Institution: University of Reading

Unit of Assessment: 8 Chemistry

1. Unit context and structure, research and impact strategy

1.1 Overview

Chemistry research at Reading ranges from fundamental aspects of inorganic, organic, and physical chemistry, to areas bordering the life sciences, medicine, engineering and physics. Reorganization of the University's research structure in 2015 led to the creation of the Chemical Sciences Research Division (CSD), in which the 18 staff (15.9 FTE) returned here conduct their research, whilst delivering a full undergraduate teaching programme in the Department of Chemistry (Figure 1). Research in Chemistry contributes to two (*Environment*; *Agriculture, Food & Health*) of the University's four multi-disciplinary research themes, with research management accomplished through the *Environment Theme*. The Research Division is strategically led by a Research Division Lead (RDL, Powell). Following internal review, collaborative research and research coherence were enhanced through reorganization into the following three sections, with Section Heads denoted in bold type.

- *Biomedical, Molecular and Analytical Chemistry* (*BMAC*): Brown, **Cramer**, Hartl, Harwood, McKendrick, Russell, Smith.
- *Materials and Interfaces for the Future* (*MIFF*): Bennett, **Chippindale**, Grau-Crespo, Powell, Vaqueiro.
- *Soft Matter* (*SM*): Cardin, Davis, Elliott, Hamley, **Hayes**, Lovelock.

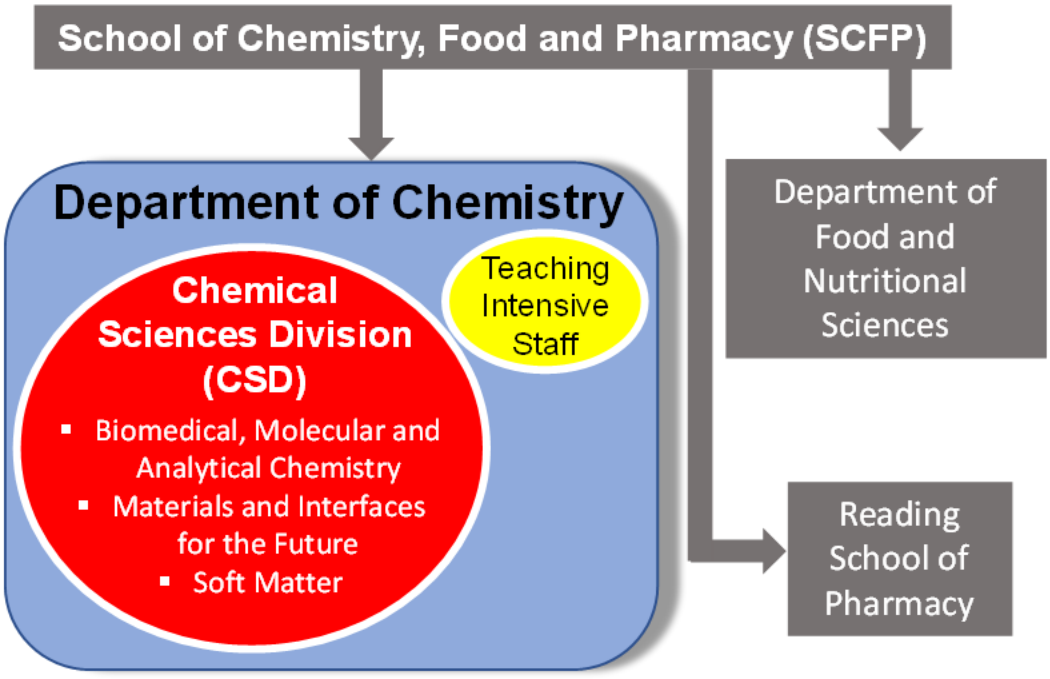

Figure 1: Schematic representation of the relationship between the School (SCFP), the Department of Chemistry and the Chemical Sciences Research Division (CSD), which comprises three research sections.

This research structure stimulates and facilitates collaboration across traditional disciplinary boundaries. The Section Heads, Impact Leader for Chemistry (Bennett), PGR Director (Vaqueiro) and Director of the Chemical Analysis Facility (Harwood) comprise the Divisional Research Committee, chaired by the RDL. The RDL sits on the Management Board of the School of Chemistry, Food and Pharmacy (SCFP, Figure 1), facilitating interaction with RDLs of other Research Divisions within the School, thereby extending Chemistry's research reach into the University's *Agriculture, Food & Health* theme. Research presentations at themed cross-

school meetings provide a further mechanism to stimulate cross-cutting activities. Interaction with other disciplines within the *Environment Theme* is sustained through a Community of Practice, of which the RDL is a member. Collectively, this promotes a collaborative environment in which Chemistry's expertise is applied to problems in cognate areas. Strong interactions between staff within the CSD to tackle key research problems is reflected in the appreciable number of outputs authored by two or more staff in the CSD (*ca*. 17% of all outputs since REF 2014), frequently from different research sections.

1.2 Research and Impact Strategy

The overall strategy identified in the REF 2014 submission was to focus on major scientific and technological challenges of the 21st Century. Four themes through which this would be implemented were identified: (a) sustainable technologies for energy production, (b) healthcare and quality of life in ageing populations, (c) anthropogenic climate change, and (d) clean drinking water.

The creation of the CSD in 2015 provided an opportunity in 2016 to refine our aim through a 5-year Vision for Chemistry research. This is to develop our base in chemical sciences and analytical technology to specialise in collaborative, high-impact research, crossing traditional boundaries of chemistry, with increasingly strong engagement with industry to address problems of technological significance. This Vision is founded on the strengths of the Chemistry return at REF 2014: in particular, the quality of outputs. Over 93% of the submission was rated 3* or 4*, with outputs in synthesis and structure of materials, catalysis and separation science performing strongly.

