Institution: University of Oxford

Unit of Assessment: 8 – CHEMISTRY

1. Unit context and structure, research and impact strategy

*All data refer to the REF period unless otherwise stated. (**Bold bracketed numbers**) refer to sections.*

1.1 Context and structure

1.1.1 Our vision

"Research in Oxford Chemistry focuses on fundamental science aimed at making major long-term impacts. We provide an environment that enables research by hiring, nurturing, and retaining talented researchers, many recognized as international leaders, across a broad spectrum of chemical sciences. Enabled by inspiring students and staff, and excellent research facilities, we undertake world-leading research crossing traditional boundaries, which engages with other disciplines, both within Oxford and across a range of external sectors. Our commitment to realising economic and societal impact from fundamental research is evident from our many industrial and clinical collaborations and our commercialisation activities."

1.1.2 Research structure

UoA8 comprises 88 Category A researchers, 86 with research based in Oxford Chemistry, one of 10 departments of the Mathematical, Physical, and Life Sciences (MPLS) Division. The Department is subdivided into three Sections, Inorganic, Organic (including Chemical Biology), and Physical & Theoretical Chemistry, each with an elected Head.

In 2015 we restructured to promote our aims of excellence in teaching and research, with appointments of Associate Heads in Teaching and Research (AHoD(T) and AHoD(R)). The AHoD(R) chairs a new *Chemistry Research Committee* (CRC), which enables research synergies (internal and external to Chemistry), identifies funding opportunities, and encourages and supports individuals in new breakthrough initiatives. The AHoD(R) engages with other Oxford departments through the MPLS Divisional Research Forum.

The *Chemistry Management Board* (CMB), which includes the AHoD(R) and AHoD(T), provides academic leadership, and is advised on strategy by the *Chemistry Departmental Committee*.

1.1.3 Research themes

Our eight research themes, introduced in the last REF, help coordinate activity, facilitate collaboration, and focus research on large-scale challenges. The themes reflect both our traditional strengths and new fields of major societal importance. Our collaborative network promotes multidisciplinary research (**1.4** and **4.5.1**), as reflected in the themes sketched below (Figure 1).

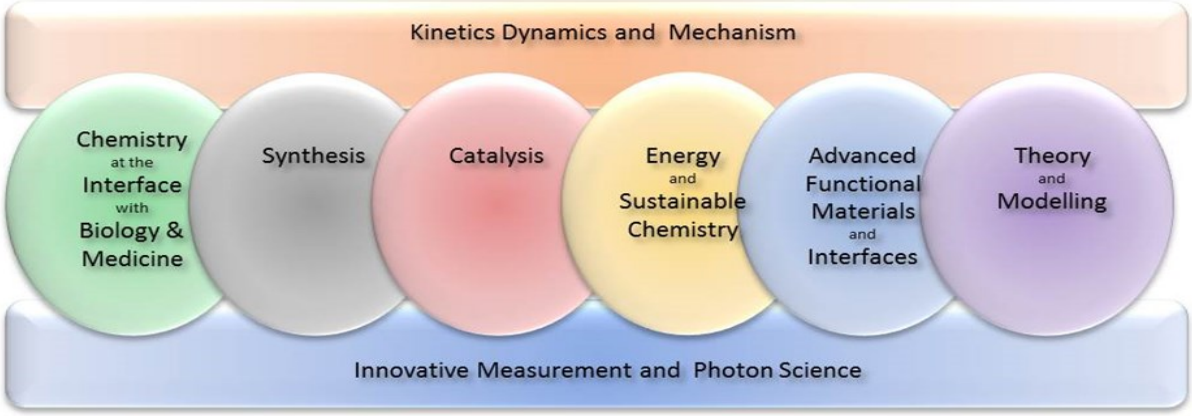

Figure 1: *Schematic of the research themes and their principal interconnections*

(Note that permanent academic staff (PAS), independent early career fellows (ECFs – typically on 5-year fellowships), and academic appointments can be in multiple themes. Category A staff numbers are as at July 2020, whilst appointments refer to the REF period.)

T1. Catalysis (29 PAS, including 2 new appointments): *Developing and understanding new catalytic processes to make societally-important products, materials, and chemicals more efficiently and with more precision.*

T2. Synthesis (32 PAS, including 1 new appointment, and 3 ECFs): *Producing new chemical compounds by reaction from simpler materials, through the invention of new reactions, catalysts, and techniques*.

T3. Chemistry at the interface with biology and medicine (39 PAS, including 3 new appointments, and 3 ECFs): *Applying chemical methods to observe, quantify, exploit, and re-programme the mechanisms of life.*

T4. Energy and sustainable chemistry (18 PAS, including 1 new appointment): *Using chemistry to inform scientific strategies and underpin clean and green sustainable technologies that improve our environment and mitigate climate change.*

T5. Kinetics, dynamics, and mechanism (32 PAS, including 2 new appointments, and 3 ECFs): *Developing and using advanced analysis methods to understand chemical transformations at the molecular level.*

T6. Advanced functional materials and interfaces (31 PAS, including 3 new appointments, and 3 ECFs): *Discovering, understanding, and developing new advanced functional materials in order to provide solutions in critical areas such as energy, healthcare, electronics, and catalysis.*

T7. Innovative measurement and photon science (37 PAS, including 3 new appointments, and 5 ECFs): *Quantifying structure and dynamics from the atomic to the mesoscopic scale.*

T8. Theory and modelling in the chemical sciences (27 PAS, including 3 new appointments, and 2 ECFs): *Applying theory and computer modelling in the chemical sciences to elucidate problems at the interfaces with physics, materials science, and biology.*

1.2 Research objectives and strategy

1.2.1 Review of the REF period

We have focused on the **research objectives** defined in our REF2014 submission (in bold), briefly reviewed below.

1. **To further our research profile by appointing, training, supporting, and retaining the best people (faculty, research, and technical staff) to carry out world-leading research.**
   We have appointed eight PAS, including creating one new post, supported 14 ECFs, and provided leadership in the *Technician Commitment* initiative. We have supported colleagues for promotion, merit pay awards (**2.3.5**), and prizes/accolades (**4.6**). We have undergone major cultural change through our equality, diversity, and inclusion (ED&I) initiatives, enabling more diverse recruitment at all career stages (**2.2** and **2.5**).
2. **To develop our eight research themes.**
   We have refined our research themes and appointed theme coordinators, who have identified areas for strategic appointments and who are a focus for external enquiries, e.g., from industry and government. The themes are promoted through collaborative funding (**3.1**), graduate training (**2.4**), researcher co-location, leadership appointments, and publicity. Strength across the themes is illustrated by the quality and scientific breadth of our ~3,800 publications in the period (including nearly 200 papers in the *Science* and *Nature* family journals), which have received >80,000 citations.
3. **To develop our strong relationships with other MPLS departments, and with biological and medical sciences.**
   2,540 (66%) of our papers have co-authors from outside the Department, demonstrating our collaborative and interdisciplinary research (**4.1** and **4.5.1**). Of these, >13% involve collaborations with other Oxford departments. Collaborations are promoted through our continued joint academic appointments, joint grants, and multidisciplinary centres for doctoral training (CDTs), e.g., the Wellcome Trust *Chemistry in Cells* (WTCIC) CDT (**2.4**).
4. **To build and sustain long term strategic and effective engagement with industry and other external partners (e.g., Diamond Light Source, Rutherford Appleton Laboratory, and Harwell Science and Innovation Campus), capitalising on the success of existing collaborations.**
   We have strengthened our collaborations with industry (e.g., with *Siam Cement Group* (SCG), *Union Chimique Belge* (UCB), and *Siemens*), and with other external partners (e.g., the *Harwell Campus*, and the *National Physical Laboratory* (NPL)) (see **4.1** and **4.5.1**). As a result, >270 (7%) publications are joint with industry and a further 7% are with staff from UK research facilities.
5. **To ensure that research facilities and core instrumentation match our ambition to remain a world-leading centre for innovative Chemistry.**
   Research equipment has been purchased totalling nearly £18M (**3.3**), and we have invested a further £2.5M in facilities. In 2018, we opened a new £25M Chemistry Teaching Laboratory (CTL), which includes dedicated synthetic and analytical suites used for graduate training. The latter alone represents an additional £2M investment in state-of-the-art instrumentation.
6. **To attract world-class postgraduates and PDRAs by providing a leading research environment, high-quality training, and scholarships.**
   We have seen a ~45% increase in postgraduate research (PGR) applications, due to development of our PGR programmes (**2.4**), including CDTs (the WTCIC, and our EPSRC

CDTs, namely *Synthesis for Biology and Medicine* (SBM), *Oxford Inorganic Chemistry for Future Manufacturing* (OxICFM), and *Theory and Modelling in the Chemical Sciences* (TMCS)), and enhanced training facilities (e.g., the CTL). The generation of increased industry funding has enabled significant postdoctoral research assistant (PDRA) recruitment (**2.2**).

7. **To advance translation of our work through spinouts, licensing, patents, consultancy, and multi-company industrial collaboration, taking full advantage of our strong track record.**

   The translation of our research is evidenced by numerous industrial collaborations and successful spinouts (see **4.2** and **4.3**). We have generated 11 spinouts (cf. three in the previous REF); in 2019/20 our 21 active spinouts collectively employed >700 people and had a turnover of ~£57M.

1.2.2 Future research objectives

We will focus on the following *key goals and objectives during the next REF* period:

O1. Refill statutory chair/research leader positions with outstanding candidates from across the world to **enhance academic leadership across the breadth of our research themes**. With 48% of our faculty aged 50+ (**2.2**) we anticipate a significant number of retirements over the next REF period. Appointments will be supported by development activities, which have already led to the endowment of the Chair of Physical Chemistry.

