Institution: University of York
Unit of Assessment: Chemistry

1. UNIT CONTEXT AND STRUCTURE, RESEARCH AND IMPACT STRATEGY

1.1 Context and Structure

The guiding principle of chemical sciences research at York is that it is of the highest international quality and is, moreover, distinctive for both its reach across traditional disciplinary boundaries and its impacts on society.

In this context, research within the Department is structured into nine interdisciplinary themes. Each theme has a research strategy (*section 1.2*), a route for realising impact (*section 1.3*) and is delivered by a diverse academic body (*section 2*), supported with high-class facilities and sector-leading working practices (*section 3*, *IES § 3,19–23*). These themes, which are informed by the University research strategy (*IES § 4,8*), are: *Archaeological and Paleoenvironmental Chemistry; Atmospheric Chemistry; Biological Inorganic Chemistry; Chemical and Structural Biology; Green and Sustainable Chemistry; Magnetic Resonance and Hyperpolarisation; Molecular Materials; Photochemistry and Spectroscopy; Synthesis, Catalysis and Mechanism*. The responsibility for a theme's vitality and future sustainability is overseen by lead members of the theme, usually a senior academic. They, in turn, are supported by a Department-wide strategy for the management and support of research, including provision of infrastructure and facilities (*IES § 39–41*).

This structure was put in place following REF2014 and a subsequent independent external review of the Department's research (*IES § 2*). In addition, the research strategy laid out in REF2014, '*to develop multidisciplinary chemistry through larger visions*', provided a roadmap for the Department's development in the current REF period—a strategy which has been realised. Indeed, since 2014 research in chemistry at York has thrived, as demonstrated by the increasing number of papers that appear in the top 10% of citations, growing international collaborations (*Fig 1-1, section 4*), and an increase in research funding. The average annual income of £10.1M in the current REF period is some 46% higher than the analogous figure for REF2014 (*section 3*), placing York between 5th and 9th (2015–2019) by total annual value of research income amongst Russell Group chemistry departments. In accord with the interdisciplinary ethos at York (*IES § 2,4*), the breadth of the Department's research is further evidenced by its position as the top grant-holding chemistry department in the UK for NERC and 2nd for BBSRC, alongside a portfolio that spans all the science-related research councils.

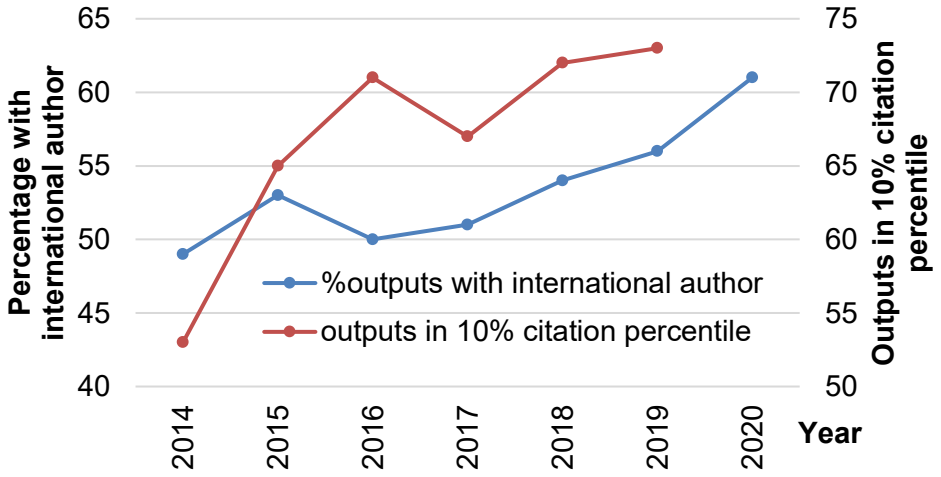

***Fig 1-1**. Plot of number of publications in top 10% of cited papers in the field and % of publications having one or more international co-authors in REF period (SciVal October 2020).*

These improvements in research performance were delivered in concert with internationally recognised commitments and actions to increase equality, diversity and inclusivity (*section 2*). The Department has held an Athena SWAN Gold Award for fifteen consecutive years and is a beacon of good practice for LGBTQ+ and disability matters.

As evidenced by the ten international research prizes/awards to research staff over the REF2021 period (in addition to 13 RSC prizes, *section 4.3*), York can now claim globally recognised research leadership in archaeological chemistry, structural biology, biological inorganic chemistry, atmospheric chemistry, and hyperpolarised NMR; all of which cut across the traditional sub-divisions of chemistry.

Further evidence of the vitality of research:

- growth in grant income (*section 3*), including increases in UKRI funding (annual average £4.1M over REF2014 and £6.1M over REF2021) and in EU funding (annual average of £0.8M over REF2014 and £1.7M over REF2021);
- success in both early career and senior fellowship schemes including ERC (x 4), Ken Murray Royal Society Research Professorship, Royal Society Industry Fellows (x 2), RS University Research Fellow, RS Dorothy Hodgkin Fellow, UKRI Future Leader Fellow (*section 4.3*);
- six **active** or *emeritus* staff who are FRS, two new in REF period: **Carpenter**, **Davies**, *Dodson*, **Gai**, *Goodby*, **Perutz**—a 50:50 M:F ratio.

Thus, following the structural changes and independent review, Chemistry at York in 2020 is different to that in 2014. The overarching themes of interdisciplinary working, alongside a commitment to equality, have borne fruit in terms of globally leading areas of research, greater citations rates, increasing collaborations, growing Research Council grant income, international research awards, significant impact case studies, and—most conspicuously—a raising of research ambition within the Department.

1.2 Research Strategy (*IES § 18*)

The wide-ranging changes made in 2015 to managing and delivering research led to restructuring of the management of research within the Department. The Chair of the Departmental Research Committee became deputy Head of Department (dHoD) and an *ex-officio* member of the Department Management Team, while a Research Office was also established, staffed by two administrators, to provide detailed research management information for performance monitoring and strategy development. These management changes were coupled with a targeted recruitment policy for new academic staff (*section 2.1*). In addition, the research strategy was rewritten to include a long-term vision that fostered multidisciplinary research and technology development. The resulting strategy, which engaged staff through research theme leaders and research fora, has since guided investments, appointments and internal organisation. In addition, retirements over the REF period allowed for a critical re-evaluation of research priorities, resulting in conscious reductions in some areas of activity. At the same time, other strategic areas were grown/refocused through targeted appointments to achieve critical mass (*IES § 22).*

The Department's current research themes are summarised below, along with highlights in the current REF period as evidence of a theme's vitality, the theme's strategic goals, and leadership in research as evidenced by internationally competitive research awards.

Archaeological and Paleoenvironmental Chemistry

This group has shown global leadership in geochronology and palaeoproteomics (**Penkman**, 2017 Pittcon award), enabling a deeper understanding of biomineralisation, evolution and climate (including sea-level) change through development of advanced techniques. By working closely with industry and policymakers, this science was used as evidence in the improved decision-making associated with the management of historical sites and major infrastructure development. Highlights include insights into the evolutionary history of Darwin's South American ungulates *via* in-depth MS analysis (**Thomas-Oates**) and resolving the phylogenetic relationships of early hominins from dental proteome analysis (**Penkman**). This research theme grew following York's institutional investment in mass spectrometry (*sections 3.2–3.3*) and commitments from NERC and ERC to a laboratory for amino acid analysis (NEaar – led by **Penkman;** ERC Consolidator Grant 2020–2025).

The theme plans to develop and apply analytical tools that provide the chemical understanding of the history of human evolution, culture and burial, including environmental markers as indicators of climatic and ecological change.

Atmospheric Chemistry
During the REF period, research in this theme delivered advances in the understanding of emissions and their links to urban and global air pollution, from diesel vehicles and fracking through to solvents and consumer products. By combining modelling and field data, work at York shed light on how the ocean influences the atmospheres of remote regions (**Carpenter** FRS 2019, ERC Advanced grant 2019–2024) and how natural emissions change ozone and aerosols. York's leadership in instrumentation delivered techniques for trace detection of chemicals as gases and in aerosols, from which the rigorous evaluation of low-cost air pollution sensors was pioneered.

Benefiting from long-term commitments and investment in both people and equipment from NERC and DEFRA, the theme's vision is to maintain its existing leadership in reactive gases chemistry, tropospheric observations and modelling, and to grow further research activity in areas related to: air pollution exposure and policy (enabled by Moller *via* a DEFRA Senior Research Fellowship starting 2019), optical and sensor-based instrumental techniques (**Edwards**, ERC Starting Grant 2019 and proleptic lectureship), non-exhaust electric vehicle emissions (**Manfred**, NERC Advanced Fellowship, 2019–2023), and biogeochemical feedbacks and responses (**Carpenter**).

Biological Inorganic Chemistry
The work of this group is distinctive for its direct study of metal-containing proteins and enzymes, using electrochemical/spectroscopic/structural methods combined with advanced protein production and isolation techniques. Highlights in the REF period include studies on the mechanisms and structures of new copper-containing oxidases (LPMOs) which led to an understanding of polysaccharide oxidation by the copper-active sites of LPMOs (**Walton**, **Davies**, IChemE Global Energy Award, 2016). This work contributes to an impact case study on biofuel production. The development of redox-switchable artificial metalloenzymes (ArMs) opened-up new methods for the production of ArMs and is underpinning new work into the catalytic potential of ArMs in organic transformations (**Duhme**).