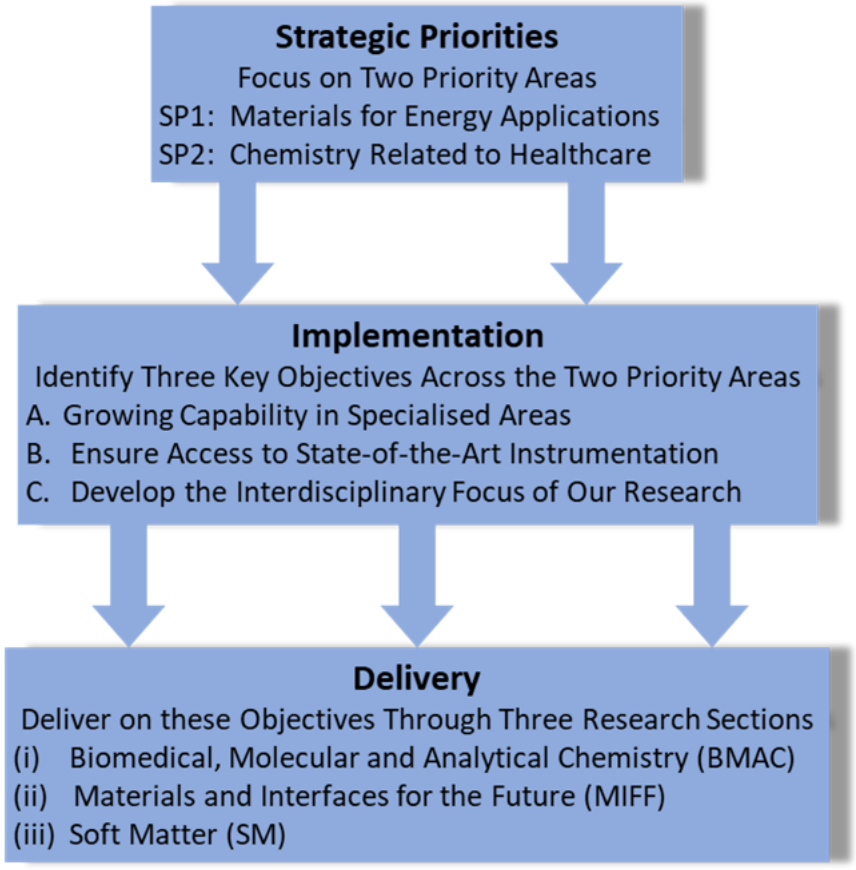

Figure 2: An overview of the research strategy of the Chemical Sciences Research Division, illustrating the relationship between strategic priorities, objectives and their delivery across three research sections.

Reorganisation of our research and rationalization of staff (reducing the size of the submission from 22 to 15.9 FTE) has enabled us to focus resources on two **Strategic Priorities** (Figure 2), evolved from (a) and (b) that reflect internationally-recognised strengths: **Materials for Energy**

Applications (***SP1***) and **Chemistry Related to Healthcare** (***SP2***). Delivered across all three research sections, these priorities are closely aligned with Research Council and Government Industrial Strategy priority areas, including *Healthy Nation: Transforming Health Care* and *Novel Materials and Novel Energy Vectors* identified in the EPSRC 2019 Delivery Plan and *Support for Emerging Technologies* and *Grand Challenge Clean Growth* of the Government's Industrial Strategy.

Impact and Knowledge Exchange were identified as areas with scope for improvement, following REF 2014. The appointment of an academic Impact Lead (Bennett) has been pivotal in driving change in the Division, increasing awareness of impact and fostering a high level of engagement with the University's Building Outstanding Impact Support Programme (BOISP). This nurtures impact over a range of timescales, through the provision of tailored and integrated support for developed, developing and potential impact projects, where significant societal/economic change may be achieved. BOISP funding for five projects was secured, covering the work of seven academics (Davis – Polytunnel films, Held – VerSoX Beamline, Hayes and Russell – Self-immolative materials, Hartl – Spectroelectrochemistry, Harwood and Smith – Selective Extractant Ligands). Support is bespoke to each project and includes: professionally-enhanced website and market analysis (Hartl); market and impact analysis (Davis, Harwood and Smith); collaborative outreach and publicity with UoR, Diamond and Johnson Matthey, describing industrial use of VerSoX beamline (Held) (https://www.youtube.com/watch?v=bM-pmlZu1II); and matched (with Defence Science and Technology Laboratory; Dstl) PDRA funding (Hayes), to improve performance and stability of self-immolative disclosure materials. This last project generated materials closer to a TRL of interest to industry and led to a new Defence and Security Accelerator (DASA) award and filing of an underpinning patent.

The research strategy of the unit is implemented through the following research objectives, underpinning our two strategic priorities, delivered through the three research sections (Figure 2).

Objective A: Growing Capability in Specialised Areas: To maximise the impact of our research capabilities, we have exploited strengths in Materials and Health-related research to consolidate existing and build new collaborations, particularly through participation in consortium-type proposals. Examples of the success of this approach are presented below. We plan to expand these areas through targeted recruitment as outlined in Section 2.1 and will also apply existing research strengths to new topics. For example, Cramer's expertise in bioanalytical chemistry offers opportunities for collaboration across the Health and Food areas, while Hamley's experience in peptides and biomaterials will be applied to new areas in Health. Hayes' specialist capability in self-immolative polymers has led to an augmented collaboration with Dstl and DASA in the area of sensing and detection, while collaboration on materials for thermal management (Powell) arose directly from AWE's recognition that our specialist expertise in energy materials was needed in this complementary field.

Objective B: Ensure Access to State-of-the-Art Instrumentation: The CSD is a major contributor to and beneficiary of the University's Chemical Analysis Facility (CAF), encompassing state-of-the-art facilities for spectroscopy, electron microscopy, X-ray diffraction, thermal analysis, chromatography and mass spectrometry (Section 3.2). Divisional staff take a leading role in the operation of this facility (Director, Harwood; NMR lead, Brown; X-ray lead, Chippindale; Mass Spectrometry lead, McKendrick) and in ensuring that instrumentation remains at the cutting edge.

Large items of equipment (> £100k), including those in the CAF, underpin multiple research programs, necessitating a broad-based inter-departmental approach to funding. A recent example is the successful application to the University's Research Infrastructure Fund, led by Chippindale, for a single-crystal X-ray diffractometer that significantly extends capabilities and cements an applications relationship with the manufacturer (Rigaku), by becoming the European demonstration laboratory. Specialised equipment requires adoption of a consortium-based approach to equipment funding, as exemplified by Cramer's membership of the Southern 4

Proteomic Consortium (Southampton (lead), Reading, Portsmouth, Surrey), awarded £448k by BBSRC for High Resolution Mass Spectrometry for Proteomic Research.

Strong links with local industry led to the donation by Johnson Matthey of a fully-equipped Escalab-250 X-ray photoelectron spectroscopy (XPS) instrument (est. £660k replacement value). This new capability in high-resolution XPS and spectroscopic imaging underpins research in all three research sections.

The CSD benefits considerably from high levels of beam time at large-scale facilities (Section 3.1). Access to world-class facilities including Diamond, ILL (Institut Laue-Langevin) and the ISIS Neutron and Muon Source is a key element of our research portfolio, facilitating correspondingly world-class research at Reading. The recent relocation of Held (in post until 2019, now Visiting Chair) to the position of VerSoX beamline scientist strengthens links with Diamond. The appointment of Lovelock (Royal Society URF) to a University Lectureship in 2017 extends the range of international facilities with which we interact to institutes including ESRF (European Synchrotron Radiation Facility) and BESSY (Berlin Electron Storage Ring Society for Synchrotron Radiation). Grau-Crespo's membership of the UK High End Computing (HEC) Materials Chemistry Consortium provides access to the National Supercomputer Facility. We also secure access to UK medium-scale facilities, including the National Crystallography Service.