O2. Enhance our research themes by **creating four new permanent academic posts and refilling ~20 existing posts** (equating to around three per research theme), with a particular focus on outstanding researchers active in interdisciplinary, strategic, global challenge areas such as materials, energy, sustainability, infectious and ageing-related diseases, and climate change.

O3. Advance **interdisciplinary initiatives**, such as the INEOS-Oxford Institute, the Oxford *Kavli Institute for NanoScience Discovery (Kavli INSD)*, which lies at the heart of a new multidisciplinary laboratory, the national *UKRI Catalysis Hub*, the *Rosalind Franklin Institute* (RFI), and the *Faraday Institution* (FI). We will forge stronger links with *Harwell* and *Diamond* through joint appointments, secondments, and collaborations.

O4. **Strengthen links to industry**, through our doctoral training initiatives, by organizing workshops, providing co-located space for partners from industry, and promoting engagement through industrial guest lecturers, advisory board representation, industrial secondments, and materials transfer with commercial research laboratories.

O5. Increase the proportion of departmentally-funded PGRs by supporting **~50 new PGR studentships** through engagement with funding agencies, key stakeholders and industry, and through a combined major University/College fundraising initiative. This will enable a more strategic approach to graduate recruitment.

O6. Enhance research facilities to enable high-level academic appointments, including developing and bringing forward plans for a new **interdisciplinary chemical sciences laboratory** to facilitate co-location with partners from other cognate disciplines and industry.

O7. Develop our instrument and workshop **Small Research Facilities (SRFs)**, investing in equipment and supporting our technicians.

O8. Enhance the impact of our research through coordinated **public engagement** activities.

Our research support staff – including two full-time *Chemistry Research Facilitators*, a *Research Information and Support Officer*, a *Development Manager*, and our *Alumni Relations and Communications Manager* – will enable delivery of these objectives.

1.3 Impact

1.3.1 Enabling impact

We have an outstanding track record in translating fundamental research to effect major change beyond the confines of the discipline: e.g., ground-breaking work on the lithium-ion battery, rapid DNA sequencing, and a pioneering glucose sensor all emerged from curiosity-driven research.

To *enable and facilitate* impact arising from our research we have:

- *Commercialized our research* through spinouts, patents, and commercial deals (**4.3**), with help from our *Research Facilitators*, and close links with *Oxford University Innovation* (OUI – the University's technology transfer office) and the MPLS *Industrial Research Partnerships* (IRP) team (**4.1** and **4.2**);
- *Engaged with external partners* to highlight and increase the relevance of our research, e.g., through industry engagement in graduate training, including *EU International Training Networks* (ITNs), CDTs, CASE and iCASE (**2.4**);
- *Collaborated extensively with industry*, for example, on research and development (R&D) of novel instrumentation and methods, and in drug discovery;
- *Promoted a culture of impact*, by encouraging nominations for *impact awards*, both internal and external to the University (**2.3.5**), showcasing impact and links with industry through our *Industry Newsletter* and our podcasts and videos, such as the *Solutions for our Future* (ITN Productions) and *Technician Commitment*;
- *Promoted entrepreneurship* through our diverse impact and IP training programmes (**2.4**), including hosting *visiting lectureships and professorships* (**4.2**);
- *Enhanced* impact through *Public Engagement with Research* (PER) and educational outreach activities (**4.4**);
- *Reflected* the importance of impact in *recruitment and retention* policies (**2.3.5**).

1.3.2 Shaping impact plans for the future

We shape and adapt our *plans* to ensure we continue to support the vitality and sustainability of our impact. Our response to the COVID-19 pandemic provides a good example of how we can adapt to a changing external landscape (**4.5**).

In the *next REF period*, we will further embed impact through the following activities:

I1. Enhancing *commercialization of our fundamental research*, through our strong links with OUI, support for academics with secondment and sabbatical arrangements, and our training for young entrepreneurs;

I2. Building stronger and larger *relations with industry*, supported by our Research Facilitators, through co-location of researchers, R&D, workshops, etc. (see Objective **O4**);

I3. Supporting the *symbiotic relationship* between our fundamental research, and the translation of that activity to generate societal and commercial impact, in the latter case through interactions with our spinout companies and industrial partners;

I4. Enhancing interactions with industry and promoting impact through *graduate training;*

I5. Promoting a *culture of both societal and commercial impact* by recognizing and celebrating success, and rewarding staff as part of our professional development strategy (**2.3**);

I6. Enhancing our *Research Facilitation Team* by focusing resource on impact and PER, e.g., through a PER 'expert in residence', embedded in the Department through academic engagement and by inclusion on CRC;

I7. Developing our *communications strategy*, building on the ongoing redevelopment of our website and supported by our *Alumni Relations and Communications Manager.*

1.3.3 Impact Case selection for REF2021

Our *Impact Cases* (ICs) provide exemplars of how we have translated fundamental research into real world benefit. Our strategy to promote commercialization led to the IC on *Oxford Nanopore Technologies* (ONT) [04Bayley], which developed the portable *MinION* DNA sequencing device used on the Zika and Ebola viruses, and more recently in high-throughput testing for COVID-19 (*LamPORE*); impact is enhanced through ongoing, symbiotic links between the company and research group. ICs concerning our spinouts *Refeyn* (Mass Photometry) [06Kukura] and *OMass Therapeutics* [03Robinson] both arose from fundamental research and industry collaboration in mass spectrometry (MS) and instrument development (theme **T7**).

Commercialization of research through the creation of intellectual property (IP) and licensing agreements, an area that we have strongly supported (**4.3**), enabled the development of the *Electrochemical sensors* IC [02Compton], with products now being marketed.

The *Oxygenases* [05Schofield] and *SCG-Oxford Centre of Excellence in Chemistry* (CoE) [07OHare] ICs reflect our strategy for forming strong links with industry, forged by hosting researchers from industry in our laboratories (e.g., from UCB and SCG), and industry engagement with our CDTs.

Our final selected IC, *Quantum Mechanical Calculations: Supporting the Destruction of Chemical Nerve Agents*, again reflects fundamental research, namely in theme **T8**, in which graduate training plays an essential role. This IC [01Clary] overlaps with the TMCS CDT, which has links with several external partners, including *Dstl Porton Down*.

1.4 Interdisciplinary research

Section **4.5.1** details support for, and exemplifies, our *interdisciplinary research*. Our focus is to promote collaboration through interdisciplinary research networks, seminars, joint appointments, and leadership roles on special initiatives. Interdisciplinary research often arises from individual collaborations, supported by our theme leads and dedicated Research Facilitators, who provide advice on funding and other opportunities, such as external collaborations. We work closely with the MPLS IRP team, whose remit is to develop links between industry and multiple academic departments (also see **4.1**).

1.5 Open research

We are engaged with University and national initiatives to promote *open research*. We appointed a dedicated *Research Information and Support Officer* in 2018. Through a combination of training, monitoring, and 1:1 advice, the role supports all aspects of Open Access publishing and Open Data, including compliance with institutional and funder policies and use of the University's online repository for both publications and data. We actively promote the *Green Route* to OA, encourage the use of Oxford-linked ORCIDs as a unique author identifier, and help ensure compliance with the deposition of electronic theses for all doctorates.

We also support several key initiatives within Chemistry. Our SBM CDT operates an Open IP and OA policy designed to ensure free exchange of information and expertise between all partners and the wider research community, and the CDT's course material is freely available to download (typically with ~900 downloads per month). We also host open-source software for molecular dynamics simulation; and provide OA data and software for crystallographic refinement and analysis, and interpretation.

1.6 Research integrity

We support a culture of research integrity across the Department. All researchers are required to follow the University's *Academic Integrity in Research: Code of Practice and Procedure*.

Research integrity education begins with an induction programme for all new researchers (including 4th Year MChem and PGR students), covering plagiarism, and data security and storage. Subsequently, we encourage participation in the MPLS Division's *Research integrity* training, which introduces good practice in research, outlines how researchers can meet their responsibilities, and sets out the key principles and practices of good research conduct. Strict compliance with relevant ethics procedures is upheld for research involving human samples (monitored by the Biological Safety Officer).

2. People

2.1 Overview

We host around 1,000 researchers, ranging from permanent academic staff (PAS) to 4th Year MChem students undertaking full-time research (Table 1). In between are those on fully-independent (typically five-year) fellowships (ECFs), early career researchers (ECRs), and PGR students. ECRs include those holding individual fellowships of 2-3 years duration, including Marie Curie Fellows (68 during the REF), but who are not yet fully independent. PAS comprise statutory chairs, associate professors (APs), and research-only professors (RPs). We host many visiting researchers, including PGRs, senior academics, and scientists from industry.

We employ around 35 technical and research support staff, key amongst whom are those working in one of the five instrumentation and three workshop SRFs (**3.3**). Oxford was a founding signatory of the *Technician Commitment* (2017), a *Science Council* initiative to support research technicians, and Chemistry provided the first institutional lead (Mackenzie).

PAS	ECFs	ECRs	PGRs	UGs
Permanent academic staff (chairs, research professors, associate professors)	***Early Career Fellows*** (independent 5-year fellowships	***Early Career Researchers*** (PDRAs and holders of individual 2/3-year fellowships)	***Graduate research students*** (largely doctoral students)	***4th Year MChem students*** (undertaking full-time research projects)
70	10	200	450	180
Visiting researchers 100				

Table 1: *Typical numbers of research staff and students.*

2.2 Recruitment and staffing strategy

Our strategy is to hire and retain the best staff possible, and to support individuals at key career transition points.