Strategic aims include integrating siderophore chemistry into new antibiotics, further development of ArMs especially towards their redox-switching in catalysis (**Duhme**), and use of advanced spectroscopic and electrochemical techniques to investigate the fundamental copper-oxygen intermediates in copper oxygenases (**Parkin**, **Walton**).

Chemical and Structural Biology
Alongside multiple insights into protein-catalysed organic reactions through structure analysis, work within the *York Structural Biology Laboratory* (YSBL) saw advances made in the understanding of the role of saccharides in microbiota and health (reported in three separate *Nature* papers, see REF2), thus cementing the link between gut biochemistry and human wellbeing (**Davies** FRS, RS Davy Medal 2015). Crystallographic computing work completed in YSBL continues furthermore to provide the cornerstone of protein structure work carried out worldwide (impact case study), and the big-data expertise that underpins this was applied to address issues in datasets related to large-scale climate modelling (**Cowtan**). Biocatalysis is an important sub-theme, notably including the discovery of a reductive *aminase* which is active across a range of compounds (**Grogan**).

Strategic aims include characterisation and production of enzymes for biocatalysis particularly in scale-up processes of relevance to industry, glycoscience (led by **Davies**, with **Fascione** and new lecturer **Willems**, ERC Starter Grant), antimicrobials, diagnostic resolved magnetic resonance imaging to study drug metabolism (with **Kennerley**), and computational methods (**Agirre**, RS-URF) and software development (**Cowtan**). The purchase of a new 200 kV cryo-electron microscope augmented by the appointment of **Blaza** (UKRI FL fellowship, 2020) and the

construction of a bespoke building to house high-field NMR with cryoprobe and state-of-the-art crystallography facilities (£6M) maintain cutting-edge facilities within YSBL.

Green and Sustainable Chemistry
This group has an international reputation in chemistry relating to green catalysis, and extraction/processing of chemicals from biomass/waste (**North**, Green Chemistry Award 2014). Highlights include the discovery of abundant-metal catalysts for cyclic carbonate synthesis under ambient conditions (**North**), creation of an evidence-based catalogue of solvents for green synthesis (**Clark**), and the study of lignin-derived polyesters obtained *via* enzyme-mediated catalysis. In accord with its application-led focus, work in this theme has commercial impact. For instance, technology for the catalytic synthesis of cyclic carbonates from waste CO_2 and epoxides was developed and licensed to a Dutch company, Alta Innovations Ltd, which then secured the financing needed to design a commercial scale plant. Other impacts include green consultancy companies led by entrepreneurial research fellows from within the theme.

Strategic aims continue to focus on industrial/environmental application, including: sustainable solvents, microwave-enhanced biomass processing (**MacQuarrie**), electrochemical CO_2 fixation chemistry (**North**, **Parkin**), and a green solvent, Cyrene, commercialised by Circa (**Clark**).

Magnetic Resonance and Hyperpolarisation
The York-originated SABRE hyperpolarisation method in 2009 was a breakthrough in the world of hyperpolarisation (**Duckett**, share of Gunther Laukien Award 2020), upon which new developments in imaging and hyperpolarisation have continued to be built during the REF period. Research work in this theme is conducted in the dedicated *Centre for Hyperpolarisation in Magnetic Resonance* (CHyM) facility, which co-locates fundamental and clinical scientists alongside a 3 Tesla MRI human-imaging facility (funded by MRC joint grant, reported under UoA 4). The appointment of **Kennerley** into CHyM, a specialist in clinical imaging research, signals the Department's long-term approach to crossing traditional boundaries. A highlight of the REF period was the discovery of SABRE-Relay, a method for hyperpolarising a wide range of biochemical substrates which opens-up medicinal molecules for potential imaging applications (**Duckett**).

Future research directions for this theme include diversification of hyperpolarisation techniques to medicinally relevant imaging substrates, development of low-field magnetic resonance capabilities for effective polarisation transfer (**Halse**), and the application of SABRE to studying low concentration intermediates in catalytic cycles (**Weller**).

Molecular Materials
Driven in part by investment in two new appointments, **Spicer** and **Avestro** (RS-Dorothy Hodgkin Fellow and proleptic lectureship), research in this theme focuses on renewable self-assembled, self-organised and nanoscale materials, and their application in next-generation technologies, from optoelectronics and energy to tissue engineering. These research areas represent an evolution of York's work on liquid crystals (*Goodby* FRS, Freedericksz Medal of the Russian Liquid Crystal Society 2016). Highlights from the REF period include the development of innovative multicomponent supramolecular gels (**Smith**), and a multi-instrumental approach to the study of structure and organisation of interfaces in ionic liquid mixtures (**Slattery**, **Bruce**).

Future work will target development of innovative gels and molecular scaffolds for stem cell growth and differentiation, with applications in tissue growth and wound healing (**Smith**, **Spicer**); the use of spectroscopic techniques to probe nanosystems, including the tailored surface properties of hydrocarbon/fluorocarbon ionic liquid mixtures, and the synthesis and understanding of π-conjugated molecular materials with inherent and emergent energy, optical and electronic properties (**Avestro**).

Photochemistry and Spectroscopy
York's long-established international reputation in time-resolved photochemistry and laser spectroscopy (**Perutz** FRS**,** AAAS fellowship 2015) was strengthened in the REF period by the appointment of **Hunt**, adding capability in 2D infrared spectroscopy. Highlights in the REF period

included the use of IR spectroscopy and XPS to study the photocatalytic reduction of CO_2 over TiO_2 (**Perutz**), and the use of DFT-calculated magnetic shielding contour plots to visualise aromaticity (**Karadakov**). **Hunt** demonstrated 2D-IR in biomedical applications (patent application), collaborating with UCB Biopharma SPRL for drug discovery, and with NPL for measurement strategies related to optogenetic protein dynamics.

Strategic ambitions for the group include the wider use of 2D-IR to investigate species in biological applications, spectroscopic studies of catalytic intermediates in metalloenzymes (**Hunt**, **Parkin**), gas-phase spectroscopy of laser-induced photoproducts important for the development of new sunscreens (**Dessent**), and determining the reaction dynamics of short-lived species relevant to environmental monitoring (**Dillon**, link to *Atmospheric Chemistry* theme).

Synthesis, Catalysis and Mechanism
Building on the Department's long-established foundations of synthetic organic and organometallic chemistry, this theme focuses on developing synthetic methodologies, alongside rigorous mechanistic work, and their exploitation in real-world applications. **Weller** (EPSRC Established Career Fellowship), **Fairlamb** and **O'Brien** (Royal Society Industrial Fellowships) exemplify this approach, with notable links to industry in the REF period (*e.g.* AstraZeneca, Bayer AG, Chemspeed Technologies, Croda, GlaxoSmithKline, Johnson-Matthey, Pfizer, Redbrick Molecular, SCG Chemicals, Shell, Syngenta). Highlights of work include: time-resolved methods for interrogation of organomanganese catalysts for C–H activation (**Lynam**, **Fairlamb**), the solvent-dependency of hydrogen-bonding *vs* halogen-bonding in co-crystallisation (**Perutz**), cascade ring-expanding cyclisation processes in synthesis (**Unsworth**), and fragment-based inhibitors of the SARS-CoV2 main protease (*section 1.4*, **O'Brien**).

The theme's on-going strategy is to solve challenging synthetic and catalytic problems in a resource efficient way. The focus will be on novel experimental approaches, *e.g.* automated synthetic chemistry, spectroscopy over wide timescales at RAL (**Lynam**), solid-state transformations (**Weller**), cascade reactions (**Unsworth**) combined with theoretical studies (with **Karadakov**), all with a trajectory towards real-world applications. In accord with this strategy, long-term relationships with the aforementioned industries are being developed, as are links to other departmental themes: *Biological Inorganic Chemistry*, *Hyperpolarisation, Photochemistry* and *Chemical Biology*.

1.3 Impact Strategy (*IES § 12*)
As described in the Impact Cases Studies, research impacts at York have emerged largely from research themes where there is critical mass of high-quality research activity, sustainable long-term funding and where the primary research has on-going engagement with end-user needs. The emphasis on integrated multidisciplinary teams in the Department's research strategy (*section 1.2*) is also, therefore, a cornerstone of the Department's impact strategy (*IES § 12, 49–50*).

In this regard, in order to enhance the translation of the Department's research into societal impact, the co-location of researchers external to the Department/University to work alongside and within the research themes is an important aspect of the strategy. For instance, the *Wolfson Atmospheric Chemistry Laboratories* (WACL) houses twelve staff from the *UKRI National Centre for Atmospheric Science* along with joint academic appointments with DEFRA and industry. YSBL houses industry-funded researchers *via* its long-term relationship with Novozymes, and has a seconded position from the Collaborative Computational Project for crystallographic software (**Wilson**). The *Green Chemistry Centre of Excellence* (GCCE) has a dedicated suite for industrial engagement, and runs RenewChem, an industry-focussed and industry-informed graduate programme. Such co-location of researchers from both within and outside the Department, who help inform the Department's research activities, maximises the translation of research into impact.

