.8	hold	On hold, pending possible collaboration.
22	CPMU/SCU plan	-	-	ongoing	Plan agreed, currently at risk
23	Computing – Experiment data storage (HPFS) and Central	-	-	FY18/19	Tender process will be initiated

Ready to start next 2 FYs

Diamond-II

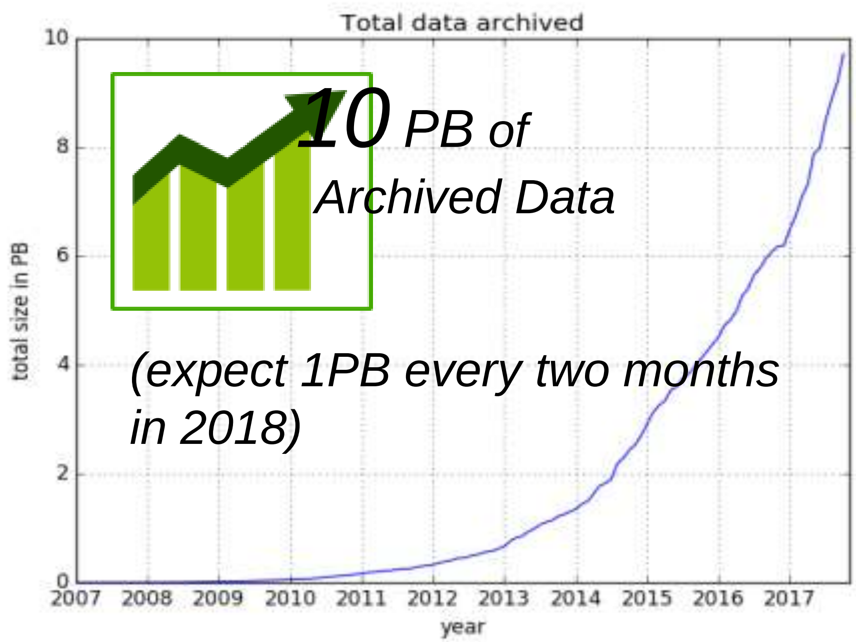
- Develop CDR, including science case, by spring 2019, for machine upgrade in period 2024-2025. Initial discussion with SAC in May 2018
- MBA designs being considered, most likely 6BA (DTBA), a possible increase in energy towards 3.5 GeV, emittance > 120 pm
- Increase *capability* with at least 10x increase in brightness
- Increase *capacity* with introduction of new, short straight section with each MBA unit – retain any BM beamlines and offer additional IDs for new beamlines



ond

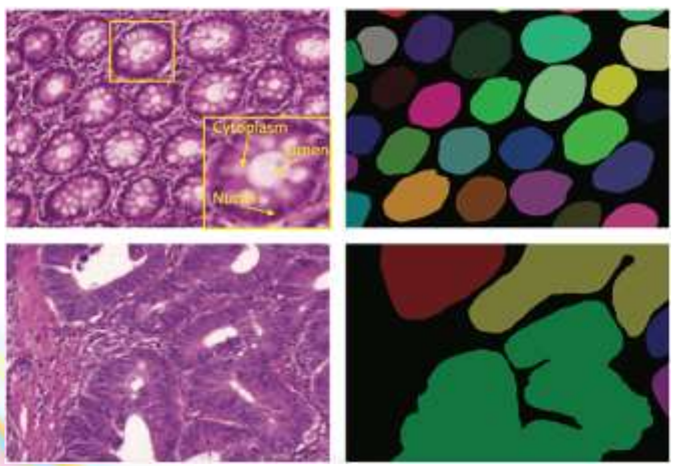
‘Big’ Data and computation

- New data centre to accommodate new servers for prompt data storage and analysis as new detectors and automation come on stream
- Size of data sets at both processing and analysis stages unsustainable – need to look for some form of ‘Cloud’ solution
- And that’s only part of the problem…



‘Big’ *and* Complex Data

- Increasingly complex, multimodal analysis, starting to involve AI and Machine/Deep Learning methods – e.g. tomography, ptychography
- High throughput, real-time results, increasingly remote
- A global challenge that requires a collective, coherent global response in partnership with other facilities, STFC universities, institutes (ATI) and industry – teams of *dozens* of people



Sustainability

http://www.esfri.eu/sites/default/files/u4/NGL_CombinedReport_300616_1515%20%281%29.pdf

Sustainability

http://www.esfri.eu/sites/default/files/u4/NGL_CombinedReport_300616_1515%20%281%29.pdf

http://www.esfri.eu/sites/default/files/u4/ESFRI_SCRIPTA_VOL2_web.pdf

Sustainability action plan

- *Ensure scientific excellence*
- *Attract and train the best staff and users of tomorrow*
- *Unlock the innovation potential of RIs*
- *Demonstrate socio-economic impact of RIs*
- *Better exploitation of data generated by RIs*
- *Establish conditions for effective governance and sustainable funding for RIs at every stage in their lifecycle*
- *Improve the international outreach of RIs*

http://ec.europa.eu/research/infrastructures/pdf/ri_policy_swd-infrastructures_2017.pdf

LEAPS League of European Accelerator-based Photon Sources

- League of European Accelerator-based Photon Sources – involves *every* European SR and FEL source – formally launched Nov. 2017
- Develop common strategy with smart specialisation for
  - Next generation enabling technology for beamlines and accelerators
  - Data processing and analysis
  - Industrial engagement and innovation
  - Wider outreach, training and integration (access) across Europe


Equilibrium
Kills