During the REF period there has been a small growth in PAS (~4%), but larger growth (17%) in ECRs and ECFs, driven in the former case by an increase in external funding, and in the latter by strategic investment in a dedicated *Research Facilitator* and better communication of the application process (**2.3.2**).

We made eight AP appointments during the period: four replaced staff who retired or moved to other HEIs (e.g., Weller to a Chair at York; Wallace to a research-leader position at King's College London); three vacancies resulted from promotion of existing postholders to RP positions; and one new post was created. Three of these AP appointments were female, and three were to academics based outside the UK (ETH Zurich (1), Stuttgart MPIs (2)). Potential areas for recruitment are now discussed widely in the Department, with decisions about appointments driven by research priorities as well as teaching need (see **3.2** for examples). We have used RP appointments to provide individuals with the freedom to focus on research.

All our Category A staff are on permanent contracts except a small number on fixed-term, part-time contracts (three in July 2020) and our ECFs (seven). We rely on external short-term funding, so the majority of our ECRs are on fixed-term contracts. Where we expect funding to continue for the foreseeable future, and there is a clear sustainable business case, an open-ended contract is used.

PAS turnover in the period was relatively low, in part reflecting the quality of our environment. Most AP appointments were of academics at a relatively early career stage, allowing us both to attract new talent and maintain a balanced *demographic profile*. However, with 48% of our PAS aged 50+, we anticipate a larger number of retirements during the next REF, including four statutory chairs. This offers a significant opportunity for strategic academic recruitment to ensure continued research leadership and shape our research portfolio (see Objectives **O1** and **O2**), with our new cross-Departmental approach to appointments laying the foundation for successful appointments.

2.3 Staff development

2.3.1 Overview

The national *Researcher Development Concordat* is implemented *via* Oxford's Code of Practice for the Employment and Career Development of Research Staff. Initiatives developed under Athena SWAN (AS) (**2.5.1**) have also helped to embed good practice.

APs and ECFs are line-managed by the Section Heads, who play an important mentoring role. APs have a 5-year probationary period, during which an advisor is appointed and they receive two formal reviews. Deadlines for these reviews have been relaxed during the COVID-19 pandemic. The review after two years provides an opportunity to identify actions and support needed for successful completion of probation. ECFs are given similar levels of support. All probationary APs have successfully completed their reviews in the REF period.

All PAS have an annual appraisal, whilst ECFs and ECRs have an annual *Career Development Review*, a scheme tailored to their needs. Chemistry has pioneered an online system to facilitate the review process. Alongside the support provided by research groups, we are also introducing more systematic mentoring for ECRs.

Staff are supported to take advantage of the wide range of development activities provided by the University. MPLS provides training designed for PGRs and ECRs, including on entrepreneurship and writing research/fellowship proposals. ECRs can also participate in departmentally-provided courses for PGR students (**2.4**).

We promote external initiatives such as the Royal Society (RS) Pairing Scheme, *Week in Westminster* (Farley, ECR 2018). We provide ECRs with opportunities to gain experience in teaching and in educational outreach (**4.4**), to raise their awareness of public engagement and support transferable skills development.

We hold an annual *Chemistry Careers Conference* for ECRs and PGRs, typically with around 40 participants. Covering careers within and outside academia, the programme includes sessions on CVs, job applications, and modern recruitment methods. We also fund ECR attendance at external events such as the RSC *Curie-Joliot Career Conference*, which focuses on breaking down barriers for under-represented groups in academia.

2.3.2 Support for and integration of those at early career stages

We strongly support early-career academics: new APs usually have teaching remission (typically up to 50% teaching remission for two or three years) to enable them to establish their research. We provide start-up funds of >£150k (e.g., for equipment, ECR resource, and consumables). We support applications to the University's John Fell Fund (JFF) for new equipment, pump-priming activity, or match-funding for external grant applications. Newly-appointed academics have received six awards from this fund in the period, totalling £520k, and our ECFs have obtained a further £230k. In addition to the direct funding support, the JFF offers valuable training in grant writing and project management.

We are committed to attracting and developing outstanding young ECFs, particularly those who complement or strengthen our themes (e.g., Kukura (**T3**), Foroozandeh (**T7**)). In 2016 we established new advertising and recruitment procedures, and employed a *Research Facilitator* explicitly to help ECFs, ECRs, and PGRs at key career stages. They provide advice on

fellowship applications and wider career development support; and hold weekly drop-in sessions (typically supporting over 60 staff and students each year). During the REF period, there have been 14 ECFs, seven of whom were in post on the census date. Four of the remainder were appointed to Oxford PAS posts, and three to similar posts elsewhere.

Integration of ECRs into our research culture has been enabled by establishing a Postdoc Forum (2015) and a Postdoc Committee (2019), and through appointing an ECR academic champion (2017). These activities, together with ECR representation on committees, ensure ECR opinion is considered in developing Departmental policy. During the first COVID-19 lockdown, the Head of Department held dedicated open (virtual) sessions for PGRs and for ECRs, each with over 100 participants.

We encourage ECR-led activities, e.g., seminar series, poster competitions, and networking events, for which we provide financial and logistical support. The *Women in Oxford Chemistry* group was launched in 2019 with such support.

2.3.3 Research, impact leave/sabbatical leave arrangements

PAS with teaching responsibilities (APs and chairs) are entitled to one term of *sabbatical leave* for every six terms worked, to enable a break from teaching or administrative duties to focus on research. 46 PAS have taken sabbatical leave in the period.

Workload allocation models enable us to adjust duties when PAS take on leadership roles, such as large-scale research projects or CDT directorships. Those undertaking significant administrative duties have reduced teaching loads to enable them to continue research. Overall, around 20 PAS have been supported in this way. For other staff, impact leave is arranged on an *ad hoc* basis with their line-manager.

2.3.4 Facilitating exchanges

PAS can use their sabbatical leave to spend time at other institutions or in industry, and we have used EPSRC Impact Acceleration Account (IAA) funding to support long-term visits of this nature. For example, in 2015 O'Hare spent his sabbatical year with *SCG Chemicals* in Bangkok, Thailand, leading to the creation of the *SCG-Oxford* CoE (**4.1.2**). We support secondments: in 2019/20, Kukura was 50% seconded to his spinout company, *Refeyn*, to provide consultancy at a critical juncture; and currently, Mohammed is 80% seconded to the RFI.

We have secured around £190k of EPSRC IAA funding for *Partnership Awards*, designed to encourage engagement with end-users of research. Such funding has supported development of an electrochemical bacteria sensor (Compton) and translation of sulfoximine catalysis to the pharmaceutical sector (Willis).

We also have a vibrant visitor programme enabling interactions with industry (**4.2**).

2.3.5 Recognition and reward

We recognize and reward PAS through two University mechanisms. In the REF period, 27 of our APs have been awarded full professor title through an annual *Recognition of Distinction* (RoD) scheme. We have mentored female APs to encourage them to apply, which has been a large contributor to us moving to 15% female full professors by 2019 (up from 6% in 2013). Since

2016, those with full title are also eligible to apply for *Professorial Merit Pay* through a biennial University-wide scheme, with 12 recipients in Chemistry.

Grade 9 and 10 research staff are eligible for award of AP title through an annual University recognition scheme, with several instrument scientists awarded title in the period (**3.3.5**).

Both research and impact are taken into account when considering academic appointments and promotions: commercial or public engagement activities are assessed alongside the applicant's research portfolio. High-profile promotions of entrepreneurial scientists illustrate the importance of these factors (e.g., Schofield, O'Hare to RPs).

We publicise the successes of our researchers, both internally (e.g., *via* our weekly newsletter) and externally (e.g., in social media, our *Periodic* magazine and *Industry Newsletter*, and special videos), including showcasing their successful start-ups. We ensure colleagues are nominated for appropriate prizes (**4.6**). We have received five MPLS *Impact Awards* (O'Hare, Vincent, Brown (2015), Booth (2018), Kukura and Benesch (2020)). A positive work environment is further enhanced by celebrating historical success of former staff, e.g., the *2019 Nobel Prize* for Goodenough (former Inorganic Chemistry chair) and Whittingham (former student), and the American Chemical Society (ACS) *Chemical Breakthrough Award* (2015) for Dorothy Crowfoot Hodgkin's work determining the structure of penicillin.

2.3.6 Supporting and enabling staff to maximize impact

In addition to leave arrangements (**2.3.3**), within the standard University contract all academic and research staff (including ECRs) can undertake up to 30 days consultancy for external organisations. 63 such staff have held consultancies in the REF period, facilitating collaborations between academia and business (**4.1** and **4.2**).

In addition, *staff are enabled to maximize impact* by:

- Enhancing their *entrepreneurship* through hosting *Innovation Champions* (five ECRs and ECFs trained by OUI to advise and mentor colleagues), providing *IP* and *Science communication skills training*, supporting the *Student Entrepreneurs' Programme* (StEP, allowing students to develop innovative business ideas), and hosting a RS *Entrepreneur in Residence* (Dr Alan Roth);
- *Adjusting workloads* through buyouts, to participate in external boards to enable impact, *e.g.,* industry boards, government, and charities (e.g., Wellcome, CRUK).

2.4 Research students

2.4.1 Overview

Graduate students are vital to our research and their training is a key contribution to the health of the discipline and to the wider economy. We run four main programmes leading to a DPhil (PhD) in Chemical Biology, Inorganic, Organic, or Physical & Theoretical Chemistry. During the REF, we have led three EPSRC-funded CDTs and the WTCIC CDT. We also participate in around six cross-departmental UKRI-funded CDTs.