As an example, in the area of atmospheric chemistry and climate, a small number of external organisations were fostered as key partners, delivering impact across a range of different scientific and environmental policy issues. The strategy was to invest resources in developing hard-wired

relationships and positioning York as a 'trusted supplier' of research, advice and evidence. This approach included joint academic appointments and meaningful workload allowances for staff who take on leadership positions (*e.g.* with government science advisory groups, advice to Select Committees on international scientific assessments, and with the United Nations). *Fig 1-2* illustrates how research interlinks between partners, which underpin three of the impact case studies in *Atmospheric Chemistry*.

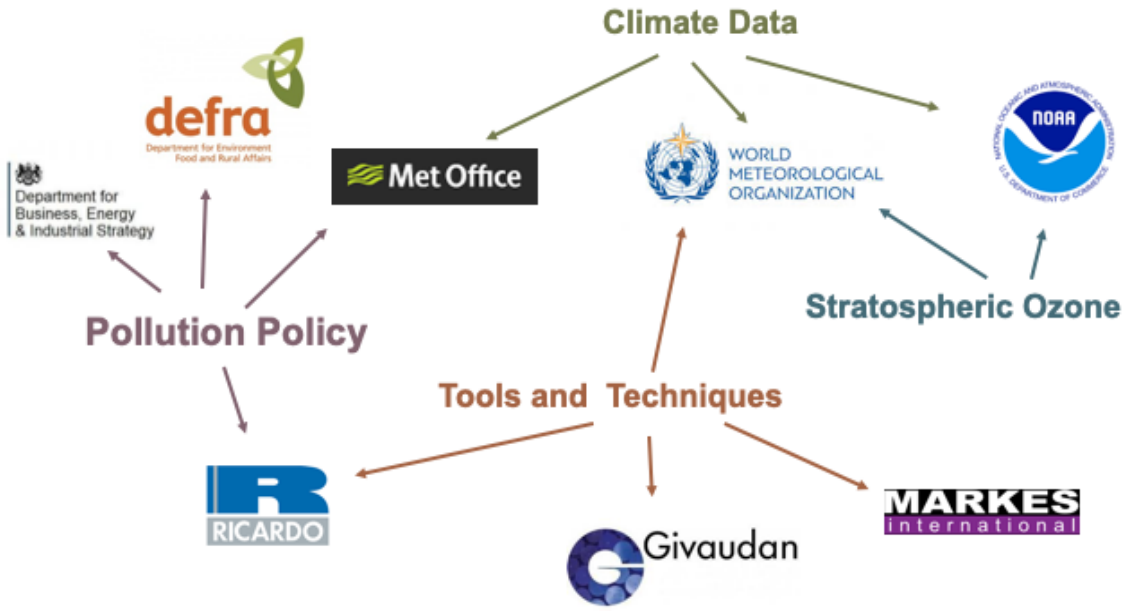

Fig 1-2. *Illustration of how individual areas of impact within York atmospheric chemistry research link with selected end-user partners.*

The success of this approach when applied to economic impact is also illustrated by the case studies relating to crystallographic software and enzymes for industry. In the latter the £billion scale of impact is created through a long-standing relationship with Novozymes, who in turn manufacture cleaning products and biofuels, involving Unilever and international biorefineries (*IES § 45)*. In the case of crystallographic software, the Department invested in the support of facilities and academic staff (**Agirre** RS-URF, **Cowtan**) whose research underpins the long-term relationship with the STFC CCP4 consortium, in turn supporting economic impacts *via* an international academic/industrial group through worldwide software provision. As evidence for the impact of the Department's research in protein science, the Queen's Anniversary Prize for 'excellence, innovation and public benefit' was awarded to YSBL in 2020.

Beyond the work described in the Impact Case Studies, the importance and value of impact is well understood throughout the Department. Accordingly, the impact strategy includes practical actions that can add value to, and complement, existing research programmes and knowledge exchange (KE) activity. To this end, there is a Departmental Impact and KE lead (**Lewis**) who provides local guidance, supported by both departmental and faculty management executives (*IES § 49–50)*. Departmental impact activities are complemented by University support provided by the Business Development Team (in partnership development, commercialisation and protecting intellectual property) and the External Relations Team, offering support through their events team and press office for issues such as publicising research and public engagement.

In this context, the Department's five impact case studies for REF2021 provide a model for the future. Accordingly, the Department's medium-term strategy is focused on the development of new areas of critical mass that can deliver impact in the late 2020s. This approach is exemplified by new investments in staff working in *Molecular Materials*, *Green and Sustainable Chemistry* and *Magnetic Resonance and Hyperpolarisation*, which are prioritised as research areas having both high scientific and impact potential, particularly for clinical applications (*sections 1.5, 2.1*)

1.4 Response to COVID-19
Perhaps one of the most vivid examples of the Department's 'impact culture' and its ability to translate research into societal benefit, is that Department researchers played prominent roles in several COVID-19-related projects (*IES § 40, COVID annex*).

1) Work on the SARS-CoV-2 nucleocapsid protein, a major immunogen implicated in the pathology of COVID-19, was initiated by **Antson** in March 2020, continuing through lockdown. The protein materials benefited UK labs and industrial companies, contributing to several studies at Universities of Oxford, Sheffield, and Imperial College, including in the testing of healthcare workers and contributing to the Oxford vaccine efforts, aiding in the development of new testing procedures with industrial partners, Avacta Life Science and Aptamer Group. The work led to a joint publication involving ~fifty co-authors, showing a breadth of interdisciplinarity.

2) Exposure to air quality was identified early in the COVID-19 pandemic as a potential risk factor increasing severity of disease and mortality rates. WACL remained open throughout with a small staff undertaking critical long-term measurements with **Evans** providing ten-day pollution risk forecasts to DEFRA and PHE. At the request of the DEFRA CSA and Minister of State, **Lewis** led a rapid evidence review on air quality/COVID-19 interactions and presented further evidence at a later Environment Food and Rural Affair Select Committee Inquiry. WACL members engaged widely with the media and Government on air quality issues during this time (*section 4.2*).

3) The spike glycoprotein (S) of SARS-CoV-2 is perhaps the most recognisable feature of the coronavirus behind the COVID-19 pandemic. Indeed, many COVID-19 survivors develop antibodies that target S. The spike glycoprotein is extensively glycosylated, creating a glycan "shield" that helps it evade immune recognition. The different atomic structures of S and its glycans, published in 2020, informed the design of many vaccines and antibody treatments against COVID-19, including the BioNTech/Pfizer vaccine.

Most structures were validated by Privateer, software produced and maintained by YSBL. Privateer ensures that critical carbohydrate components do not contain errors that could potentially mislead vaccine or antibody design (evidenced in citations). Since the start of the pandemic, the YSBL team (led by **Agirre** and **Cowtan**) focused on 1) the automatic cross-linking of structural information with glycomics data to ensure the creation of biologically sound glycan structures; 2) introduction of native support of Electron Cryo-Microscopy maps; and 3) the creation of a standalone version of the software. These developments led to the inclusion of Privateer in the validation pipeline of the CCP-EM consortium.

4) COVID-19, caused by SARS-CoV-2, requires effective therapeutics. Shorter-term approaches (one to two years) focus on repurposing known drugs and on developing vaccines. A longer-term approach (five to ten years) is to use the methods of fragment-based drug discovery to identify suitable, small-molecule antiviral therapeutics, by targeting distinct parts of the viral machinery. The York 3D Fragment Library (**O'Brien**, Hubbard) was deployed as part of a fragment screening campaign at the Diamond XChem Facility against two COVID-19 proteins (with Walsh/Ahel/von Delft, Diamond). In February 2020, a large-scale screen against the SARS-CoV-2 main protease, one of two cysteine viral proteases essential for viral replication, identified two York lead compounds. These molecules offer structural and reactivity information for on-going structure-based drug design against SARS-CoV-2 main protease (public domain in March 2020, the COVID MoonShot; fully open-initiative). In May 2020, a screen against the SARS-CoV-2 macrodomain enzyme identified four York hit compounds (**O'Brien**, public domain in July 2020).

1.5 Strategic Aims
In addition to a clearly articulated and resourced science strategy (*section 1.2*), the Department's future success also hinges on people (*section 2*). To this end, the strategy has been to support research areas through targeted senior appointments, and to attract and support future research leaders. There has, accordingly, been growth in the numbers of independent research fellows (IRFs) (*section 2.1*) since REF2014. In addition to the recruitment of ECRs, the Department made

recent strategic appointments into the new research themes: laser spectroscopy, MRI, Cryo-EM, glycoscience, organometallic/catalytic chemistry and molecular materials.

Looking to the future, the well-established themes of *Atmospheric Chemistry*, *Biological Inorganic Chemistry*, *Chemical and Structural Biology* continue to thrive, delivering world-leading research alongside societal impact. These themes thus provide compelling models as to how this can be achieved. In this regard and following this model, ECR appointments during the REF period safeguard the future (**Blaza**, **Willems**, **Agirre** in YSBL and **Manfred**, **Edwards** in WACL). Additionally, over the coming period new appointments within *Green and Sustainable Chemistry* will be made, including the recruitment of a new Director (**Clark** reduced his fte), offering opportunities for new research directions in sustainable industries, low carbon futures, chemical engineering and the circular economy. The Department will further strengthen *Archaeological and Paleoenvironmental Chemistry* as a proven enabler of influential, often profoundly interdisciplinary research that reaches across science and the humanities.