Objective C: Develop the Interdisciplinary Focus of our Research: Interdisciplinarity is a core strength, central to our long-term vision and key to success in our two strategic priorities. We have created an open and collaborative research environment, where the expertise of staff complements that of researchers in other disciplines, both within and beyond the University. For example, CSD researchers make significant contributions to the University's *Agriculture, Health and Food* theme, exemplified by collaborative projects with the Departments of Food and Nutritional Sciences (Davis, Cramer), Agriculture (Davis, Cramer, McKendrick, Pfrang (in post to 2018)) and Pharmacy (Hayes, Cardin, Vaqueiro). Interdisciplinarity has extended to problems of environmental significance through the work of Pfrang in ozone oxidation of organics and Grau-Crespo in trace element incorporation in stalagmites, through projects carried out in collaboration with agriculturists, ecologists and archaeologists at Reading. We have exploited our strengths in materials, particularly in polymer chemistry and in thermoelectrics that complement those of physicists, engineers and manufacturing specialists, by engaging in large-scale projects with researchers in academia, industry and government laboratories.

The increasing focus on interdisciplinarity has seen us increase the number of industrial collaborations (by *ca*. 40%) since REF 2014. Projects where CSD provides underpinning expertise include those with Dstl/DASA (Hayes, Russell); BP International, Gnosys Global (now Kinetrics), Henkel AG, Domino Printing Sciences (Hayes); LNC Therapeutics, Mondelez (Cramer), AWE (Powell, Grau-Crespo); Kymira, European Thermodynamics, Dycotec Materials (Powell, Vaqueiro), BP Lubricants (McKendrick), Medimmune Ltd (Hamley).

Examples of how each research section has **delivered** on our strategy are described below:

*Biomedical, Molecular and Analytical Chemistry***:** Experimental activities encompass synthesis and the development and application of advanced analytical techniques to challenging and complex problems, including those at the chemistry-biology interface. Harwood's expertise in the creation of bespoke ligands for selective extraction of metal ions from solution, supported by the EPSRC (£320k), has resulted in key contributions to the remediation of nuclear waste (***SP1***), through invited membership of research consortia. He contributed core synthetic expertise to the multi-disciplinary project PACIFIC (*Providing a Nuclear Fuel Cycle in the UK for Implementing Carbon Reductions*), securing £155k UoR/£3M total (EPSRC) and involving significant interaction with the nuclear industry. The synthesis of ligands with actinide:lanthanide selectivities exceeding 100:1 led to the follow-on consortium-based project ATLANTIC (*Accident ToLerANT fuels In reCycling*), securing £168k/£2.5M (EPSRC). The participation of Smith (appointed 2015) in ATLANTIC provides succession planning, maintaining vitality in this

important area that complements activities in Materials for Energy Applications elsewhere in the CSD. Smith also brings a new capability in flow chemistry (EPSRC first-grant £98k) that complements the work of Russell in the synthesis of bioactive molecules.

Cramer's development of novel mass-spectrometric techniques (**Objective B**) has been strongly supported by BBSRC, EPSRC and Defra (over £1M in total) and Waters Corporation (3 jointly-funded PhD positions), with additional industrial PhD funding from Mondelez, and LGC. This has resulted in diversification (**Objective A**) of the range of health-related problems (***SP2***) to which MS techniques are applied, including analysis of proteomic markers for penile cancer and high-throughput MALDI as a large-scale classification method for animal health. This work is complemented by McKendrick's research with BP into the application of mass-spectrometric techniques to problems of industrial significance (**Objective C**). New NMR methodologies developed by Brown are applied to problems of biological relevance, including novel, scalable production systems for high-value diterpenoids in a consortium (**Objective A**) led by the University of York (£176k/£3.1M, BBSRC). Hartl's expertise in synthesis and electrochemistry is increasingly applied to problems of technological importance, including participation in a COST Action (21 partners, £520k) in photocatalytic water splitting (***SP1***) and collaboration with researchers at Wuhan in China, supported by a Royal Society International Exchanges Award. The development of novel spectroelectrochemical cells (>140 cells of all types sold to more than 130 customers worldwide, *ca*. £280k) introduces a strong inter-disciplinary element; this includes collaboration with Cardin on the binding of complexes to DNA, at the boundary with life sciences.

Materials and Interfaces for the Future: The core activities of this group revolve around the experimental solid-state chemistry of Chippindale, Powell and Vaqueiro, complemented by the expertise in surface chemistry of Bennett and the computational modelling of Grau-Crespo (and Bartok-Partay, in post to 2019). Bennett's investigations of the surface chemistry of ultra-thin films led to collaboration in the catalytic work of Held and extensive use of X-ray synchrotron facilities. Chippindale has developed metal cyanides as potential negative thermal expansion materials through collaboration with physicists (**Objective C**) at the ILL (joint PhD project, 6 joint papers) which has provided new insights into dynamical properties through inelastic neutron scattering.

Powell and Vaqueiro have established a leading position in the synthesis and evaluation of novel, high-performance thermoelectric materials (***SP1***). This work benefits from an inter-disciplinary approach (**Objective C**). Their materials expertise was central to an EPSRC award (£317k/£988k) to a consortium (**Objective A**) led by Loughborough University to investigate energy recovery from vehicle-exhaust streams. Collaboration with electrical engineers (Cardiff) and automotive engineers (Loughborough) resulted in delivery of a skutterudite-based demonstration generator, which met the 500 W output target of the industrial partners (Johnson Matthey, Dana Corporation and Ricardo PLC). This followed the success of an EU FP7-funded, nine-member consortium (£357k/£1.03M, 2012-14) in developing thermoelectric technology for building applications. Powell and Vaqueiro were the sole academic partners in an industry-led consortium (Kymira, Dycotec Materials Ltd and European Thermodynamics) funded by Innovate UK (£135k/£373k) to develop materials for wearable thermoelectrics.

Thermoelectrics research extends into measurement capabilities (**Objective B**), including construction of an in-situ cell for measurement of electrical properties simultaneously with the collection of powder neutron-diffraction data (joint PhD student with ISIS Facility, £39k) and novel measurement techniques (collaboration with Universitat Jaume I, Spain, 3 papers). Experimental research in thermoelectrics is enhanced by the computational expertise of Grau-Crespo (3 joint papers) within his wide-ranging programme of computer simulation of materials that encompasses photo catalysts, thermoelectrics and electron-phonon structure and transport in solids. This has facilitated research across the CSD, particularly the surface chemistry and catalysis of Bennett and Held, (4 joint publications) and has attracted international collaborations, including partnerships with India (British Council, £15k) and South Korea (Royal Society, £12k).