2.4.2 Recruitment

Our annual DPhil intake is ~100 students, including ~30 on CDT programmes (~6 of which are on cross-departmental CDTs). 51% of our PGRs are non-UK residents (18% EU, 33% other

overseas). Applications have increased by over 45% (Table 2), largely reflecting the popularity of our CDTs. We hold three open days to help attract a diverse range of applicants. Interviews are held for candidates applying for scholarships and CDT places. Most successful applicants have a first-class UG degree (or equivalent).

2013/14	2014/15	2015/16	2016/17	2017/18	2018/19	2019/20
297	389	389	342	351	411	441

Table 2: *Chemistry PGR application numbers.*

We provide an inclusive culture taking account of all *protected characteristics*, where necessary making adjustments tailored to individual needs. For those with a physical or learning disability we hold detailed discussions about any adjustments required. We support the University UNIQ+ scheme (a summer graduate access research internship programme), hosting one project in 2019 and mentoring seven students in the online 2020 programme. The WTCIC CDT is currently operating a blind recruitment process, which will be assessed for wider roll-out.

2.4.3 Studentship funding

Figure 2 provides a typical snapshot of PGR funding for the cohort starting in 2016/17 (with 106 starters). Whilst research councils (UKRI) provide 24% of the external funding, there is a variety of funding sources, and a significant proportion of students are either self-funded or funded through University scholarships. Around 5% of studentships are CASE awards, with a further 25% of our EPSRC DTA studentships having partial industrial support. In the REF period, we have also been awarded 19 EPSRC iCASE DTA studentships allocated strategically by the MPLS Division to encourage industrial collaborations.

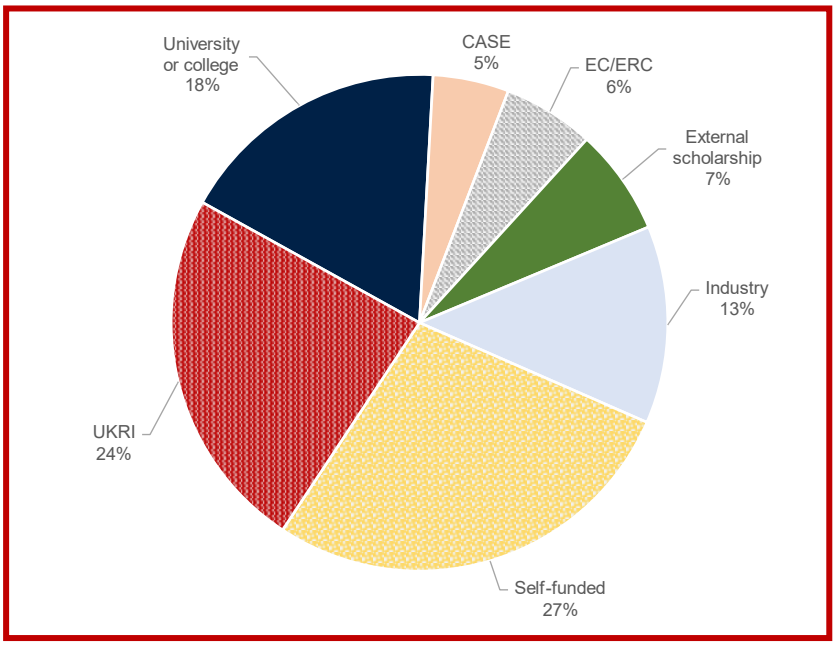

Figure 2: *Summary of PGR student funding sources for cohort starting in 2016/17.*

We have hosted three competitively awarded EPSRC CDTs in the REF period, which have attracted considerable funding from industry: e.g., the SBM CDT secured industrial support (>£4.5M) to enable an Open IP research collaboration to be established with 11 global companies. The CDT is funded by EPSRC until 2022, but with a new cohort from 2019/20 funded through a combination of industrial (~£2M), philanthropic, Departmental, and University

support. Strong industrial support has also been realized for the new OxICFM CDT, with eight industrial partners. In addition, our EU ITNs have industrial links: we have coordinated four ITNs during the REF period and participated in 12 others.

Supported by our *Development Manager* since 2017, we have launched a campaign to fund PGRs through philanthropy and other means (see Objective **O5**). With the availability of funding the greatest barrier to entry, this will enable us to attract and support a more diverse pool of talented students.

2.4.4 Monitoring and support mechanisms

Programmes are overseen by one of three Chemistry Directors of Graduate Studies, who monitor supervision arrangements, review termly reports, troubleshoot any concerns, and organize examinations. Students receive considerable formal and informal supervision and are expected to have regular one-to-one meetings with their supervisory team. WTCIC CDT and cross-departmental CDT students typically have co-supervisors from outside Chemistry. First-time supervisors receive mentoring support from an experienced co-supervisor. We also run workshops for new supervisors.

PGRs are formally assessed around the end of their first and their third years of research, for which they submit written reports and give presentations. These provide an opportunity to review progress and obtain advice on the steps required for successful completion.

In Chemistry, the *rate of completion* within four years is around 85%, and ~95% of DPhil students complete their degree, mostly within five years. Typically, just under 100 DPhil degrees are awarded annually (Table 3).

2013/14	2014/15	2015/16	2016/17	2017/18	2018/19	2019/20	Grand Total
91.3	106	97.8	97.5	88.3	99.7	97.5	678.1

***Table 3:** UoA8 doctoral (DPhil) degrees awarded.*

2.4.5 Skills development and future careers

We aim to engender in our PGRs the skills and qualities required to become outstanding researchers, to educate them with a broad understanding of the subject and its relevance to the major global challenges, and to equip them for successful careers both inside and outside academia.

PGRs have access to a wide variety of training, helping them to develop research and transferable skills. We provide a choice of introductory courses, including in nuclear magnetic resonance (NMR), MS, and X-ray crystallography, and in IT, mechanical workshop, and glassblowing skills. CDT and masters' level courses are also available to all PGRs (where capacity permits). The MPLS Division provides training courses which have had >1,600 Chemistry attendees over the REF period, including on scientific writing (213 attendees), thesis and report writing (83), scientific entrepreneurship (44), and presentation skills (176).

PGRs can also develop teaching skills through practical demonstrating on the UG course, and delivering UG classes in mathematics, physics, and quantum chemistry. Training is given for each of these activities.

PGR training needs are reviewed termly as part of the reporting process. Students are expected to keep a portfolio of training received, which is reviewed at the formal assessment milestones.

We hold a wealth of regular seminars which PGRs are encouraged to attend. Research themes and groups also organise their own meetings, e.g., in Chemical Biology and Soft Matter, which students sometimes organize themselves. As part of the formal assessment process, Sections organise PGR student symposia, in which 3rd year students give a short talk.

Towards the end of their programme, PGRs are encouraged to talk to the University *Careers Service*, which has a designated Chemistry contact. DPhil graduates go into a *wide variety of careers*. Typically, nearly 40% stay in academia, becoming ECRs, with a further 20% pursuing research careers in industry or other non-university environments. Just over 10% of PGRs follow careers in management, with the remaining 30% pursuing careers including medicine (5%), teaching (4%), and IT (2%).

2.5 Equality, Diversity, and Inclusion (ED&I)

2.5.1 Overview

ED&I issues are now central to Departmental life and are a standing item on all committee agendas. We have a Chemistry E&D Committee, which has broad membership and is chaired by a member of CMB. It has led initiatives that enabled us to achieve an AS Silver award in 2015 (renewal submission due November 2020).

Our 2020 ED&I Action Plan includes a focus on ethnicity and race. We have recently appointed an ED&I Fellow who has a particular interest in race-equality issues, and we encourage participation in University networks, including BME, Disability, and LGBT+. Since the last REF, BME representation in the researcher population has increased from 16% (July 2013) to 22% (July 2020). Additionally, we have placed increasing focus on neurodiversity, e.g., publicising activities around *Neurodiversity Celebration Week*.

The University has well-developed policies and procedures covering all aspects of human resources. Recently revised academic recruitment procedures explicitly aim to increase the diversity of those shortlisted for and offered jobs. The proportion of women in PAS posts (chairs, full professors, and APs) has risen from 9% in 2013 to 16% in 2019. During the REF period, 36% of our ECFs were women, and the percentage of female ECRs increased from 31% in 2016 to 35% in 2019. Female PGR applications rose from 37% in 2016 to 42% in 2019, with the percentage of female starters rising in line with this.

An important emphasis has been on improving Departmental culture, with consideration given to work/life balance and to supporting returners after breaks. Whilst there is more to be done, our annual survey data indicate real progress (e.g., 90% of respondents would now recommend the Department to a friend, c.f. 58% in 2012). There is greater visibility of the existing diversity within Chemistry, including through staff profiles featured on the website. We actively promote the achievements of women, such as *Women in Science* awards (**4.6**). Our female academics are increasingly taking on leadership roles, including co-directing CDTs, serving on CMB, or leading spinout companies (three out of the 11 Chemistry spinouts founded in the period).

2.5.2 Consideration of ED&I issues

In areas such as promotion, reward, and recruitment, we give explicit consideration to ED&I. All recruitment panel members undertake ED&I and implicit bias training, and a gender balance is also sought for all recruitment/promotion panels. Most leadership positions (e.g., Heads of Section and Department) are by election, with a preliminary process to encourage candidates to come forward, particularly from underrepresented groups. Decisions about access to internal and, where necessary, external funding are generally taken by CMB, with ED&I issues explicitly discussed.