Notwithstanding a clear direction of travel for academic appointments, there are many challenges ahead, including the effects of the COVID pandemic and the transition period from Brexit. In particular, the uncertainty that always exists in re-securing current DTP/CDT funding in a volatile UKRI environment is a concern. The Department's approach therefore has been to diversify the funding base for research, especially for PGR students (*section 3.1*). In particular, this funding base includes a focus on philanthropic donations—an area in which the Department has been successful through the establishment of a major benefaction for the recruitment and support of PGR students (>£1M in REF period) from Dr Tony Wild, a York alumnus (*section 3.2*). This approach to funding, placed alongside the long-term research strategy and cohort of talented and young researchers (*section 2.1*), means the Department is well placed to meet future challenges.

1.6 Open Research Environment and Ethics

The Department was an early adopter of open access of research data, driven in large part by the existing open cultures. This culture led to a high degree of compliance and, between 2016 and 2019, >95% of the Department's outputs were open access. Further, since 2015, 140 datasets were deposited to the University data repository in addition to datasets deposited in subject domain archives such as the Centre for Environmental Data and Analysis (CEDA), the Protein Data Bank, CCDC and NOAA (National Oceanic and Atmospheric Administration).

In other examples of making data open access, the Department deposited 360 X-ray single crystal structure datasets to the Cambridge Crystallographic Data Centre; and, over the period from 2014–2019, 356 datasets were deposited in the Protein Data Bank. The Department's work in open access data, through **Cowtan**, contributed to University management of research data. In particular, the University formed an open research strategy and operations groups within the REF period (*IES § 16–17*), of which **Cowtan** is a protagonist.

Sector-leading Practices

In protein structure research, it is and has been routine practice to deposit experimental X-ray data. As such, YSBL also has an archive of processed experimental data back to at least the 1980s. Additionally, YSBL has retained all unprocessed image data since 1998 – these are made available on request to users.

Penkman co-established the open access aminostratigraphy database kept at NOAA.

The atmospheric chemistry group at York ensures all data meet all open accessibility and metadata requirements, which are deposited with CEDA, a petabyte storage and analysis capability offered by STFC. Since 2000, York has made ~70 million atmospheric observations publicly available *via* CEDA, comprising ~1,200 individual datasets, involving 42 different instruments. WACL is active in advising global bodies such as the WMO in ensuring long-term datasets on global change are also open access, including working to create standards for reporting of pollutants such as VOCs and NO_x. Research data from the York-led Cape Verde

Atmospheric Observatory are open access through the UN World Data Centre for Greenhouse Gases and as part of the UK data submissions to UNFCCC.

Research Ethics (IES § 14,29)
All staff and students are made aware of their ethical responsibilities at the time of recruitment and/or upon submitting a research proposal, through university policies. Notwithstanding the clear University expectations on research ethics however, the Department also sees this as a matter of culture, with engagement and accountability at its heart. As such, the Department adopts progressive data sharing procedures (see above). This is coupled with regular open seminars across the Department, in which PGR and postdocs are encouraged to speak about results and data in an open and friendly atmosphere. These seminars—organised by academic staff—happen at group, theme and departmental levels. During the REF period, the Department held several research fora specifically dedicated to discussing research ethics.

2. PEOPLE

2.1 Staffing Strategy and Staff Development

The Department is people-focused. We seek to appoint the best and then retain this talent within a supportive and positive culture (*IES § 9*). Indeed, as might be expected of an Athena SWAN gold Department, equality principles inform much of what we do (*section 2.3*, *IES § 24–26, 35–37*). This approach has borne fruit in terms of staff engagement and also in terms of intra-Departmental collaborations. For instance, in the Employee Engagement survey in 2017, 96% of staff said that they liked the work they did and that their work was interesting to them, 87% said that colleagues cooperated to get work done even if it meant doing something outside the usual activities. 94% confirmed that their Manager / Supervisor treated them with respect. Moreover, a 2020 culture survey revealed that many felt that the Department is a 'great place to work' (87% of academic, research and professional support staff). 90% of academic staff, 92% of professional support staff, and 83% of PGRs confirmed an understanding of the Department's policies in relation to equality; these figures underline the emphasis on a supportive, fair and sustainable culture.

56.8 fte are returned to REF 2021, with a total active headcount of 62 Category A staff. As one of the largest UK chemistry departments, the strategy during the REF period was to maintain rather than grow academic staff numbers. As such, staff turnover has created most of the new opportunities for academic recruitments, by which areas of critical mass identified within the research strategy were strengthened (nine appointments in period, see below). The approach was twofold: to appoint talented ECRs into lectureships and, where required, established researchers into leadership positions. This strategy, alongside best practice in the support of existing staff, means that there was an increase in the quality of outputs and income/academic staff fte (*section 1.1*) during the REF period, even while transitioning through a period where several of the Department's research leaders (**Clark**, **Gai**, **Perutz**, **Taylor**, **Wilson**, *Goodby*, *Hubbard*) retired or moved to part-time working.

Academic Appointments in REF period

Avestro (*Molecular Materials*; RS-DHF), **Blaza** (*Chemical and Structural Biology*; Lecturer), **Carslaw** (0.4 fte, *Atmospheric Chemistry*; Reader – p/t appointment, also p/t with Ricardo plc), **Halse** (*Photochemistry and Spectroscopy*; Lecturer), **Hunt** (*Photochemistry and Spectroscopy*; Professor), **Kennerley** (CHyM; Lecturer), **Spicer** (*Molecular Materials*; Lecturer), **Weller** (*Synthesis, Catalysis and Mechanism*; Professor), and **Willems** (*Chemical and Structural Biology*; Lecturer). All except **Hunt**, **Weller** and **Carslaw** are appointed to their first academic post.

Nine ECRs (*section 4.3*) were appointed during the REF period, up 60% since REF2014. Part of his increase is the result of a new process (led by **Halse**) for identifying and selecting the strongest IRF applicants, as follows. Following an Open Day for interested future ECRs, guidance is given on CV and research proposal preparation and formal assessment of fellowship applications is then made in consultation with senior academic staff. Promising candidates, who are aligned with the research strategy, are selected for submission of bids to fellowship funders, and provided with departmental support, including mentoring and matching funds and/or research studentship support. All staff applying for fellowships are supported through a funded PhD studentship or PDRA provision. New fellows appointed through this process are assigned a mentor and hold regular discussions with the HoD during their probationary period (*IES § 29*). In this regard, the Department has an excellent record of moving independent research fellows to permanent lectureships (>90%).

Staff Development

In addition to the support given to new appointments, all staff are supported in their personal and career development *via* senior academic mentoring of each of six management/teaching sections. This management structure deliberately cuts across the research themes. The senior academic, labelled as academic group leader (AGL), provides support including enabling internal peer review of papers and grant proposals, career development advice including helping to identify key training needs. Probation for these staff is conducted by the HoD in consultation with the AGL.

The Department has a rolling programme of research leave for academic staff, in which staff are encouraged to spend time at other institutions and use the period to establish new research areas. A formal process is in place to oversee research leave applications and outcomes. Over the REF period, there were 26 individual periods of research leave, each of approximately ten weeks (*IES § 23*).

Postdoctoral Researchers
Postdoctoral researchers are an integral part of the Department's research effort. As befits the Department's people-centric approach, this group of staff is supported both during their research projects and in career development. There is a member of academic staff (**Avestro**) who is their named Champion, who provides bespoke and personal support to PDRAs. For instance, working closely with the University's Research Excellence Training Team, the Department provides PDRAs with a training package including access to PGR training programme, the University coaching scheme and award-winning Leadership Training (*IES § 22, 27–29*). In addition, the Concordat to Support the Career Development of Researchers is embedded into the Department's Athena SWAN action plan to ensure oversight and proactive monitoring of actions by the Equality and Diversity Group (EDG, *IES § 35–37*).

All PDRAs are provided with a peer mentor and one-to-one career development support, a scheme developed from running a successful pilot for PDRAs in partnership with the institution. Importantly for research career development, PDRAs are also offered opportunities to sit on departmental committees, to co-supervise undergraduate and postgraduate students related to their project, to deliver a small number of tutorials/workshops and to offer their own undergraduate summer research projects, enabling professional experience to be gained for next career steps. Finally, as part of the Department's commitment to equality, the HoD works with the EDG to monitor the balance of protected characteristics (*e.g.* gender, race) within the PDRA cohort (*IES § 27–28*). As part of its commitment to the careers of its staff, the Department employs a dedicated Employability and Diversity Officer who provides one-to-one careers support for all staff and students, including specifically for PDRAs, *e.g.* through networking events and CV workshops.

Response to COVID-19 (IES § COVID19 annex)
The COVID-19 crisis brought significant pressure on researchers and research staff. In response, during the crisis the Department took a proactive stance towards protecting staff wellbeing, most notably though actions towards mental-health support, *e.g.* mental health fora, stress management classes (*IES § 25*). The Department also worked towards the early reopening of research laboratories. At the end of the first lockdown in March 2020 technical staff were specifically tasked to open research labs and repurpose teaching labs, allowing a restart of research activity in July, albeit at reduced occupancy levels. Access to research labs under COVID-secure working arrangements has continued uninterrupted since.