Soft Matter: Polymer chemistry was a core element of the research emerging from REF 2014, through the work of Colquhoun (in post to 2018), Hayes and Davis. With BBSRC support (£495k), Davis' interdisciplinary collaboration (**Objective C**) with the School of Agriculture (Hadley) and BPI-visqueen, has developed innovative polymer films with controlled spectral response. Their use in polytunnels improves crop yields as described in an Impact Case Study. Innovate UK (£243k) funding has extended the work to a higher TRL applied to tea growth in Kenya. Hayes has consolidated and built on the solid foundation established in REF 2014 to achieve a leading position in stimuli-responsive polymers. The synthetic expertise of Russell has been instrumental to the success of this patented work, affording another example of a highly productive inter-sectional collaboration. The potential of these materials in detection and sensing has led to growing interest from the industrial and defence sectors, thereby advancing **Objective C**. A series of projects funded by Dstl/DASA (total £499k) produced materials that show a colorimetric response to electrophilic alkylating agents; offering a means of detecting chemical warfare agents, fumigants and pesticides that avoids the need for instrumental techniques. Hayes' expertise in polymer design contributed to an EPSRC award (£375k/£3.5M) to a multi-disciplinary team of academics and industrialists, led by the additive manufacturing group at University of Nottingham, to exploit 3D printing in a range of industrial sectors, exemplifying the success of the consortium-type approach we have increasingly adopted (**Objective A**).

A further example in *Soft Matter* of the success of this inter-disciplinary approach is the work of Hamley in peptide chemistry applied to biomaterials (***SP2***). Interdisciplinary collaboration (**Objective C**) involving polymer chemists (Hayes, Colquhoun), mathematicians (Wang) and pharmacists (Connon) has been supported by a £1.5M EPSRC Platform Grant in *Nanostructured Polymeric Materials for Healthcare*. The theme of biologically-relevant systems is continued by Cardin's work in understanding binding of metal complexes to DNA, and their potentially therapeutic benefits (***SP2***), carried out in an inter-disciplinary team (**Objective C**) involving researchers in the School of Pharmacy, that has attracted BBSRC funding in excess of £2.4M. Elliott's work on templated formation of porous structures, in collaboration with Squires (in post to 2017), has led to the controllable growth of mesophases and, subsequently through an inter-sectional collaboration with Bennett, the exploitation of nanostructured electrodes in gas sensing. This work is complemented by the fundamental studies of Lovelock, appointed in 2017 and already securing significant funding (£239k across two awards). His research, to link reactivity in liquid media to electronic structure, benefits from the computational expertise of Grau-Crespo and the synthetic skills of Smith. It also extends to collaboration with Bennett into the geometric and electronic structure of ionic liquids and their interaction with surfaces and to templated materials growth (with Elliott).

1.2.1 Future Developments

The future strategic vision for Chemistry at Reading is increasingly to bring expertise to bear on new and challenging technological problems of societal importance, commensurate with our two **Strategic Priorities**, thorough collaborative, high-impact research that crosses the traditional sub-disciplinary boundaries of chemistry. Recent substantial awards, where the bulk of the spend will occur in the next REF period, reflect this ambition and address our two **Strategic Priorities**. They include £1.05M (two awards, BBSRC and EU) to Cardin to extend collaborative work with the School of Pharmacy and international partners into DNA complexation and Gene Editing Immunotherapy (***SP2***); £892k (EPSRC) to Cramer for the development of high-speed diagnostics for large population screening (***SP2***); £220k (Leverhulme Trust) to Vaqueiro to work with the ISIS Facility and international partners on materials related to energy harvesting (***SP1***) and £609k for a collaborative project (University of Manchester, JNCASR Bangalore) led by Powell to develop new affordable thermoelectric materials for energy harvesting from traditional Indian cook stoves (***SP1***).

We will pursue new opportunities for collaborative research in healthcare (***SP2***). Cramer's proteomics and AP-MALDI MS work readily lends itself to analysis of biomarkers in a range of diagnostic fields. This has recently included development of a high-speed MS-based test for the detection of COVID-19. Brown's expertise in NMR techniques offers opportunities to impact on drug development, including cost-effective antimalarial treatments. Hamley's expertise in self-

assembling peptides will be extended to applications in healthcare, including vaccine adjuvants and antimicrobial peptides with enhanced activity and selectivity.

Similarly, we will extend our research in Materials for Energy Applications to new sustainable energy production and storage technologies (***SP1***). Existing expertise in chalcogenide chemistry and structure-property relationships will readily translate to battery technology (Chippindale, Powell, Vaqueiro), while expertise in hydrothermal synthesis and semiconductor design will be applied to new photovoltaic materials (Vaqueiro, Chippindale, Grau-Crespo).

We will continue to nurture research impact, both through the Impact Lead fostering an impact culture and by accessing funding through the BOISP programme. This will be coupled with broader approaches to developing engagement, supporting events and initiatives with external partners and collaborators to strengthen networks and increase the impact achieved across CSD. Support will be delivered by the Impact Team, Knowledge Transfer Centre (KTC) and Research Communications, in collaboration with the CSD Impact Lead

2. People

2.1. Staffing Strategy:

Our staffing strategy is to focus appointments in areas of existing strength to consolidate and expand areas where we have recognized world-class expertise. This allows new appointees to benefit from an existing infrastructure, mentoring by researchers familiar with the field and immediate opportunities for collaboration, thereby accelerating their early-career trajectory.

Since REF 2014, we have recruited Smith (2015), whose expertise in synthesis expands and invigorates our research in ligand design for selective ion-extraction, while his specialism of flow chemistry brings a new dimension to the synthesis of pharmaceutically active compounds. Lovelock, recruited in 2017, is a Royal Society Research Fellow with an associated permanent lectureship. He brings a new dimension to research into materials for energy applications through clean fuels and CO_2 capture and processing. He strengthens our facility interactions and has established collaborations with Bennett, Held (visiting chair), Smith and Grau-Crespo. In Autumn 2020, Dr James Cooper joined from the Stoddart group, Northwestern University, as a lecturer in the *Soft Matter* group. His expertise in supramolecular switches and molecular replication complements that of Hayes and Russell.

The challenging climate for undergraduate recruitment into Chemistry has restricted our ability to recruit T&R staff to replace all who have retired or moved institution since 2014, reducing the size of the submission from 22 to 15.9 FTE. In seeking to balance research and teaching workloads effectively, we have, over the REF period, appointed seven teaching-intensive posts (permanent and fixed-term). This has helped maintain time for research and contributed to an increase in the Division's research-output volume (+29% outputs/submitted FTE; +10% outputs/submitted FTE/year) and income (+30% total income/submitted FTE; +16% average annual income (excluding income-in-kind)/submitted FTE) with respect to the previous assessment period.

We will seek growth in targeted areas by pro-actively encouraging high-calibre candidates to apply for fellowships, through personal contacts and publicising available schemes. Our specialist research themes and excellent infrastructure have created an environment that is attractive to outstanding researchers at the beginning of their careers. Since 2014, we have hosted two Royal Society University Research Fellows (Sacchi and Lovelock), a Royal Society Dorothy Hodgkin Fellow (Bartok-Partay) and a Daphne Jackson Fellow (Benny, now a lecturer in Further Education). Research Fellows are assigned a senior member of staff as mentor, who provides advice and support on launching an academic career, seeking funding, and establishing a profile through publication and conference participation. Research Fellows can elect to do a small amount of lecturing, supported by their mentor, to gain experience. In this way, we support their career development so that they emerge well placed to secure a

permanent academic position. The success of this approach is reflected in the permanent positions secured by Sacchi (Surrey, 2016) and Bartok-Partay (Warwick, 2019).