CMB is made up of *ex officio* members, and at one time all academic members were male. To address this, after consultation with a group of our senior women, a female academic "without portfolio" was added to the committee. From October 2020 the AHoD(R) role will be held by a female academic, further improving the gender balance on CMB.

2.5.3 Leave and flexible working

Entitlement to *sabbatical leave* (**2.3.3**) is consistent for all eligible PAS. Staff are reminded regularly of their entitlement and applications for sabbatical leave are very rarely declined.

Flexible working is encouraged, and many staff change their working patterns, either formally or informally, as their caring and other responsibilities change (e.g., in 2019, 12 academic and research staff were working part-time). We have clear support mechanisms for all those returning to work, e.g., from parental leave (**2.5.4**). The recent experience of the COVID-19 lockdown has led us to explore how remote working can be supported, and this will be carried forward into more normal times.

The support described above is available to all staff regardless of their contract. We have shown our commitment to promoting *part-time flexible* working by a joint campaign with Somerville College, raising around £380k to support an ECF designed for individuals returning from a career break and/or needing flexible working arrangements. The first such Fellow will start in January 2021.

2.5.4 Support and wellbeing

Individuals returning from leave arising from ill-health, disability, or caring responsibilities are offered tailored support. Workload is often reduced in the first year after return, and part-time/flexible working offered. We sponsor four University nursery places. A PGR maternity-pay policy was introduced in 2018, with Chemistry covering the cost if grant-providers do not.

Individuals are encouraged to apply to the University's *Returning Carers Fund*. All nine ECR/academic women who returned from maternity leave during the REF period have received grants from the fund (totalling £42k), including paying for additional researcher support, equipment, administrative support, and additional childcare to enable *conference attendance*.

We publicise the support available for staff and students with *protected characteristics* and, working together with the University's *Disability Advisory Service* (DAS), take a case-by-case approach to ensure that support is tailored to the individual. In consultation with the DAS, adjustments have been made to research laboratories and, on occasion, personal support provided.

Wellbeing is an increasingly important focus for us, particularly with respect to mental health. Responses to staff and student surveys suggest that the measures implemented have been beneficial (e.g., 90% of staff say they are satisfied in their job). A comprehensive guide to the support available is included on our intranet and has been highlighted on its front page during the COVID-19 pandemic.

Since 2014, we have used the national *Anti-Bullying Week* to highlight the issue and run a series of events such as *Think Differently - Choose Respect* (2018) and *Change Starts Here* (2019). Those with concerns about bullying or harassment can seek advice and support from one of five Departmental *Harassment Advisors*. Our achievements have been recognised by MPLS ED&I Awards, including *Best Initiative* for our *Anti-Bullying Week* activities.

2.5.5 ED&I and the REF process

In line with Oxford's REF 2021 Code of Practice, our primary criterion for output selection was research quality, based on an academic-led peer review process.

Eligible staff nominated up to six outputs, which were read and scored by at least two reviewers, with a sample of scores calibrated by external reviewers. A diverse and balanced output selection review panel was established, comprising CMB and five other academics. Explicit consideration was given to diversity in the reviewing team, and in decisions made on output selection, such as the gender balance of selected outputs (~20% female) versus that of submitted staff (18% female).

3. Income, infrastructure, and facilities

3.1 Research funding

3.1.1 Overview

At the census date our research grant portfolio was over £120M, with an average annual research grant income during the period of £28.5M (up 57% compared to REF 2014 - Table 4). Average annual industry funding increased very significantly (by over 300% to >£5M), reflecting our impact strategy. Annual income from UKRI remained broadly constant over the period, whilst EU income increased significantly (by nearly 250% to an average of >£7M), with 19 major ERC grants commencing (three Starting Grants, six Consolidator, six Advanced, one Synergy, and three Proof of Concept Grants). Sources of funding are now significantly more diverse than in REF 2014.

UoA8	REF 2014	REF 2021
Average annual income	£18.2M	£28.5M

Table 4: *UoA8 average annual research income.*

Significant industrial sponsors have included SCG (£12.3M), UCB BioPharma SPRL (£1.7M), UCB Celltech (£0.8M), and Novo Nordisk A/S (£0.7M).

Our spinouts have invested significantly in our research, including OxSTEM (£4M), ONT (£1.9M), and Osler Diagnostics (£1.7M), reflecting the synergy between our fundamental research and its translation through the company (**1.3.2**).

3.1.2 Major grants and links to quality output or impact

Table 5 lists our top ten competitively awarded (non-industry, non-CDT) grants in the period. The selection includes a range of funders (EU, UKRI, charities), and both single investigator and collaborative grants (e.g., EPSRC Programme and EU Synergy grants).

Oxford PI	Start date	Funder	Grant type	Amount (£k)
Conway	01/10/2019	EPSRC	Programme	5,019
Hore	01/04/2019	EU	Synergy	3,370
Vincent	01/01/2016	EPSRC	Standard	2,941
Goodwin	01/10/2018	EU	Advanced	2,587
Brouard	07/04/2020	EPSRC	Programme	2,544
Robinson	13/02/2015	Wellcome Trust	Senior Investigator	2,366
Hore	01/12/2013	EU	Advanced	2,212
Gouverneur	01/07/2019	EU	Advanced	2,000
Bayley	01/08/2019	EU	Advanced	1,942
Fletcher	01/05/2016	EU	Consolidator	1,873

Table 5: *Chemistry major (non-industry) grants awarded in the REF period.*

Exemplifying links with quality outputs and impact, Hore's funding supported fundamental research into the mechanism of bird migration resulting in highly-cited work in *Nature* and elsewhere, whilst Robinson's supported research underpinning the *OMass* IC. Vincent's EPSRC grant supported fundamental research into new routes to drive enzyme-catalysed chemical synthesis using hydrogen.

3.1.3 Strategy for generating income

Our *strategy* seeks to enhance funding by:

- Supporting applications for *major funding* by providing relief from teaching and administrative responsibilities, through buyouts and secondments;
- Raising awareness of opportunities *via* our dedicated *Chemistry Research Facilitation and Grants (Finance) teams*, provide advice and feedback on draft proposals, and practice with interviews;
- Through CRC and CMB, focusing attention on *high-level funding initiatives*, such as EPSRC/BBSRC equipment initiatives, and making prioritization decisions on bids;
- Supporting greater use of *University-administered funding* to provide follow-on funding for technology development and for secondments or partnerships (**2.3.4**). During the REF period, we have received 30 awards totalling £1.4M from IAA funds (EPSRC, BBSRC, and Global Challenges Research), and we have secured nearly £4M from University funds, including £2.2M from the JFF and ~£600k from the Oxford Martin School, adding significant impact to grants obtained from external sources;
- Through the work of our dedicated Research Facilitator, *supporting those applying for ECF funding* (**2.3.2**);
- Promoting *income diversification* (e.g., through increased EU and industry funding), by highlighting opportunities, providing support for initiatives, and publicising our links with industry in our industry-facing webpages and regular *Industry Newsletter*;

- Enhancing our *philanthropic activities* through the support of our Chemistry *Development Manager*, who has catalysed a six-fold increase in annual philanthropic income, with over £2M being received since 2017 (funding equipment, studentships, and the endowment of a statutory chair). Philanthropy will be a focus of activity during the next REF (see **O1** and **O5**).

3.2 Organisational infrastructure supporting research and impact

The AHoD(R) and CRC provide a strategic focus for considering new funding initiatives (e.g., for equipment), promoting support for researchers, particularly at early career stages (**2.3.2**), and developing initiatives to support the SRFs (**3.3.2**). The theme coordinators also help identify funding opportunities. As a result, we have invested significantly in the underrepresented area of Materials Chemistry (two academic appointments, one a newly-created post), and strengthened capability in Theoretical & Computational Chemistry (making academic appointments in Computational Organic Chemistry, Computational Inorganic Materials, and Electronic Structure Theory).

Co-location of researchers to reflect our research themes is increasingly a priority. Such clustering of activity is illustrated by the co-location of researchers involved in the EPSRC Programme Grant, *REDOX* (PI: Conway), and in the new interdisciplinary *Kavli INSD* (Director: Robinson; see **4.5.1**).

Our *Chemistry Research Facilitation* and *Grants* teams also provide support for research and impact. They work closely with Divisional teams to develop interactions with funding agencies and industry.

3.3 Operational and scholarly infrastructure supporting research

3.3.1 Buildings

Research is currently located in three main buildings, with 65% of staff housed in our modern Chemistry Research Laboratory (CRL). Over the next REF, a key objective is to develop and bring forward proposals for a new research laboratory to replace the other two ageing laboratory buildings (see Objective **O6**).

During the period, we invested over £2.5M in laboratory refurbishments. This includes newly-purposed space for biological NMR (Baldwin), new MS facilities (Robinson), an interferometric scattering microscopy (iSCAT) facility (Kukura), a new diffractometer (Goodwin), an ultracold chemistry laboratory (Heazlewood), a soft condensed matter laboratory (Krishnan), a mass selective ion deposition laboratory (Rauschenbach), inorganic synthesis facilities (Williams, Edwards), and new imaging MS and femtosecond dynamics laboratories (Burt, Brouard, Mackenzie, Vallance). A new facility for high performance computing has also been created.

3.3.2 Instrument and workshop facilities

Our instrument and workshop SRFs provide vital elements of research infrastructure. The instrument SRFs include dedicated facilities for MS, NMR, electron spin resonance (ESR), chemical crystallography and magnetometry, and surface analysis; whilst the workshop SRFs include the glassblowing, mechanical, and electronics facilities.