2.2 Training/Supervision of PGR students (IES § 30–34, *section 3.2*)
All PGR students in Chemistry undertake the Innovative Doctoral Training in Chemistry (*i*DTC) programme, which offers the advantages of a cohort-based postgraduate experience to all research students studying Chemistry. Students participating in other doctoral training networks can also opt into *i*DTC activities. Graduate training is offered to all students to support the development of scientific, transferable and employability skills, and to enhance the research skills of each student. This core training is progressive and takes place at appropriate points throughout a student's degree programme, with most of the training taking place in Year 1. In conjunction with Core training, students select training related to their research area to enhance skills, techniques and knowledge. One further distinctive aspect of the *i*DTC is its focus on supporting international PGRs, which includes a bespoke English language course. For PGR students undertaking interdisciplinary projects (*e.g.* in Chemical Biology or Atmospheric Chemistry) tailored training across traditional discipline boundaries is provided, *e.g.* NERC DTPs ACCE, ECORISC and PANORAMA, EU ITNs and the BBSRC White Rose Mechanistic Biology DTP.

Integration of PGR Students into the Research Culture
As in all chemistry departments, PGR students at York are intrinsic to the success of the Department's research and are, therefore, integral to the research cultures of both their immediate research groups and the wider department. In terms of the latter, integration and collaboration between research groups are fostered through the shared training experience, research seminars and group meetings, academic co-supervision, mentoring and other support (*e.g.* disabilities, well-being). In addition, all new PGR students are assigned a mentor from the existing research student community. PGR students have local access to state-of-the-art research facilities and analytical services – nearly all of which are free at the point of access. Students are also allocated a personal consumables and conference budget, the latter enabling network development, presentation of their work to a wider audience and learning first-hand of international developments. Additional opportunities to present research include regular student-led graduate seminars, annual poster competitions and regional seminars.

The Department earmarks funds to recognise and reward its best PGR researchers. For instance, the Kathleen Mary Stott Prize is awarded by an independent panel to final-year PhD students for performance in research and involves a prize-winners' departmental seminar. Recently the Department established an Overseas Visiting Scheme which allows York PGR students to visit the laboratories of prestigious international research groups (*e.g.* Borovik and Green groups at the University of California, Irvine, USA; Vocadlo group, Simon Fraser University, Canada; ShuLi You group, Shanghai, China) as part of their PhD studies.

Research Student Numbers
The Department is committed to maintaining PGR numbers *via* use of internal funds, industrial support through matched funding and CASE award schemes (co-funding 25 PhD students since 2013/14), Marie-Curie training networks, charities and through the philanthropic schemes, including the Wild and University overseas scholars schemes *(section 3.2*). PGR student numbers grew from 125 in 2013/14 to 155 in 2017/18, with the number per academic staff/fte growing from 2.7 to 3.4. Flexibility in these schemes allowed the Department to attract talented PhD students from around the world, increasing cultural diversity. Accordingly, specific provision for overseas students is made by the Department. For instance, *Chemical InterActions*, which is led by international research students, is a social network for all Chemistry students and staff that runs regular social and academic events. International students are also invited to regular informal international coffee mornings to assist cohort integration.

Student Outcomes
The Department has on-time thesis submission rates (2013–14 starters 82%; 2014–15 starters 93%; 2015/16 starters 89%), with low withdrawal rates (<5%) and low failure rates over the past five years (<3%), resulting in high overall successful outcomes (94% over the REF period).

2.3 Equality and Diversity
The Department is internationally recognised for its equality work. Most notably, it was the first academic department in the UK to hold an Athena SWAN (AS) Gold Award (*IES § 37*) which it has held uninterrupted since 2007.

Support for people at all stages of their career is a priority and the Department's proactive EDG continues to address all forms of inequality, aiming towards a working environment in which all participants can reach their full potential (*IES § 19,22–23*). Key equality measures for the Department include: **1)** F and M appointment rates for researchers are equivalent, indicating a gender-neutral recruitment process; **2)** actions linked to direct appointments and named researchers (ECRs) led to substantial improvement in %females recruited *via* these means (from 16% for the 2015 AS submission to 46% for 2018). Of note in this context is the lack of gender 'leaky pipeline' amongst academic staff in the Department. 25% of professors are female (October 2020) with 28% female total academic staff; **3)** eliminating median gender pay gap for professorial staff (20% in 2010, <1% in 2018). (*IES § 21*)

Activities in REF Period
The work of the EDG group informs, encourages and supports policies and working practices, especially flexible working, informing and influencing institutional guidance (*IES § 35–37*). In 2018, ten research staff (6F, 4M) and ten academic staff (21%; 5F, 5M) were formally working part-time including five members of professorial staff (2F, 3M).

At a functional level, meetings and seminars are all held at family-friendly times and diversity training is embedded in the UG and PGR curriculum and during staff induction, which includes a workshop on neurodiversity and positive LGBTQ+ actions. The Department introduced specific 'all genders welcome' toilets; 'Trans 101' training for all staff; personal pronoun discussion at initial UG supervision meetings and has developed nationally shared pronoun usage guidance. The Department provides baby changing facilities and a quiet/prayer room. In addition, there is active invitation of female seminar speakers (~40% to 2019) and PGR external examiners (*e.g.* 35% in 2016–17), and a well-supported maternity, paternity and adoption leave policy. These Departmental guidelines later became institutional policy.

Ensuring the prominent profile and sustainability of equality practice, in 2015 the Department recruited an Employability and Diversity Officer (Jones).

The Department improved the ethnic diversity of its staff and students, using the philanthropic Wild fund (*section 3.2*) to recruit and retain PGRs from different ethnic backgrounds. Use of the fund enabled 79 students to accept postgraduate research positions since its inception, 63 of whom have so far graduated of whom 49% are female. At a national level, **Dessent** led a successful bid to the RSC for a project to study the experiences of BAME individuals working in Chemistry.

Recognition of those with disabilities, which includes academic, technical and support staff, is built into the inclusive ethos of the Department (*section 2.1*). This support directly adds to the research endeavour of the Department, and graduate students with significant long-term health issues graduated successfully in the REF period. Support is provided by Disability Officers, **Perutz** and Sarju, the former of whom also brings influence to bear nationally as a member of the HE-STEM Disability Committee.

Leadership in Equality and Diversity
York is a beacon department nationally and internationally, as evidenced by its staff members giving numerous invited external presentations over four continents in the REF period. **Dessent**, Jones, **Wann** and **Walton** serve on Athena SWAN judging panels. **Walton** has an international reputation for gender equality; he has served on multiple university and governmental panels for equality in academia. **Smith** is noted for his work and public profile around LGBTQ+ issues and parental/caring roles, and is an appointed member of the RSC Inclusion and Diversity Committee. **Matharu** is Chair of the University Staff Race Equality Forum. The Department specifically credits these activities in its workload model.

Commensurate with its role as a beacon and in addition to its annual Equality and Diversity Lecture, the Department plays host to many seminars and national events focused on equality and diversity, *e.g.* 2016 RSC Joliot Curie Conference, dedicated to supporting the aspirations of ECRs, particularly women and those who are underrepresented in academia; the LGBTQ+ STEMinar 2018; and a two-day celebration of its ten-year anniversary as an AS Gold holder. The Department introduced an unconscious bias observer scheme for all stages of the appointment processes, which contributed positively to an increase in % female researchers to the Department's highest ever level of 40%. This best practice has been shared widely within the academic sector. In accord with the institution's guidelines, this practice extended to the internal REF process, where selection of outputs for submission was monitored against protected characteristics including age, disability, ethnicity and gender throughout. No significant evidence of bias was found, when grade/seniority of staff members was taken into account. The fraction of outputs returned under UoA8 associated with female authors is 16% (*cf*. %F fte Category A staff of 20%).

3. INCOME, INFRASTRUCTURE AND FACILITIES

3.1 Research Income Overview

Combined with the structural changes described above (*section 1*), the Department is active in supporting staff to seek funding, for example by implementing a new research workload model which specifically encourages bids for funding that enable large-scale science (*IES § 38b*). In this regard, the Department won several multi-institution and/or large research grants in the REF period, representing a distinct shift in funding patterns since the last REF exercise. For example:

- Large EU consortium bids, for example in sustainable synthetic chemistry (*e.g.* CHEM21, ReSolve, RenewChem) and biocatalysis (*e.g.* CoEBio3).
- EU-funded Synergy award in glycoscience (**Davies**).
- Four European Research Council (ERC) grants; one Advanced, one Consolidator and two Starter; competitive personal awards (*section 4.3*).
- Champion (EU) materials chemistry with fifteen academic / industrial partners.
- Multi-centre EPRSC grants (**Clark**).