2.2 Staff Development

We encourage and support the personal and professional development of all staff through University-level programmes, such as the *Academic Practice Programme* and *People Development*, which provide training in leadership, management, and mentoring. Within SCFP, career development workshops for ECRs focus on career transition points, obtaining funding, becoming independent, and the grant writing and review process. Feedback led to the establishment of a monthly grant-writing forum to support ECRs for fellowship and grant applications. This is complemented by centralised provision of training in teaching and learning available to all academic staff.

Career development, progression and identification of training needs are discussed at annual performance development reviews (PDRs), conducted by Research Section Heads. This process is complemented by Personal Research Plans (PRPs). These provide a space for reflection on research goals and needs and identification of barriers to research, without the limitations of performance measures or objectives. Common issues and research needs identified in PRPs are incorporated into the Annual Research Operating Plan, submitted to the University Committee for Research & Innovation. All staff present short overviews of their research achievements during the year at an Annual Research Day. This helps maintain a flow of information on research activities in the Division and stimulates new research collaborations.

The CSD adopts a pro-active and highly transparent approach to promotion. The SCFP Personal Titles Committee discusses the position of all staff in the School, with a particular focus on encouraging all candidates who meet promotion criteria to apply. Staff are supported in the process through University-level training and by promotion mentors in SCFP (Chippindale and Almond in Chemistry), who provide advice and feedback on individual applications. There have been eight staff promotions in Chemistry since 2014: seven to Associate Professor (Brown, Cranwell, Grau-Crespo, Nutt, Pfrang, Squires, Vaqueiro), and one to Professor (Chippindale). These include three staff that were appointments in REF 2014.

2.3 Training and Supervision of PGR Students

All Chemistry PGR students have a minimum of two supervisors, more for joint projects with facilities or industry, ensuring students have sources of advice beyond their primary supervisor. PhD students produce two reports during year 1, the supervisory team providing feedback on the first. Progression to year 2 is determined by assessment of the second report by an internal assessor and satisfactory performance in an oral examination. Subsequent progress is monitored through annual reports submitted by students and supervisors. These are reviewed by the Departmental Director of Postgraduate Studies, who acts on any issues raised.

In-house PGR training includes specialist training in instrumentation in the CAF and mandatory Health and Safety training. In addition, all PhD students select an advanced UG course in Chemistry in Year 1. Research Section meetings improve presentation skills of PGR students, with feedback provided by the supervisory team. Complementary training in transferable skills is delivered centrally through the Reading Researcher Development Programme (RRDP). Doctoral students can also access skills training for teaching through the Graduate School's *Preparing to Teach* programme. PGR students also attend external training courses, including those provided by the British Crystallographic Association and central facilities. These provide specialist training that would be difficult to deliver internally in a cost-effective manner. International students are supported through courses to help with their academic English, developed by the International Study and Language Institute.

All PGR students are expected to attend weekly research seminars and are encouraged to embrace outreach and public engagement opportunities (for example, the Royal Society of Chemistry (RSC) initiatives, *Spectroscopy in a Suitcase* and *Chemistry for All*; and primary/secondary school events, including the successful Salters' Days). PGR students deliver oral presentations and posters at an annual Divisional Research Day, which also provides

networking opportunities with potential employers and representatives of the Society of Chemical Industry (SCI). PhD students participate in the UoR Graduate School Annual Doctoral Research Conference, at which in 2019, a CSD student received the Environment Theme PhD Researcher of the Year award. External conference attendance is strongly encouraged, with funding available through the Graduate School, University Research Travel Grants and departmental funds. PGR students are encouraged to join the RSC and the SCI, and to apply for travel funding available from these organisations.

The Division typically has around 40 postgraduate research students (PhD and MSc). Our PGR programmes attract many international students, with approximately 33% from overseas, funded by their governments (Mexico, Thailand, Nigeria, India, Malaysia, Indonesia, Colombia, Ecuador, Saudi Arabia) or by prestigious scholarships (Felix, Commonwealth). We have succeeded in maintaining the number of PGR students per FTE at *ca* 2.2 throughout the assessment period (Figure 3). Many projects are supported through sole- or co-funding in collaboration with central facilities (Diamond, ISIS, ILL), industry (AWE, BP, Dstl, Johnson Matthey, Kinetrics, LGC, Mondelez, Waters) or other departments within UoR (Pharmacy, Food, Agriculture, Archaeology). We participate in the SCENARIO NERC DTP, which typically funds one Chemistry PhD student per year to investigate important environmental problems. The interdisciplinary approach to PhD funding extends to the Food BioSciences DTP, which supports a collaborative project with Biological Sciences, Aberystwyth.

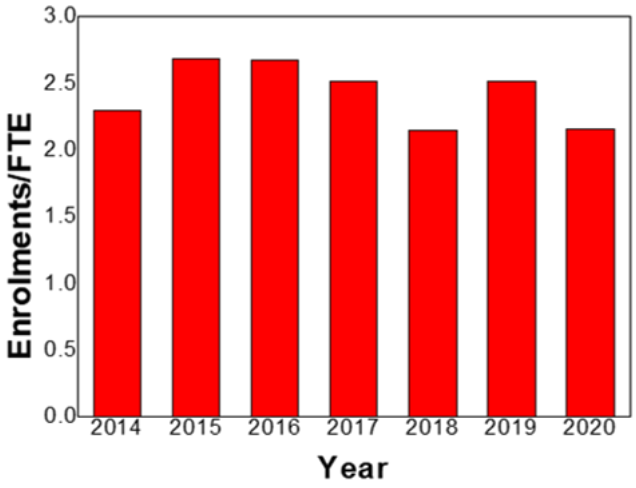

Figure 1: PGR (PhD and MSc by Research) student enrolment in each year of the REF period, expressed per staff FTE for that year

2.4. Equality and diversity

SCFP holds an Athena Swan Silver Award in recognition of our efforts to eliminate potential gender bias and promote an inclusive culture. CSD staff actively participate in annual Diversity and Inclusion Away Days to discuss challenges and formulate effective policies. They also sit on the SCFP Diversity Committee. An Academic Support Network, comprising a database of staff who provide advice in areas such as work-life balance, the writing of publications and teaching development, supports both new and existing staff, including PDRAs, within SCFP.

The gender composition of our staff and research students is broadly in line with national trends. Of the 18 individuals returned in the UoA, four (22%) are female. Two of our eight professors are female, which exceeds the UK average of 9% (RSC). The percentage of female postgraduate students in Chemistry has been in the range of 34% to 41% during the assessment period, which compares favourably with the ~40% of females securing undergraduate qualifications in the chemical sciences in the UK. *Ca.* 20% of staff originate from outside the UK providing cultural diversity that benefits the division.