A key objective has been to increase the level of SRF costs recovered from external grants with a view to improving their long-term financial sustainability. This has increased more than three-

fold during the REF period to ~£600k in 2019/20. Paid work for external users (totalling >£800k over the period) has also been undertaken by the SRFs where capacity has allowed (**3.3.8**).

3.3.3 Specialist research infrastructure and facilities

In addition to the SRFs, we host a radiochemistry laboratory (Gouverneur), which provides labeled radiopharmaceuticals for Positron Emission Tomography scanning research. We also host some of the most sophisticated MS facilities worldwide, including a new mass photometry facility (Kukura). We have substantial Chemical Biology facilities, which have supported the fundamental research leading to two of our ICs.

3.3.4 Equipment investment

During the REF period, we have invested nearly £18M in equipment. This includes >£4.6M spent on cutting-edge instrumentation costing >£50k, essential for the SRFs, funded primarily from UKRI and EU sources (£2.2M), Wellcome (£1M), and institutional co-investment (£1.3M). A significant fraction was for core and advanced NMR, magnetometry, diffractometry, and MS equipment, in the latter case to establish high-sensitivity IC-MS methods (£1.6M), and to enhance bioscience research (£1.2M). Our researchers and SRF leads work closely with instrument manufacturers not only to get good value, but also to develop novel instrumentation, as reflected in four of our ICs.

Through the work of the Development team, we have received ~£350k in donations for research equipment, including £120k to support ECFs and new APs.

3.3.5 Technical and support staff

Having a strong team supporting our core activities is critical, and recruitment and retention of staff is essential. Of our 35 technical staff, the instrument SRFs have seven senior staff (Grade 8 or above, including five SRF managers), and seven technical staff (Grade 7 or below). Four senior instrument SRF staff have received AP or full professor title in the REF period (Cooper, McCullagh, Claridge, Mohammed).

Seven technicians are employed in each of our mechanical and electronics workshops. We recently employed an apprentice in the latter and plan to recruit one also in the mechanical workshop. The work of our technical staff is recognised both internally and externally. Two workshop staff received Honorary MAs in the period. Our glassblower (Adams) was profiled nationally in both *Chemistry World* and *The Guardian*, raising awareness of issues around training, recruiting, and retaining qualified scientific glassblowers. She was also invited to the *House of Lords* in 2017 to an event highlighting the importance of science technicians.

3.3.6 IT support

Our IT is maintained by eight staff. In addition to providing day-to-day support, they also lead on special initiatives, such as introducing electronic lab books and electronic sign-on for the SRFs. The team leads in providing data storage and automated backups, and also supports our high-performance computing (HPC) facilities, including clusters, workstations, and software. The clusters, used particularly by our theoreticians, provide for both serial and parallel computing, as well as massive memory systems, and are housed in a new purpose-built cooled server room (costing £180k). This service complements the HPC provided by the University, such as the *Advanced Research Computing* service.

3.3.7 ED&I related to access to funding and infrastructure

In support of ED&I initiatives (**2.5**), the Facilitation team mentors ECRs in applying for independent fellowships: the gender balance of our ECFs on the census date (over 40% female) suggests that this investment in support has been effective. We have a buyout scheme for PAS requiring time to apply for major grants, including those requiring extra support, e.g., due to caring responsibilities. Typically, around 20 colleagues have buyout arrangements at any one time. We have also strived to ensure that our main decision-making committees (e.g., on space allocation) have a diverse representation in terms of career stage, gender, etc..

3.3.8 Use of infrastructure, facilities, and expertise for impact

Our interactions with industry are often initiated though the external work undertaken within our SRFs (**3.3.2**). For example, links with UCB Celltech were catalysed through the work undertaken in the EPR facility, leading to three publications and around £800k in total funding. ECRs from UCB have also been co-located with researchers in the CRL. Interactions with SCG (one of our ICs) have also been enhanced through the access we provide to our SRFs, and the laboratory space made available to SCG on a commercial basis at the University *Begbroke Science Park*.

Access to novel instrumentation is often an initial driver for impact activities, as exemplified by the *Mass Photometry* IC, in which early access to prototype instrumentation was provided in the Kukura group, leading to the spinout of the company *Refeyn*.

3.3.9 Shared infrastructure

We make significant use of shared UKRI-supported facilities, such as *Diamond*, *ISIS*, and the *Lasers for Science Facility*, with associated average annual UKRI income-in-kind of >£1.8M in the REF period. For example, the *UKRI Catalysis Hub* (Williams, Davis, Aldridge, Vincent), which brings together 27 UK HEIs and industry, involves shared labs (*Research Complex at Harwell*) and beamtime. We also make use of UKRI co-funded facilities located outside the UK, including the *European Synchrotron Radiation Facility* and the *Institute Laue Langevin*.

Staff from other UK HEIs often make use of our unique facilities, including in MS, ESR, and NMR. Developing links with the *RFI* and *FI* (**4.1.2**) offers further opportunities for sharing infrastructure, with the former particularly in MS and MS imaging.

3.3.10 Major benefits-in-kind

During the REF, companies have supplied in-kind equipment support equivalent to over £1.1M, e.g., from *OMass* (£150k to support MS as a platform for drug discovery), and the *SR Thermo Fisher* commercial venture (£715k Orbitrap MS as part of a collaboration to develop metabolomics technologies). There have also been significant donations of equipment in the CTL analytical suite (£160k).

3.4 Non-UKRI infrastructure and facilities

We make considerable use of non-UKRI funded facilities, totalling well over ~125 days, including FLASH (DESY, Hamburg), SACLA (Free Electron Laser (FEL), Japan), SLAC National Accelerator Laboratory (Stanford University, USA), the FHI FEL Facility (Max Planck, Germany), ANSTO (Australia), KOALA (Laue neutron diffractometer), SNS ORNL, and FERMI (FEL Radiation for Multidisciplinary Investigations, Italy).

4. Collaboration and contribution to the research base, economy, and society

4.1 Collaborations

4.1.1 Support for collaboration

Collaborations are supported by joint appointments, secondments, and sabbatical leave (**2.3.3** and **2.3.4**). We have three joint academic appointments with other Oxford departments, Oncology (Brown), Pharmacology (Russell), and Biochemistry (Mohammed), and externally with the *ISIS Neutron and Muon Source* (David). Joint appointment (B Davis) and secondment (Mohammed) arrangements with the *RFI* further enhance interactions with the Harwell Campus.

Collaborations are facilitated by networking activities established with Departmental or institutional seed funding: these bring together researchers from multiple departments, and sometimes external partners. We lead or participate in the *ChemBioPlants* hub, *Comp Chem Kitchen* (**4.2**), and the *Oxford Energy* and *Oxford Photonics* networks. The latter forged a collaboration between Chemistry (Vallance) and Materials (J Smith) resulting in the formation of the spinout *Oxford HighQ*, winner of the *Institute of Physics* Business Start-Up Award (2020).

We support collaboration by hosting ~100 visitors at any one time, including those on external schemes such as Newton International Fellowships (11 during the REF). Student visitors on the Erasmus scheme and other exchange programmes provide a vibrant community of international researchers.

Our *collaborations with industry* are supported by the SRFs providing analytical services (**3.3.8**), partnering in doctoral training (**2.4**), and facilitating joint research initiatives, licencing agreements, and consultancies. We also encourage and support applications for BBSRC and EPSRC IAA and other translational funds (**3.1.3**). We showcase our industrial partnerships through an electronic *Industry Newsletter,* published twice yearly and circulated to nearly 200 subscribers.

Three PAS participate in the multidisciplinary *Oxford Suzhou Centre for Advanced Research* (OSCAR), based in Suzhou, China. This aims to enhance collaboration with Chinese industry and research institutions. Our OSCAR chemists have recently patented a surface modification technology which imparts antibacterial, antiviral, and antifungal activity. The first Chinese spinout company, *OSCoat*, is being created to commercialise application to personal protective equipment and commercial collaboration is planned for the scale-up phase.

4.1.2 Effectiveness of research collaborations

In the REF period, 2,540 (66%) of our papers included co-authors from outside Chemistry and 43% had international co-authors. The vibrancy of our collaborations with the wider University is demonstrated by our joint publications (480; 13%) and joint funding (totalling nearly £48M), with links to the Medical Sciences (£35M) and MPLS (£12M) departments being particularly strong.

We are involved in several collaborative EPSRC programme grants. Conway leads a grant in *REDOX* chemistry (with partners from Oxford Oncology, CRUK/MRC, and KCL). Oxford chemists have also been co-investigators on four programme grants led by another Oxford department (e.g., Materials, Physics) or another HEI (including by Bristol (£2.4M to Oxford) and by Heriot Watt (£2.5M to Oxford), both with Brouard, Vallance, and Mackenzie).

We contribute to several multi-institutional initiatives. In addition to the *UKRI Catalysis Hub* (**3.3.9**), we also have close ties with the *FI* on battery research: Williams is involved with *SOLBAT* (led by Bruce, Oxford Materials); Clarke, Hayward and Goodwin are co-investigators on *FutureCat* (led by Sheffield, with around £1.4M to Oxford); David, through his joint appointment with STFC, is involved in *NexGENNA*. We are partners in research themes of the *RFI*, including Next Generation Chemistry (B Davis, Mohammed), and Biological MS (Benesch, Brouard, Burt, McCullagh, Rauschenbach, Robinson, Vallance).

The effectiveness of our *industrial collaborations* is illustrated by our PGR training programmes (**2.4**), with which companies actively engage and benefit from the research our students undertake. Our industry partners are also keen to recruit our qualified PGRs once they complete: e.g., over half of those SBM CDT students who have thus far completed (42 in total) have taken up positions in the pharmaceutical industry.