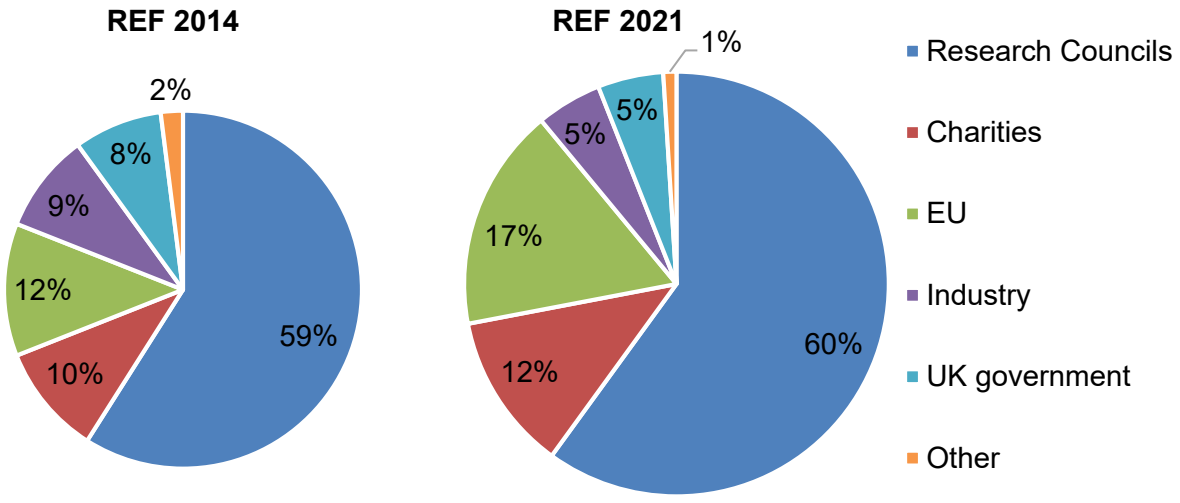

***Fig 3-1**. Pie charts of average per annum research income for REF2014 period and REF2021 period (does not include income-in-kind). Areas of circles reflect total value: REF2014 period average annual income is £6.9M pa and REF2021 average is £10.1M pa (not including major facility time allocations).*

Overall, during the REF period, the Department's direct average research income grew by 46% compared to the last REF period (*Fig 3-1*), now placing it in the top-10 of UK Chemistry departments. The annual research income per fte rose similarly, and over the REF period is £178k per Category A staff, based on 56.8 fte, and >£200k per RE/OFS-funded staff, based on 45–50 fte. Annual average Research Council, charitable and EU funding grew over the same period by 48%, 86% and 108% respectively.

3.2 Research Infrastructure and Support

The Department has benefited from an infrastructure programme over the last decade that replaced much of the old 1960 CLASP structure, continuing during the current REF period. In addition to new buildings for *Green and Sustainable Chemistry*, *Magnetic Resonance and Hyperpolarisation*, and laboratories for chemical synthesis and materials chemistry reported in the last REF submission, in this REF period further investments include:

1) Capital of >£6M (Wellcome, Wolfson, University of York, BBSRC and philanthropic donations) funded a bespoke and integrated facility (551 m^2) for protein structure determination, with a new 200 kV cryo-electron microscope, a new rotating-anode X-ray source and detector for protein crystal screening, and high-field NMR spectroscopy with cryo-probe.

2) WACL, established by the Wolfson Foundation in 2014, expanded in 2018 with funding from NERC and the University, adding a further 450 m^2 of research space, including an air pollution sensors lab, additional PhD space and new computing facilities, making a total of >1200m^2 of dedicated space for atmospheric chemistry research, the largest of its kind in any university in Europe (*IES § 40*). The most recent £1.5M buildings expansion was further supplemented by a £4.3M capital award from NERC for new instruments for air pollution science. Alongside new facilities and equipment there were new high-level technical appointments, including an Instrument Engineering Manager, High Performance Computing specialist and a Global Modelling Fellow.

3) Mass spectrometry Orbitrap (x2), for atmospheric chemistry (in WACL, led by **Hamilton**) and CoEMS (>£1.2M, *section 3.3*). The Orbitrap MS (WACL) has been used to study secondary organic aerosol (SOA) formation in the atmosphere, stimulating a new collaboration with the Guangzhou Institute of Geochemistry (GIG), in China, and has since been incorporated into multiple projects studying toxic species in particle pollution supported by UKRI and industry. A Synapt G2Si high definition mass spectrometer was funded through a BBSRC ALERT grant (**Thomas-Oates**, **Davies**).

4) Infrastructure investments for photochemistry/photophysics (>£500k) include a Ti-sapphire laser system which supports enhanced time-resolved spectroscopy capability, spanning UV to mid-IR wavelengths and a temporal range covering 100 fs to hours. This facility supports research ranging from gas-phase electron diffraction experiments (**Wann**) to solution-phase photochemistry measurements and is complemented by the addition of 2-D IR spectroscopy capability (**Hunt**).

5) Upgrade to magnetic resonance facilities (NMR >£800k) and EPR (Q-band Jeol XES-320 EPR ~£80k) equipment. The latter investment has provided an enhanced capability in the *Biological Inorganic Chemistry* theme.

6) EPSRC strategic capital award (£3.25M) of a double aberration-corrected microscope to the York-JEOL Nanocentre (*section 3.3*), now part of the EPSRC SuperSTEM national facility for microscopy. Electron Backscatter Diffraction detector for SEM, funded from EPSRC (£250k).

Interdisciplinary infrastructure and support
As described above (*section 1*) interdisciplinary science is a distinguishing feature of York's current research and its research future. To ensure a suitable working environment, therefore, the Department has invested in and maintained equipment/infrastructure which allow diverse teams to work in one place, including on-site co-working with external organisations. For instance, YSBL researchers are housed in dedicated laboratories located in the Biology buildings. Accordingly, YSBL researchers maximise the biological context in which they work, particularly in the areas of microbiology, glycoscience, tissue engineering, and computational methodology including software. Researchers in the *Atmospheric Chemistry* theme are housed in WACL, another dedicated building with labs and office space, accommodating researchers from the Chemistry and Environment departments. Researchers in the *Green and Sustainable Chemistry* theme occupy the GCCE and enjoy close links with the Biorenewables Development Centre (a not-for-profit University company). The latter of these is a scale-up facility that supports the translation of fundamental research in green chemistry into sustainable commercial products. CHyM is a dedicated Wellcome-funded building co-located with the York Neuroimaging Centre (part of the Medical School and Psychology department). CHyM provides a laboratory equipped to support the work of both clinical and chemical scientists, thus facilitating translation into the clinic of the York-originated technique of SABRE-polarisation.

In accord with the department's research ethos, staff also play central roles in several University interdisciplinary initiatives, including the York-JEOL Nanocentre (with Physics and Electronic

Engineering); the Centre of Excellence in Mass Spectrometry (CoEMS, with Biology); the Biophysical Sciences Institute (BPSI, with Physics, Mathematics and Biology); and the scientific archaeology research of BioArCh (with Biology and Archaeology). In addition, staff contribute to collaborative efforts with the York Plasma Institute (YPI, with Physics) and to partnerships with external research partners in academia, industry and government (*sections 1.3, 4.1, 4.3*).

Further reflecting the interdisciplinary outlook of research, the Department is part of five Doctoral Training Partnerships: BBSRC White Rose DTP, three with NERC (PANORAMA, ACCE, ECORISC schemes with multiple Universities), and the EPSRC DTP Mobility Training Pilot. The last, which is led from the department, continues the theme of inclusivity within the Department's graduate school. It helps UK businesses up-skill their employees (eight PhD studentships awarded over two cohorts) and to attract applicants from non-traditional backgrounds.

The investment in equipment/infrastructure has been accompanied by a commitment to technical staff, who are essential contributors to the department's research (*IES § 40*, National Technician Commitment). In this context, the Department recently completed a partial restructuring of technical staff which saw each research laboratory provided with a dedicated research technician for the on-going maintenance/management of laboratory facilities and environment. In addition, the Department has dedicated administrative support for research, including a departmentally funded research office which provides alerts on funding opportunities, support with grant applications and provision of management information for the department's Research Committee. The office has a specific remit to support the coordination of large multi-investigator, interdisciplinary bids (*section 3.1*), the growth of which in the REF period has become a hallmark of the Department's interdisciplinary approach.

Philanthropic Funding
In a challenging funding context, especially for PGR students, the Department has grown additional and sustainable sources of support, distinctively raising £3.8M of direct investment from multiple philanthropic sources. Much of this investment comes from 'The Wild Fund', a benefaction to the Department from Dr Tony Wild, an alumnus (>£1M in REF period alone). The Fund has principally been used to support PGR studentships. Notably, use of the fund is more flexible than most UKRI training investments allowing the Department to bring-in talented PhD students from around the world, particularly from developing countries (35 PhD students, M:F 4:3, 2014–2020). In addition, during the REF period, philanthropic funding also supported two independent fellowships, PGR studentships, PDRA positions and a Knowledge Transfer Fellowship (leading to a spin-out consultancy). Such funds also underpinned the RenewChem scheme (*Green and Sustainable Chemistry*), departmental contributions to new DTPs, and have provided cutting-edge equipment (to WACL from Givaudan).