We ensure diversity on committees and recruitment panels and are attentive to equality and diversity issues, when considering promotion or other staff rewards. Our pro-active approach to promotion (Section 2.2) is designed to compensate for reported differences in application rates among genders and ethnicities, while we also take care to eliminate bias against part-time staff.

We have taken affirmative action to address the lower representation of female speakers on our research-seminar programme. Before 2015, the proportion of female speakers annually never exceeded 30%, with no female speakers for two terms. Since then, at least a third of speakers have been female (~40% in 2018).

We organise an annual "Heroines of Science" event for local schools, to promote female role models in research. We also seek to provide male and female role models for young people, through a programme of lectures based on research in the CSD, targeted at schools with low numbers of pupils progressing to higher education, to promote widening participation.

The CSD offers a supporting environment to staff with caring responsibilities. Options include part-time working, flexible working hours, compressed working hours and working from home. We also support maternity/paternity/parental leave by providing teaching cover, paying 'Keeping in Touch' days during the leave, and reducing workload in the first term after return. Over the assessment period, one member of staff has benefitted from a reduction in hours; two have taken advantage of flexible working to allow for caring responsibilities, while child-care responsibilities of another two staff have been supported through flexible working from home. Two staff also took parental leave, where flexibility surrounding return to work and ongoing child-care responsibilities exceeded legal requirements. In the recent past, we have also supported staff through flexible working following family bereavement.

Senior staff in the CSD attended two E&D Training Modules specifically designed for REF-related processes to ensure E&D factors were considered during the construction of the submission. As described in the University's Code of Practice, final selection of outputs was informed by peer-review quality assessments and metrics as relevant (in line with University policies on responsible use of metrics). Our aim was to optimise for quality whilst remaining mindful of E&D issues. We have reflected on the outcomes of the University's interim Equality Impact Assessment (2020) and bias analysis on the final pool (2021), which showed no statistically significant differences for Main Panel A units of assessment, providing assurance that our processes are effective.

3. Income, infrastructure and facilities

3.1 Research Funding Portfolio

Our research funding portfolio (total spend since 2014 = £8.75M, with a further £5.14M of UKRI in-kind income) includes funding from three research councils (EPSRC, BBSRC and NERC), The Royal Society, charitable foundations, UK Central Government, UK Public Corporations, Innovate UK and the European Commission. Average annual income per FTE is £125k. Excluding income-in-kind, annual income per FTE has increased by *ca*. 16% relative to REF 2014. The substantial element of RCUK/UKRI in-kind income reflects our leading position as facility users, with 50% of the submitted staff securing facility time in the assessment period. Over 600 days of experimental facility time (> 35 days per FTE) have been awarded in the UK and overseas through competitive processes. This includes: Diamond (143 days), ISIS (75 days), Central Laser Facility (113 days), ILL (22 days), ESRF (35 days), BESSY (34 days), MAX-Lab (29 days), LaserLab Amsterdam (105 days), Elettra (33 days), together with computing time on Archer (130 MAU).

Facility usage has led to the establishment of close collaborations with scientists at large-scale facilities, including jointly funded studentships. Proximity to the Harwell campus, in particular, fosters a genuinely collaborative environment, with researchers moving freely between sites on a daily basis. This is exemplified by funded projects with ISIS (Pfrang, atmospheric oxidation of

organics; Powell, Vaqueiro, thermoelectrics; Squires, amyloid fibrils) and Diamond (Hamley, bioactive peptides; Squires, nanomaterials; Cardin, DNA; Bennett, surfaces; Held, catalysis). Eighteen PhD studentships have been directly funded by industry, contributing to an increase in the total number of doctoral awards per FTE from 2.97 in REF 2014 to 4.69 in the current period, despite the challenging UK PhD funding environment. We have taken steps to maintain this momentum through the enlargement of our MSc-by-Research programme, which has seen an increase in enrolments since 2014. The MSc is beginning to act as a feeder to our PhD programme, with 4 students making the transition in the last two years.

3.2 Research Infrastructure and Facilities

Besides the classical provision of glassblowing and other workshops, together with IT and librarian support, the CSD hosts the Chemical Analysis Facility (CAF), founded in 2008 with an initial University investment of ~ £4.5M, supporting research in the CSD and more widely across the University. This now incorporates other facilities, such as the BioCentre Facility, previously established with an investment of > £8M. The CAF Director (Harwood) is supported by academic leads (three from the CSD), six full-time technical staff in NMR, mass spectrometry, spectroscopy, electron microscopy, thermal analysis and X-ray diffraction, and an administrator.

New instruments, funded by the University's Annual Research Equipment & Infrastructure Fund, installed over the current REF cycle complement or replace existing equipment. They include a JEOL 2100Plus cryo-TEM (£463k); a Thermo Scientific Delta V Advantage Light Isotope Ratio Mass Spectrometer with capabilities for multi-isotope (CNSOH) analysis (£250k) and a Rigaku Synergy-S dual micro-focus source, single-crystal X-ray diffractometer (£431k). In addition, to this £1.3M (ex. vat) investment, complementary funding was secured for a Vitrobot preparation unit for the TEM and a 400 MHz NMR console (£70k). The step-change in crystallographic capabilities afforded by the state-of-the-art X-ray diffractometer includes an order-of-magnitude increase in data-collection rates - hugely beneficial to directing synthetic work - and the ability to investigate crystals previously too small to study in-house. It is the cornerstone of a diffraction suite (SXD, SAXS and 3 powder instruments) with a world-class capability and capacity.

Cramer received an EPSRC instrument development grant for a high-performance hybrid ion-mobility mass spectrometer (list price >£700k) to develop his novel technology. The purchase of the associated IP by Waters Corporation includes provision for royalty payments on commercialization of the technology. This has also deepened collaboration with the company, in the form of support for studentships, a cash contribution to a BBSRC IPA project and investment in equipment in the Cramer laboratory. MS capabilities were further enhanced by the subsequent donation by Waters of a similar instrument in 2019. Additional capability is provided through Cramer's membership of the Southern 4 Proteomic Consortium. Grau-Crespo's membership (supported by £33k p.a. of UoR investment) of *The Materials and Molecular Modelling Hub* consortium affords similar benefits in providing access to Tier 2 HPC, funded by a £4.5M EPSRC award to UCL, with Grau-Crespo as a co-investigator.

External funding enabled the purchase of an Agilent UV/near IR spectrometer (£100k) in 2016 (Davis, UoR/Innovate UK). We have also benefitted from the purchase by individual groups of equipment for next-generation experiments, including those to support polymer chemistry (£98k, Hayes) and flow chemistry (£30k Smith). Lovelock secured £30k through the EPSRC ECR Capital Equipment scheme for a glove box and recirculating fume cabinet.

Phase 1 of refurbishment of the Division's Research Laboratory Space (2019) received £745k of University investment. Refurbishment of the teaching laboratories (£800k) has additionally provided new space for research activities, including pump-priming projects and the expanded MSc by research programme. Increased MSc numbers (and the space to accommodate them) has facilitated new research avenues, including photovoltaics (Vaqueiro) and batteries (Chippindale), which will stimulate future funding applications. A new research data archive, implemented during the assessment period, allows free time-unlimited archiving of research data, in alignment with Research Council data policies.