Specific examples of our *successful collaborations with industry* include:

- *Siemens & Tsang,* developing new catalysts for a green ammonia process powered by renewable energy, and establishing the world's first such pilot plant (with colleagues at STFC and Cardiff, supported by the MPLS IRP Team);
- *SCG & O'Hare,* supporting the *SCG-Oxford CoE*, which has generated ~70 publications during the REF, over £15.7M investment by SCG in the UK, licensing to SCG of four Oxford-developed technologies, granting of 37 patents, and the award of the RSC Industry-Academia Collaboration Award (2019);
- *Unilever & Williams,* collaborating on testing new polymers, i.e. making, testing and understanding the performance benefits of sustainable and degradable polymers in formulations and products;
- *UCB BioPharma & Schofield, Dixon, Willis, Smith and Paton,* a collaboration arising from links with the SMB CDT which led to the discovery of new late-stage functionalisation methods to modify drug-like molecules, e.g., *Linezolid*, an antibiotic used to treat bacterial pneumonia;
- *Waters Corporation & Benesch,* developing next-generation labelling methods for MS instrumentation to elucidate the structure of proteins and their interactions, particularly with respect to biotherapeutics and drug-discovery.

4.2 Interaction and engagement with research users, beneficiaries, or audiences

We promote interaction and engagement with research users through PGR training (**2.4**), research conferences, industry-sponsored symposia/prize events, and academic involvement on company boards and advisory roles. We hold research grants and contracts with industry and provide analytical services to our partners. We also support sabbatical leave and secondment arrangements to enable such collaborations (**2.3.3** and **2.3.4**).

We regularly host *visiting professorships*, including Vipul Patel (Head of Flexible Discovery Unit, GSK), Ian Churcher (GSK), Malcolm MacCoss (facilitating links with UCB), Allen Orville (UK XFEL Hub leader, Diamond), Henrik Mouritsen, (Universitat Oldenburg, collaborator on Synergy Grant), Jeffery Penfold (ISIS:STFC collaboration), Vernon Gibson (President's Envoy, Imperial College

London), Tadhg Begley (Texas A&M University; Newton Abraham visiting professor), and the annual Hinshelwood visiting lectureship (e.g., Joanna Aizenberg, Harvard (2016/17)).

51 of our 88 Category A staff were directly involved with commercial activities and consultancy. Over 20% of our annual research income is generated from industrially sponsored research and these interactions have led to >270 joint papers (7%) with industrial co-authors in the REF period. In addition, we engage with research users and beneficiaries by:

- *Advising industry*, e.g., Schofield (Member, Syngenta scientific advisory board), Goicoechea (consultant to BASF), Dixon and Smith (scientific advisory board for Avra, India), and Compton (Senova advisory board);
- *Enhancing the performance of our spinouts* through new research (see **1.3.2**, activity **I3**), e.g., reinvestment of over £2M by ONT in Bayley's research to advance DNA sequencing;
- Hosting 29 *industrial funded studentships* from 19 different companies totalling £5.4M, providing both research support and potential future employees (**2.4**);
- *Co-organizing and hosting a series of public computational chemistry meeting*s, *Comp Chem Kitchen*, encouraging engagement with industry which has resulted in new partnerships and iCASE studentships (with Vertex and Evotec).

4.3 Wider activities and contributions to the economy and society

We created 11 spinout companies in the period (cf. three in the last REF period). As of July 2020, University investments in the 21 active spinouts from Chemistry were valued at £20.1M. Investments in ONT (**1.3.3**) alone were valued in Jan 2020 at £12M, with ONT itself valued at £1.7Bn. In the REF period, our active spinouts (including those incorporated before the REF period) have secured well over £650M in follow-on funding; and during 2019/20 they employed >700 people and generated a combined turnover of ~£57M.

Further evidence of our *wider activities and contributions to the economy* include:

- Filing 453 *patent applications* (205 granted to date), with a further 335 PCT and Priority filings, a significant increase in total on the previous REF;
- Completing 170 *consultancies*, 75 *commercial deals* (generating around £150k per annum), and a further *44 assignments* (of IP and other entities);
- *Supporting industry through R&D*, with >180 industrially funded projects involving >60 different companies, with REF period research income totalling £37M.

Our *fundamental research frequently impacts on wider society*, particularly in the medical arena, from Bayley's development of the first synthetic retina to Farrer's work on less invasive treatments for paediatric brain cancer. Other examples include:

- *J Davis* – developing diagnostics and protocols to assay disease biomarkers, leading to the spinout company *Osler* (2016) producing a universal healthcare diagnostic;
- *Wong* – developing new environmentally sustainable methods of producing grapefruit flavouring, brought to market in 2018 by spinout *Oxford Biotrans*, and being used by two top flavour and fragrance companies;
- *Edwards* – 2017 spinout *Oxford Sustainable Fuels* transforming plastic waste into transportation fuels, providing a viable route to utilise waste previously left for incineration or landfill.

We have also *influenced society* by advising external bodies, for example:

- *Influencing Government*, e.g., Schofield (Scientific review of DSTL and MoD through the Defence Scientific Expert Committee), Williams (partner, World Economic Forum, *Global Plastic Action Partnership*; participant in HM Treasury's *Plastics Call for Evidence*);
- *Serving as expert witnesses*, e.g., Donohoe, Brown, Adlington, Schofield (patent revocations and disputes), and Aldridge (advisor to the UK Government's Environment Agency on chemical contamination);
- *Presenting to policy makers*, e.g., Vincent and Reeve (exhibited at the EPSRC *Science for a Successful Nation Showcase*), and Williams (co-authored three RS policy briefings, including *Synthetic carbon-based fuels for transport*; led the *CS3 Symposium and white paper* on *Science to Enable Sustainable Plastics*; attended the RS Lord Prior Discussion on *The UK Industrial Strategy*; and presented to Parliament on the *Plastic Waste Challenge*, engaging with ~50 attendees including MPs, industry, and NGOs).

4.4 Engagement with diverse communities and publics

We engage with the wider community through social media. Our *Twitter* feed has ~18,000 followers, and frequently engages with science journalists, researchers, and the general public. We host a popular *Facebook* page with over 5,000 followers, and our website typically receives 7,000-12,000 visitors per day.

Our *Alumni Relations and Communications Manager* and *Educational Outreach Officer* promote our research to external audiences and support PER activities. We publish an annual magazine, *Periodic*, circulated to around 8,000 alumni and publicly available through our website, which highlights our research. Amongst other activities, our *Educational Outreach Officer* promotes our research to those of school age (e.g., the *Electrochemical Sensors* IC), typically making around 30 schools visits per year, and hosting visits of both teachers and pupils to our laboratories.

We support PER through training, and by providing opportunities to participate in PER events at local and national levels. A PER committee with an academic lead (Cooper), reporting to CRC, develops our PER strategy, and supports initiatives such as awarding two £2K bursaries annually (to fund projects to develop activities) and establishing a science communication training event for students to produce PER infographics. We work closely with the MPLS Division through its PER facilitator, with over 80 Chemistry staff/students attending MPLS training sessions.

We have contributed to multiple PER initiatives including:

- *Held exhibitions* at the Oxford University Museum of Natural History, e.g., *Bacterial World* (Flashman) and *Biosense* (Schofield), which were seen by 175,000 and 245,000 visitors, respectively; and Museum of the History of Science, e.g., *Back from the Dead* (Schofield);
- Participated in *public engagement events*, e.g., *Oxford Open Doors* (annually) with themes including *Chemistry for a Sustainable Future*, *Cardiac Chemistry*, and *Chemistry for Cancer Research*, in total attracting nearly 400 participants; *Crystallography Ideas Cafe* at *Cheltenham Science Festival* (2015), involving a panel discussion with 30 members of the public; and *Curiosity Carnival* (Reeve), part of European Researchers' Night (2017);
- Engaged with the *media*, e.g., BBC radio's *The Life Scientific* and *Woman's Hour* (Robinson, 2014);

- *PER seed-funded projects*, e.g., Reeve (concerning *HydRegen*) was awarded an MPLS-BSA Media Fellowship to spend a week at *The Mirror*;
- *Production of video animations* (e.g., *Shedding Light on the Situation* (Heazlewood) and *What can Chemists learn from Nature?* (Vincent)) and *podcasts* (e.g., *Robert Robinson's Chemical Box*, *Learning from Nature* (Vincent), *How do you turn plastic in to fuel?* (Edwards), *How garlicky is your garlic?* (Compton), and *The Fastest Camera in the World* (Vallance and Brouard)) *via* the Oxford Sparks online science engagement portal;
- Involvement in *International Year of Crystallography* (2014), e.g., the *Crystals at the Garden* exhibition at the Oxford Botanic Garden, involving eight Oxford Chemistry research groups, which was subsequently included in a public exhibition in Toronto during an international crystallography congress.

Many such activities involve or are led by female chemists, who thereby act as excellent role models for women considering studying or working in science.

4.5 Contribution to the sustainability of the discipline

We contribute to the sustainability of the discipline by training MChem and PGR students and ECRs. We help shape national policy, e.g., through roles in the RSC, including the presidencies of the *RSC* (Robinson), and its divisions (Conway, Vallance, Brown, B Davis), and the *Heads of Chemistry UK* (Softley, Brouard) and its standing committee (Brouard). We participate in advisory boards and on UKRI colleges and prioritization panels (EPSRC, STFC, ERC). Colleagues are frequently asked to give invited lectures and seminars, and actively participate in journal reviewing and editing (**4.6**).