3.3 Research Facilities
The Department enjoys state-of-the-art facilities for its research. Almost all facilities are free at the point of use and they are supported by an expert technical staff cohort, many of whom are equipment specialists. Facilities include: X-ray diffraction (powder, single crystal and rotating anode for proteins), protein production (two dedicated labs), mass spectrometry, NMR, EPR, elemental analysis, chromatography, each of which is led by a technical staff member. More specialist high-end facilities are also available through other access arrangements. These include the Centre of Excellence in Mass Spectrometry (see below, led by **Thomas-Oates**) offering Qh-FT-ICR MS with dual ESI/MALDI sources, Orbitrap with ES, nanospray and APCI sources) and ultraflex III. High-field NMR (600 wide bore and 700 MHz equipped with cryoprobe, 400 MHz solid state). Protein production and characterisation through the Department of Biology's Technology Facility, offering amongst other services, advanced genomics/proteomics and eukaryotic expression. High level microscopy provided by the Nanocentre (SEM with EDX, ultra-high resolution (<1 Å) TEM with aberration correction, AFM). Additionally, University-level facilities which are extensively used by departmental members, include a 7,500 core cluster for high-speed computations (*IES § 41*). All of these facilities are complemented by in-house glassblowing, electronics and mechanical workshops with experienced technical staff, who provide dedicated

and expert support especially for research carried out in the *Photochemistry and Spectroscopy,* and *Synthesis, Catalysis and Mechanism* themes.

3.4 Use of non-UKRI Facilities

Staff have been successful in winning time on major international facilities: Felix laser laboratory, Netherlands (**Dessent**, £9.5k value); Bragg Institute, Australia (**Weller**, £14k + £47k value); IDo2 at ESRF, Grenoble (**Shimizu**, £28k value); Phoenix XAS at the Swiss Light Source (**Duhme**, £135k value); Guangzhou Institute for Geochemistry, China (**Hamilton**, £45k value); XMaS facility at ESRF Trieste (**Fairlamb**, £43k value).

4. COLLABORATION AND CONTRIBUTION TO THE RESEARCH BASE, ECONOMY AND SOCIETY

4.1 Research Collaborations

There is an ethos of departmental collaboration at York, with shared PGR students being the norm (currently 70% of PhD students have more than one supervisor). Many examples of research collaborations exist within and between research groupings and across the university. Indeed, 34% of the Department's outputs returned to REF2021 have two or more co-authors from departmental academic staff.

Regional research collaboration is promoted through the N8 Universities network (including EPSRC-funded work) and the White Rose Consortium involving York, Sheffield and Leeds, which allocates PGR studentships to research projects involving staff from at least two universities (*IES §* 6). Nationally and internationally the Department collaborates across academia as seen in the Department's returned outputs, where 80% have at least one non-York author. Moreover, the percentage of all publications that include at least one international author grew over the REF period to >60% (*Fig 1-1*).

Collaboration and translation of key findings to academic and industrial end-users are aspects of many projects *e.g.* EU networks, knowledge exchange programmes, direct industry funding (including CASE schemes), and involvement in Knowledge Transfer Networks/partnerships (Moller). The Department actively encourages links to end-users. Examples include *Hubbard* who had a 40% contract with Vernalis during the REF period; **Lewis** is an NCAS Director, a long-term UKRI position which aligns atmospheric chemistry research with Government and industry end-users (100% externally funded contract); and the Department has two Royal Society Industrial fellows (**Fairlamb**, **O'Brien**).

There are many examples of collaborative research with outside bodies, which include the following:

1) Research on the discovery and dissection of enzymes for biofuels has been conducted by **Walton** and **Davies**, with Henrissat (CNRS Marseille, France). With techniques ranging from phylogenetics to EPR spectroscopy, the York and CNRS teams studied enzymes needed to create biofuels from plant wastes or energy crops, leading to an impact case study. The collaborative effort was recognised by the Institution of Chemical Engineers Global Energy Award (2016), and the RSC's Rita and John Cornforth Award (2020), the latter of which specifically recognises collaborative research.

2) GCCE participated in Europe's largest public-private partnership (CHEM21) dedicated to the development of manufacturing sustainable pharmaceuticals. The €26.4M (£21.2M) project, brought together six pharmaceutical companies, thirteen universities and four small-to-medium enterprises from across Europe, to develop sustainable biological and chemical alternatives to finite materials. The CHEM21 Metrics Toolkit provided a unified resource to evaluate the sustainability of chemical and bio-chemical reactions. A book '*Green and Sustainable Medicinal Chemistry: Methods, Tools and Strategies for the 21st Century Pharmaceutical Industry*' was led by **Clark**. Outputs from the project were shared publicly through an on-line learning platform.

3) The research in WACL is delivered as a collaboration between NERC and the university. NERC, through its centre NCAS, provides resources for the co-location of twelve research staff on a long-term basis (ten-year rolling contract ~£1M pa). Collaborative delivery of national capability in atmospheric chemistry is enhanced with DEFRA support and engineering consultancy (Ricardo), which collaborate on academic appointments (Moller and **Carslaw**). WACL collaborates with other government departments to deliver research on the broader issues of chemical hazard detection, with AWE plc for the national nuclear security programme, with Dstl on malicious materials detection and with BEIS on UK oil and gas emissions and the impacts of the development of shale gas in the UK. The labs have long-term links (*via* KTPs, and industrially-funded fellowships) with two instrument manufacturers, Markes International and Syft

Technologies who have commercialised York research (impact case study), and with Givaudan, who have provided support *via* equipment and multiple contracts for research in chemical metrology and indoor air chemistry. These collaborations have underpinned three impact case studies.

4) Renewable Solvents (ReSolve) is a €4.3M (£3.8M) York-led EU project (2017–2020; eleven partners from five countries) focused on replacing traditional, fossil-based solvents, with safer bio-based ones with high performance in applications and improved toxicity profiles. Two bio-based solvents, Cyrene and Cygnet, were developed departmentally, commercialised by Circa, who set-up a Yorkshire-based company enabling Cyrene supply internationally.

4.2 Contribution to the Research Base, Economy and Society (*IES § 18*)

The Department has wide-ranging collaborative research projects with industries, charities and government, many of which are exemplified by the Impact Case Studies (*Fig 4-1*). These ICSs are not repeated here, other than to highlight the breadth of impact reported therein: academic/commercial (crystallographic software), governmental policy and environmental (WACL research) and industry (enzymes). In another indication of the breadth of the Department's interactions with outside bodies, since the last REF period, departmental research has included 223 collaborative partners from 36 countries over six continents.

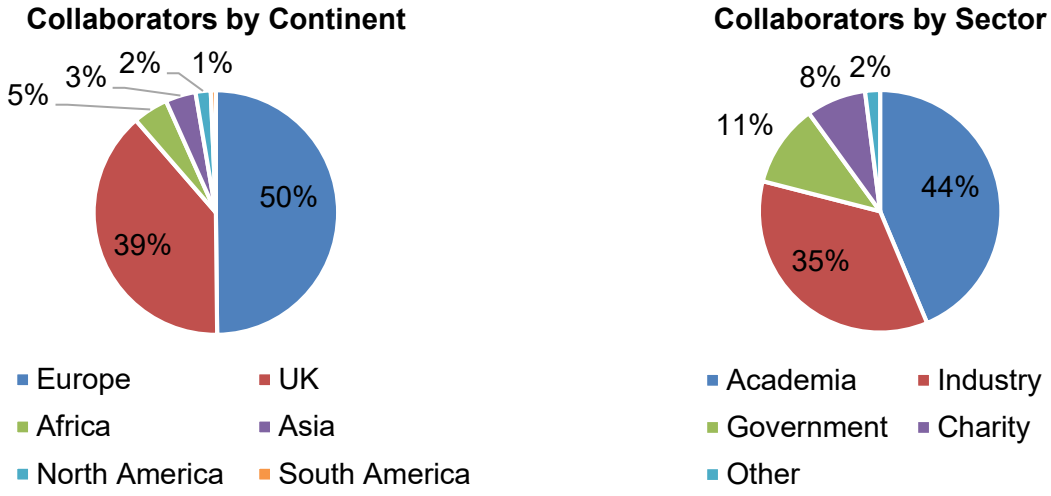

Fig 4-1. *Pie charts of collaborations by continent (left) and by sector (right), as a fraction of numbers of projects.*

To achieve this breadth and depth, the Department has put strategies in place to ensure that research reaches out beyond higher education. For instance, the departmental research committee incentivises PhD studentship bids that grow connections with either industry or major science facilities, *e.g.* STFC. Furthermore, departmental facilities and expertise are made available to outside users (local industry, schools, public), often planned as part of the original research proposals. Examples of these links from the REF period are as follows:

1) In *Green and Sustainable Chemistry*, expertise and equipment are offered to external organisations, in particular SMEs, to help them deal with chemical problems and to collaborate on joint research projects. These interactions often start as short contract projects but can lead to longer-term collaborations. An example of this approach is a small contract feasibility project (£14k) with Biome Bioplastics in 2014 where the Department assessed the potential to synthesise novel compostable plastic films from lignocellulose-derived monomers. The results led to a collaborative project (Innovate UK, 2016–19, £303k to York) and Biome have recently filed a patent on this family of new bio-based and bio-degradable polyesters.

2) York has a portfolio or activities linked to policy and public engagement. For example, WACL houses an NERC Knowledge Exchange Fellow (Moller) who focuses on impact in environmental policy and heritage management. Moller's fellowship (2018–2022) is the result of a long-term relationship with DEFRA. During the REF period, this has developed from a role leading the secretariat for the *Air Quality Expert Group* to providing liaison between the UK air quality science research community and the DEFRA Air Quality Team, advising them and research councils on strategic evidence needs for science and policy. Moller works directly with the Chief Scientific Advisor as a DEFRA Senior Fellow, supported by NERC, NCAS, DEFRA and the University, providing benefits to all partners, and creating new opportunities for evidence-informed policy and science with impact, for example enabling expert input from UK academics to the development of the *Government Clean Air Strategy*.