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

4.1 Collaborations, Networks and Partnerships

Interdisciplinarity, a core element of our strategy (**Objective C**), necessarily entails the establishment and nurturing of strong collaborations and partnerships and participation in research networks. Harwood's research into ligands for nuclear waste remediation in collaboration with the nuclear industry, through ATLANTIC and PACIFIC projects, provides a template for multi-disciplinary collaborative projects, where specialist expertise at UoR provides key input into a larger-scale project. This is exemplified by Hayes, whose expertise in supramolecular polymers was instrumental in creating the "*Formulation for 3D printing: Creating a plug and play platform for a disruptive UK industry*" collaborative project between 15 academics and 5 industrial partners (GSK, Malvern Instruments Ltd, PPG Industries, Syngenta and Unilever), supported by EPSRC. Similarly, Brown's expertise in NMR underpinned the BBSRC-funded project "*Synthetic Biology of Diterpenoids*" (2015-2020), led by University of York, with University of Cambridge, GSK, Croda, Unilever.

Consortium and network building have been particularly beneficial to research into thermoelectric materials for energy recovery (Powell, Vaqueiro). This includes: an international collaboration with the Central Michigan University (Royal Society International Exchange Grant); an EU-funded project (InnovTeg) with nine partners, including CRISMAT, Caen, France with whom nine joint publications have resulted; two EPSRC-funded UKTEG projects with the Universities of Loughborough and Cardiff (three joint publications), Dana Corporation, Ricardo PLC, Johnson Matthey (one joint publication); and the Innovate UK TEG-Jacket project on wearable thermoelectrics with Kymira Ltd, European Thermodynamics Ltd and Dycotec Materials Ltd. Deeper links with Johnson Matthey have involved funded use of equipment at UoR, an invited presentation at an industry day at the JM Technology Centre (2017) and organization of a *Thermoelectrics and Exhaust-Gas After Treatment* workshop at UoR in 2015.

Further examples of international collaborations include Cardin's internationally-leading DNA work, such as the Japan Society for the Promotion of Science's (2018-present) support of a studentship and 3yr programme of visits to FIBER institute (Kobe, Japan), and BBSRC-supported collaboration (2013-2016) with Trinity and University Colleges, Dublin that led to the RSC Cornforth Award (2016). Hartl has participated in extensive collaborative networks, including three funded by China: Central China Normal University Wuhan; Shanghai Institute of Organic Chemistry (China) and University of Malaga (Spain); Huazhong University of Science and Technology, Wuhan and Yiching Entrustech Environmental Co. Ltd. (Yixing, Jiangsu Province, China). These are in addition to the EU-funded COST Action CM1202 – *Supramolecular Photocatalytic Water Splitting* (*PERSPECT H_2O*; 2013-2016), involving 21 groups from EU countries. Hamley has had numerous national and international collaborations, including with China (supported by The Royal Society), India (through UKIERI/DST), and Brazil (via a FAPESP-funded collaboration). Grau-Crespo led a UKIERI Trilateral Partnership collaboration on carbon/boron nitride materials (2013-2015) with the Jawaharlal Nehru Centre for Advanced Scientific Research JNCASR (India) and Purdue University (USA). He subsequently extended the collaboration with JNCASR through organization of an India-UK joint workshop in Thermoelectric Materials in Bangalore (2018), funded by The British Council.

4.2 Industry and Facility Collaborations

Long-term collaborative research with industry is a core aspiration of the Division through pursuit of **Objectives A** and **C**. In addition to engagement through large-scale research consortia outlined in Section 4.1, individual research groups collaborate directly with companies. For example, Davis' polymer chemistry underpinned the collaboration with BPI-visqueen to produce polymer films with controlled spectral response. Similarly, Bennett's knowledge of oxide surfaces led to a London Underground supported contract to solve intermittent signalling through the rail-wheel interface, leading to identification of Si incorporation and oxidation as the culprit. The development of novel analytical techniques has proven to be a fruitful area. Cramer's close ties

with Waters, to advance MALDI-TOF MS technology to permit detailed analysis of biological samples, offers potential for step changes in multiple diagnostic fields and is finding application in agriculture, veterinary sciences (collaboration with Reynolds, Centre for Dairy Research, UoR and Defra), clinical diagnostics and biomedical research. Waters have noted "*The agricultural community would gain a whole new toolbox for the rapid and large-scale analysis of animal health, your technology would be far more specific and accurate than current mid-IR tests*". This complements McKendrick's collaboration with BP to develop effective analytical methods for the study of complex lubricant formulations.

Hayes has successfully pursued funded projects with BP, Domino Printing Sciences, Gnosys Global Ltd and Henkel over an extended period of time to translate supramolecular polymer technologies from the research laboratory into marketable materials. Henkel hold a patent on supramolecular polyurethanes discovered at Reading that have thermal-reversibility characteristics suited for use in hot melt adhesives and pressure-sensitive adhesives. Work carried out with Domino Printing Sciences has resulted in a patent on new inkjet ink formulations, while in conjunction with Gnosys Global Ltd, the University has filed a patent on healable organic materials. Hayes and Russell have a long-term relationship with Dstl (supporting 2.5 years of PDRA time and two fully-funded PhD studentships) to develop highly effective disclosure systems for chemical warfare agents using novel self-immolative chemistries discovered at Reading. Dstl have patented the technology and are looking to exploit it with third parties. Hamley has led projects with Medimmune (2015-2019, co-funding two PhD studentships) to investigate self-assembly and its relation to bioactivity of gut hormone peptides.

Hartl has developed commercially-successful, optically-transparent, thin-layer electrochemical (OTTLE) cells adapted for optical spectroelectrochemistry, using a variety of spectroscopic probes. The room-temperature OTTLE cell, manufactured by spin-out Spectroelectrochemistry Reading since 2013, has been sold to over 90 customers globally and has been cited in >700 peer-reviewed papers. Profits support postgraduate research in the Hartl group and the sponsorship of international conferences, such as the 23rd International Symposium of Photochemistry and Photophysics of Coordination Compounds 2019, in Hong Kong.

Powell co-chairs with Freer (University of Manchester) the UK Thermoelectric Network (TEMPEST), established with EPSRC support. This fosters industry engagement through regular meetings that bring academics from a wide range of disciplines together with industrialists. The network gives leadership to the UK community by providing a focal point for stakeholders, input into consultation exercises by Government bodies and publication of a UK Thermoelectric Roadmap (Powell, Freer) that highlights opportunities to increase scope and efficiency of heat-energy recovery systems.

Many of our collaborators enrich our environment through membership of our External Advisory Board. This comprises members from Unilever, Syngenta, BP, Johnson Matthey, Diamond, Cytec Aerospace Materials, CEMAS, AWE and Waters Corporation. The Board meets biannually to provide advice and constructive criticism on matters including Divisional research strategy and PG research, ensuring we remain responsive to the evolving industrial research landscape and aware of topical new directions where our specialised skills may be applied.