4.5.1 Support for and exemplars of interdisciplinary research

We support *interdisciplinary research* through our collaborations across the University and with external partners. These are enabled by our involvement in multidisciplinary networking initiatives and joint appointments (**4.1**), and cross-departmental/divisional CDTs (**2.4**).

Links with other Oxford departments are strengthened by roles on advisory boards (e.g., Robinson as scientific advisory board member for Oxford Biochemistry), joint academic appointments, and jointly-funded projects. Collaborations with colleagues in the Medical Sciences Division alone have generated over 350 papers (9%) during the REF period. We have strong links with the *Target Discovery Institute* through Huber and Brennan (both returned within UoA8), who are PAS in the Nuffield Department of Medicine. They are frequent collaborators with Chemistry (e.g., Kawamura, Flashman, Schofield, Dixon, M Smith, and Conway) in a range of fields including hypoxia, epigenetics, and cancer research.

In the period, we published more than 650 papers (17%) with members of other national and international facilities and institutes, including over 250 with UK research facilities such as *ISIS* and *Diamond*. Our industrial partnerships provide additional impetus for cross-disciplinary research.

Further support for and examples of *interdisciplinary research* include:

- *Training PGRs* through our CDTs and other programmes (**2.4**), e.g., the WTCIC CDT (joint with Oxford Pharmacology, the Francis Crick Institute, the RFI, GSK, Janssen and Merck, Sharp & Dohme UK), the OxICFM CDT (with over 40 academics from across MPLS, eight

industrial partners, two national facilities, and 17 international institutions), and our EU ITNs (e.g., DiSTRUC, with partners in Physics and elsewhere);

- *Collaborative work involving multi-disciplinary teams*, e.g., Williams and Imperial College London teams working with *Shell* to deliver catalysts transforming CO_2 to dense energy carriers, like methanol;
- *Jointly-funded projects and collaborations*, e.g., Flashman (with Plant Sciences), Kawamura (Oncology), Schofield (Medical Sciences Division, XFEL Hub at Diamond), Conway (King's College London), and Brouard, Vallance and Mackenzie (Bristol and, separately, Heriot Watt);
- *Leadership of interdisciplinary initiatives* such as Robinson's directorship of the new *Kavli INSD*; involvement in the *FI* (Clarke, Hayward, Goodwin, Williams, David), and the *RFI* (B Davis, Mohammed);
- *Nominations for awards and prizes* (**4.6**), e.g., Schofield (RSC Interdisciplinary Prize for work on the activity and resistance to antibiotics).

4.5.2 Responsiveness to national/international priorities

We have responded to national/international priorities, including addressing the recent challenge of the COVID-19 pandemic, e.g.:

- *Circular economy*, a growth departmental activity in the REF period, e.g., Williams (sustainable routes to new polymers), Edwards (plastic waste to fuels);
- *Energy security/sustainability*, e.g., Tsang (catalysts to generate new energy vectors), David, Clarke, Hayward, Goodwin, Williams (novel battery technology), Compton (Oxford Martin Programme on Monitoring Ocean Ecosystems);
- *Strong economy/manufacturing*, e.g., EPSRC OxICFM CDT – providing doctoral training to increase capacity and capability in future manufacturing and materials (**2.4**);
- *Food security*, e.g., Flashman (plant oxygen-sensing enzymes and the molecular response to flooding, supported by €1.9M ERC Consolidator grant); B Davis (with Rothamsted Research, a chemical yield enhancer based on a natural sugar);
- *COVID-19 response activity*, including grants totalling over £1.1M (from UKRI, University and other sources) supporting six research groups during the first wave of the pandemic. Colleagues also served on NHS COVID-19 working groups (Brown - Manufacturing Industry Coalition and the Molecular Diagnostics Consortium) and collaborated in clinical trials (McCullagh, with partners in Oxford and Edinburgh).

4.6 Wider influence, contributions, and recognition

4.6.1 Wider contributions to the research base

We *contribute to the research base* through *training highly skilled* PGRs, ECRs, and visitors. They contribute directly to research whilst in the Department, and many continue to do so after they leave (**4.1.2**).

We further *contribute to the research base* by:

- *Disseminating research through publication* (>3,800 papers during the period, receiving on average 20+ citations per paper), and *presenting plenary lectures, invited talks, and research*

seminars, with over 1,000 invited lectures, and over 50 visiting professorships and lectureships in the REF period;

- *Engaging in peer review activities* for journals;
- *Serving on UKRI colleges and panels,* e.g., more than 25 academics serve on the EPSRC College and regularly participate on prioritization panels;
- *Participating on grants committees*, e.g., Perkin (RS panel member for Newton International Fellowships); Compton (ERC Starting, Consolidator and Advanced Grant panels); and Timmel (Foreign member of German Research Foundation Priority Programme – EPR).

We make wider contributions to research by *influencing research policy*, e.g.:

- *Serving on UKRI strategic advisory teams and panels,* including Williams (EPSRC *Manufacturing the Future* SAT), Brouard (STFC EPSAP), and Brown (BBSRC *Exploring new ways of working* SAP);
- *Supporting the RSC*, e.g., President (Robinson), Divisional Presidents (Vallance, Conway, Brown, B Davis), and Council membership (Brown);
- *Supporting external institutions and facilities,* e.g., Clary (chair, review committee of the *Max Planck Institute*, Heidelberg), Compton (scientific advisory board, *Centre for Spectroelectrochemistry*, *Leibniz Institute*, Dresden), and Kukura (international advisory board, *J. Heyrovsky Institute*, Prague);
- *Supporting learned societies*, e.g., Robinson (council member, Royal Society), Hore (chairman, International Spin Chemistry Committee), and Benesch (chair, Molecular Biophysics subgroup of the Biophysical Society, Los Angeles);
- *Advising/supporting major research collaborations*, such as the *UKRI Catalysis Hub*, e.g., Williams (Steering Group and Management Group Member) and Weller (Steering Group);
- *Supporting other societies and charities*, including Robinson (chair, L'Oreal Women in Science Programme; advisory board, Royal National Children's SpringBoard Foundation; and board of directors, the Vallee Foundation), Goodwin (advisory panel, Leverhulme Trust), Schofield (advisor to Cancer Research Technology; CRUK Multidisciplinary Committee member), and Moloney and Schofield (scientific advisory board, Antibiotic Research UK).

4.6.2 Recognition by the research base

Our staff have received numerous accolades for their achievements in the REF period, including an impressive *38 awards and prizes from the RSC* – including the Tilden Prize (twice), the Norman Heatley Award (twice), the Interdisciplinary Prize (twice), the Corday-Morgan Prize (twice), and the Harrison-Meldola Memorial Prize (twice). Six colleagues were elected as *Fellows of the Royal Society*. Dame Carol Robinson, FRS, was elected President of the RSC for 2018-20, and [Sir] David Clary, FRS, was knighted in 2016 for services to international science. We are typically ranked as one of the top departments worldwide (6th in 2018, 2019, and 2020 QS Chemistry Rankings).

Below we give examples of how staff have been *acknowledged for their wider influence* during the REF period, and their contributions to and recognition by the research base:

- Around 25 *journal editorships/associate editorships*, including Clarke (associate editor, *Journal of Solid State Chemistry*), Clary (editor, *Chemical Physics Letters*), Manolopoulos (deputy editor, *Journal of Chemical Physics*), Brown (editor-in-chief, RSC Book Series on

Chemical Biology), Conway (associate editor, *Journal of Medicinal Chemistry*) and B Davis (senior editor, *ACS Central Science*);

- *Editorial Board membership* of over 70 journals, including Hore, Timmel, and Mackenzie (editorial board, *Molecular Physics*), Robinson (international advisory board, *Angewandte Chemie*), Compton (editorial board, *Science*) and McCullagh (editorial board, *Nature Scientific Reports*);
- *Award of Fellowships*, including six FRS (Gouverneur, David, B Davis, H Anderson, Schofield, and McCulloch (taking the total to 12 current staff)), Clary (elected Einstein Professor of Chinese Academy of Sciences), B Davis (fellow, Academy of Medical Sciences), and Robinson (foreign associate, US National Academy of Sciences).
- *Award of prizes*: including 38 RSC prizes, three RS medals or awards, inaugural awards of the *Blavatnik Chemistry Laureate* (2018 and 2019) and a Blavatnik Chemistry finalist (2018), two ACS awards, two BBSRC Innovator awards (including Brown, Commercial Innovator 2016), one European Academy of Sciences medal, and one Leverhulme Prize;
- Receipt of *Women in Science awards*, e.g., Robinson (IUPAC *Distinguished Women in Chemistry or Chemical Engineering*, 2019), Farrer (L'Oréal–UNESCO *Women in Science Fellowship*, 2018), Robinson (L'Oréal–UNESCO *Women in Science European Laureate*, 2015);
- *Award of honorary degrees*, e.g., Robinson (six honorary degrees/doctorates including from Aarhus, Ben-Gurion, and Southern Denmark), Davies (Salamanca), Beer (Murcia), and Compton (Xiangtan);
- *Award of honorary fellowships/membership*, e.g., Edwards (American Academy of Arts and Sciences), Robinson (RSC, and the British Biophysical Society), and Bayley (British Biophysical Society);
- *Award of visiting professorships*, around 25 in total, including at New South Wales, Australia (Goodwin), Sapienza, Rome (Kukura), Indian Institute of Technology (Schofield), JILA/NIST Boulder (Mackenzie), and Kyoto and Perugia (Dixon);
- *PGR students and ECRs* have received >100 prizes for poster and oral conference presentations, etc., including the *Springer Thesis Prize* (2).