3) A Knowledge Exchange Fellowship (High, 2016–2020) engages and collaborates with the non-academic stakeholders Historic England and York Archaeological Trust, to maximise the translation of research to these bodies. A particular example here is the research carried out in the Department on the rapid deterioration of organic remains at the famed Mesolithic site of Star Carr. The work highlighted the need for the better use of scientific techniques in understanding when and why archaeological sites are at risk.

Response to COVID-19
Lewis provided direct advice to Government and SAGE on issues including emergency management of crematoria, and worked with the Office for National Statistics, DEFRA and PHE to quantify air pollution impacts on UK COVID-19 mortality. **Lee** engaged with media outlets including the BBC, *Daily Telegraph*, *The Economist*, *Financial Times* to provide real-time data visualisation of the effects of lockdown on urban nitrogen dioxide. **Carslaw** provided support to multiple government departments linking transport volume changes with pollution and weather data, including an early identification of non-linear effects during the lifting of travel restrictions, reported in *The Guardian* (front-page).

Contributions to Society (IES § 13)
Departmental staff engage whole-heartedly in outreach activities, with many researchers initiating activities both locally and nationally. The Department's commitment is demonstrated by having a long-term Departmental Schools Liaison and Outreach Officer. Distinctively, the Department supports CPD activities in science for primary teachers, as well teaching resources from the unique *Centre for Industry Education Collaboration*. Colleagues are encouraged to publicise their work, and the University collects annual data, ensuring that outreach is allocated in the departmental workload model. Examples include:

Smith is in demand as a schools' lecturer and influences policy and processes within science, particularly regarding diversity. He has a presence on Twitter (>20k followers) and YouTube , using the latter to explain the chemistry of a number of everyday experiences as well as providing some more specialised content. **Carpenter** delivers atmospheric chemistry lectures, including recent York research to A-level students (ca 2k students annually; Science Live). Moller, **Lee, Hamilton** and **Lewis** are all active in promoting debate around contemporary issues associated with air pollution, making multiple TV and radio contributions (Radio 2,4,5; World Service; Inside Science; The Inquiry; Costing the Earth; Newsnight; Trust Me I'm a Doctor; Channel 4 News), and publish regularly though The Conversation, reaching >350k readers in the REF period. All were active in 2020 supporting public understanding of the science linking air quality, aerosols and COVID-19. **Lewis** worked with Aardman Animations and broadcaster Marcus Brigstocke to produce an animated film on air pollution, released at the 2018 Hay Festival. **Cowtan** has been an advisor on the BBC 4 documentary 'Climate Change by Numbers' and has been active in explaining climate science to the public (Hay Festival, National Geographic website, New Scientist, BBC World Service, news article in *Science*).

4.3 Indicators of Influence

Prizes

Almost one third of staff (31%) have received prizes during the REF period. Election of **Davies** as Fellow of Academy of Medical Sciences and award of the Ken Murray Research Professorship, and the Fellowship of the American Association for the Advancement of Science (AAAS) awarded to **Perutz**. **Gai's** (FREng 2014) contributions to science were recognised by the Royal honour of Dame Commander of the British Empire (DBE) and being elected to a Fellow of the Royal Society (2016). **Carpenter's** leadership in atmospheric chemistry was recognised by election to a Fellow of the Royal Society (2019), a Royal Society Wolfson Research Merit Award (2018), and the Royal Society Rosalind Franklin Award and Lecture (2015).

RSC Prizes and Awards to **Davies** (Haworth Memorial Lectureship, 2018, Khorana Prize, 2014), **Bruce** (Peter Day Award, 2014), **North** (Green Chemistry, 2014), **Unsworth** (Hickinbottom Award 2018; RSC/BMOS Young Investigator Award, 2015), 2020), **Davies** and **Walton** (Rita and John Cornforth Award, 2020), **Walton** (Joseph Chatt Award, 2016), **Penkman** (Joseph Black Award, 2016), **Fairlamb** (Corday-Morgan Prize, 2016), **Carpenter** (Tilden Prize, 2017), **Clark** (Green Chemistry Award, 2018). **Duckett** (Tilden Prize, 2018), **Parkin** (Roger Parsons Medal and Sir Edward Frankland Fellowship, 2019), **Weller** (EPSRC Established Career Fellowship, 2015. Frankland Award 2016).

Davies was awarded a Royal Society Davy Medal (2015); **Davies** and **Walton** received the IChemE's Global Energy Award, 2016, **Walton** was awarded the 2020 Jubilee Professorship of Chalmers University, **Thomas-Oates** was named British Mass Spectrometry Society Lecturer (2019–2021) and Goodby awarded the Freedericksz Medal of the Russian Liquid Crystal Society and the Royal Society Royal Medal (2016). **Edwards** (*Nature* Research Awards for Global Impact. **A. Wilkinson** was awarded the International Prize of the Slovak Academy of Sciences (2015). **Penkman** was awarded the Blavatnik Award (2020) for Young Scientists. **Duckett** was co-recipient of the Laukien Prize (2020). Industry-facing research was recognised by the awards to Goodby (AkzoNobel UK Science Award, 2014), **O'Brien** and **Fairlamb** (SCI/industry-sponsored prizes for Process Chemistry Research, 2017 and 2019, respectively).

Panel Memberships

Staff are influential at UKRI: (**Carpenter** and **Lewis**, both NERC Panel Chairs, and **Carpenter** is a member of the Excellence Panel for the Evaluation of NERC Centres 2020 and UKRI Future Leaders Fellowships Panel Chair), STFC (**Lewis**, Panel Chair), EPSRC (**Duckett** and **O'Brien**, Panel Chair), internationally with the Academy of Finland (**Lewis**, Panel Chair; **Lee**, **Hamilton, Bruce**). Staff serve regularly as advisors to scientific panels; **North** is co-Chair to CO2Chem, which brings together researchers, industrialists and policymakers from across disciplines to utilise carbon dioxide as a feedstock. **Lewis** served as advisor to the Royal College of Physicians, NPL, AWE plc and UKRI and was invited to give evidence to multiple House of Commons Select Committees and Ministerial round-tables. **Evans** was an Advisor to NERC and the Met Office. **Lewis** and Moller are both members of the Natural Hazards Partnership, and chapter authors for the Cabinet Office National Risk Assessment. **Lewis**, Moller and **Carslaw** are all public appointments to the DEFRA Air Quality Expert Group, with **Lewis** Chair of that group since 2019. **Carpenter** is Chair of the World Meteorological Organisation (WMO) Global Atmospheric Watch (GAW) Scientific Advisory Group on Reactive Gases, a lead author of the 2014 and 2018 WMO/United Nations Environment Programme (UNEP) Scientific Assessments of Ozone Depletion and from 2020 a member of the Assessment Scientific Steering Committee. Staff have made panel contributions to the national Athena SWAN review group (**Walton**), EU iNEXT project (**Wilson**), Fundação para a Ciência e a Tecnologia, I. P. (FCT) - the Portuguese public funding agency (**Fairlamb**), ERC (**Dessent**), Hungarian National, Research, Development and Innovation Office (**Duckett**), Israel Science Foundation (**Duckett**), Wellcome Trust (**Antson**, **Thomas-Oates**), Ministry of Education Singapore (**Clark**), Royal Society (**Bruce**, **Davies**, **Duckett**, **Fairlamb**, **Perutz, Walton**), STFC-Central Laser Facility (**Perutz**), the Irish Higher Education Authority (**Walton**).

Current Research Fellowships (with Proleptic Appointment)*
Antson (Wellcome Trust Senior fellowship, 2nd renewal), **Agirre** (Royal Society University Research Fellow), Mahon (Marie Curie reintegration fellowship, 2019), **Avestro*** (RS Dorothy Hodgkin RF, 2019–2023), **Blaza** (URKI FL fellowship, 2020), **Carpenter** (ERC Advanced 2019–2024), **Davies** (Royal Society Ken Murray fellowship), **Edwards*** (independent funding from philanthropic support and then ERC Starting Grant, 2019–2024), High (NERC Knowledge Exchange Fellowship, 2016–2020), Moller (NERC Senior Knowledge Exchange Fellowship, 2014–2022; DEFRA Senior Fellow, 2019–2022), **Manfred** (NERC/DfT Independent Research Fellow, 2019–2023), **O'Brien and Fairlamb** (Royal Society Industry Fellowships), **Penkman** (ERC Consolidator, 2020–2025), **Unsworth*** (Leverhulme Trust, 2016–2019; Eleanor Dodson Fellow from 2019), **James** and **L. Wilkinson** (Leverhulme Trust Early Career Fellows, 2019–2021), **Willems** (ERC Starting Grant, 2019–2024).

Contributions to Learned Societies
There are 26 entries for council membership, Advisor, Trustee or Chair of a Learned Society, with major contributions made to the Royal Society of Chemistry and the Royal Society, and 23 staff have been involved in Editorship or Editorial contributions.