A significant example of the way staff in CSD have influenced the facilities-enabled research agenda is provided by the VerSoX beamline at Diamond. The vision for an interdisciplinary facility for soft X-ray spectroscopic analysis in a controlled atmosphere was first proposed to STFC by Held and Bennett in 2009, subsequently garnering the support of a community of ~50 research leaders. This secured ~£6M capital expenditure and ~40 person-years of work during the REF period for a new beamline. Held was part-seconded to Diamond (~60% FTE, 2012-2019) to design, build and run the beamline. It became operational in 2017 with Bennett as first user and now supports a growing interdisciplinary user base (see Impact Case Study). In mid-2019, Held relocated to Diamond full time but remains a visiting Professor at Reading.

4.3 Awards and Fellowships

Staff in the CSD have been recognized through the award of prestigious prizes and fellowships. Notable examples include: Hamley - *Macro Group UK Medal of the RSC/SCI* (2016), *RSC Peter Day Award* (2016), *The Royal Society Wolfson Merit Award* (2011-16); Cardin – *RSC Rita and John Cornforth Award* (2016); Colquhoun - *President's Medal, Materials Chemistry Division of RSC* (2016), Leverhulme Emeritus Fellowship, 2019-20; Lovelock - Royal Society University Research Fellowship, 2016-date; Bartok-Partay - Royal Society Dorothy Hodgkin Fellowship, 2014-19; Sacchi - Royal Society University Research Fellowship, 2014-16; Benny, Daphne Jackson Fellowship, 2015-17. Both Davis (CDRSP, Leiria, Portugal) and Hartl (Central China Normal University, Wuhan, PRC) have held visiting professorships at overseas institutions.

4.4 Journal Editorships

During the REF period, members of the CSD have held over twenty senior editorial and board member positions in fields relevant to our areas of strength. Current examples include: Chippindale (Co-Editor, *Acta Crystallographica E,* 2012-date; Editorial Board, *Journal of Chemistry*, 2017-date); Harwood (Letters Editor, *Synlett*, 2001-date; Editor-in-Chief, *SynOpen*, 2017-date); Powell (Associate Editor, *Journal of Solid State Chemistry*, 2019-date); Cramer (Associate Editor: *Frontiers in Plant Science*, 2019-date); Grau-Crespo (Editorial Board, *Scientific Reports,* 2014-date); Hamley (Advisory Board, *Soft Matter*, 2013-date); Hayes, Editorial Board, *Reactive and Functional Polymers*, 2012-date); Vaqueiro (Editorial Board, *Journal of Physics: Energy,* 2018-date; Editorial Board, *Materials,* 2017-date).

4.5 Leadership and Contributions to the Research Base

Chemistry staff have played key leadership roles in instigating and organizing important meetings and conferences in the field and have influenced decision making, through advice to learned societies and funding organizations, as chairs and members of committees and panels.

Since 2014, we have contributed to the organization of 37 meetings (2.3 per FTE). For example, Hamley chaired the RSC Faraday Division Meeting on *Self-Assembling Materials for Biomedicine* (2016); the *3rd International Conference on Peptide Materials, PepMat* (2018); the Royal Society Theo Murphy International Discussion Meeting *Self-assembled peptides: from nanostructure to bioactivity* (2016). Held chaired the *3rd Workshop on Ambient Pressure-XPS* (2016), and Grau-Crespo co-chaired the *UK-India Workshop on Thermoelectric Materials* (2018).

Examples of significant leadership in learned Societies include: Cramer's positions of Executive Committee Member (2007-date) and Vice President (2018-date) of the British Society for Proteome Research; Colquhoun's Presidency of the Materials Chemistry Division of the RSC (2012-15); Held's membership of Faraday Division Council of the RSC (2016-18); and Chippindale's membership of the Royal Society International Exchanges Committee (2020-date). Mentoring and support has propelled ECRs from the REF2014 period into leadership roles. For example, Grau-Crespo was a Member of the Executive Committee CCP5 Network (2012-14), while Vaqueiro has been a Committee Member of the RSC Solid State Chemistry Group (2014-2018) and of the BCA-IOP (Institute of Physics) Physical Crystallography Group (2018-date).

Hartl's membership of the International Evaluation Board of Charles University, Prague, Czech Republic (2019-2020), Hamley's membership of the RSC MacroGroup UK Committee and European Polymer Federation Representative (2008-15), and Bennett's role as Evaluator of Institutes of the Czech Academy of Sciences, Chemical Sciences Panel (2015) bring an international dimension to our leadership contributions.

Since 2014, the CSD has provided 11 members of the EPSRC Peer Review College, and panel members and chairs for national and international organizations. These include EPSRC (20 panel members, 4 chairs; a participation level of 1.5 per FTE), The Royal Society, BBSRC, NERC, STFC and Heinz Maier-Leibnitz Zentrum (Munich). Staff also provide leadership through membership of selection panels and advisory boards at ISIS (Vaqueiro), Swiss Light Source, Helmholtz-Zentrum Berlin, MAX-Lab and Advanced Light Source (Held), user committees at

Diamond (Chippindale) and ISIS (Powell, Crystallography Chair, 2011-16), and the Diamond-II User working group for a new nanofocus beamline (Chippindale, 2020-date), reflecting our commitment for engagement with the facilities beyond that of routine users.

Over 180 keynote/plenary/invited lectures have been delivered across the world (11.3 per FTE). Notable examples include: Hamley, "*Bioactive Peptides and Their Conjugates: From Nanoscale Self-Assembly, towards Therapeutics*", keynote, e-MRS Spring Meeting 2015, Lille, France; Vaqueiro, "*Layered Oxychalcogenides as Thermoelectric Materials*", 12th European Conference on Thermoelectrics, Madrid, Spain, 2014; Powell "*Materials Design Strategies for Sulphide Thermoelectrics*" 37th International Conference on Thermoelectrics, Caen, France, 2018; Held, "*In-Situ Investigation of Energy Systems using Ambient-Pressure X-Ray Photoelectron Spectroscopy*", 254th ACS National Meeting, Washington DC, USA, 2017; Cramer, "*Developing new diagnostic tests using biobank samples, robotic sample preparation and mass spectrometry*", keynote, Lab Automation and Robotics 2016, Berlin, Germany, 2016; Cardin, "*Targeting DNA with ruthenium complexes*", plenary, ISNAC2017, Tokyo, Japan.

Beyond our core scientific communities, we engage with a variety of audiences in disseminating our research. This includes an extensive outreach programme offering a 'menu' of research-focused lectures delivered by CSD staff (Chippindale, Colquhoun, Grau-Crespo, Vaqueiro) from which schools select; research-focused presentations at meetings of the Association for Science Education (Squires, Vaqueiro) and talks for the general public, including events at *Café Scientifique* (Harwood) and The Wilmslow Guild (Colquhoun).