

Unit-level environment template (REF5b)

Institution: Durham University

Unit of assessment: UoA 8 CHEMISTRY

Section 1. Unit context and structure, research and impact strategy

Unit context: Chemistry is one of eight departments within the Science Faculty and is a thriving centre for research and education. We have an academic staff of: 22 Full, 11 Associate and 8 Assistant Professors; 5 Fellows (RS URF, GCRF, BBSRC) and 5 Teaching staff (total male/female 40/11; BAME 4; REF headcount 46; Cat. A FTE 44.2), supported by cohorts of ca. 40 PDRA and ca. 90 PhD students. Four current staff (Badyal, Howard, Hutson, Parker) are Fellows of the Royal Society. The academic community is supported by 45 non-academic staff (41.8 FTE) (technical, administrative, analytical). We teach ca. 600 FTE undergraduates via 4-year MChem (Research, International and Industry routes) and 3-year BSc courses as well as multi-disciplinary degrees under the Natural Sciences programme. We have a strong ethos for collaborative research and impact within the Department, with the University's Research Centres and Institutes, and with strategic external partners.

The Department is ranked highly in 2021 Chemistry league tables (UK: 4th Times, 4th Complete University guides, 2nd Guardian) and Top 100 in the world (85th Physical sciences, Times Higher; 51-100 QS(2020)). In the REF period, the Department has published 1413 outputs with a total citation count of >22,000 and combined h-5 index of 47 (SciVal, Aug 2020).

Research strategy, themes and structure: Durham Chemistry's research is organised to enable the discipline-focussed breakthroughs that come from individual PIs tackling specific research problems, whilst simultaneously targeting the larger societal-scale research themes that can only be tackled by building multi-investigator collaborative teams (Figure 1). This approach was developed under the University 2017–2027 strategy and outlined in the institutional environment submission.

Following REF2014 we collectively identified three central interdisciplinary grand-challenge themes where we have the critical mass and core skills to have impact: “New Materials”, the “Bio-Economy” and “Manufacturing the Future”. The New Materials theme allow us to target the technology-enabling new compounds, composites and treatments identified as needed for economic success by Innovate UK; the Bio-Economy theme clusters activities around bio-based products, sustainable and resource-efficient solutions to challenges in the food and chemical sectors, health and the environment; while Manufacturing the Future helps tension research against delivering real-world impact. The themes link to our 41 PI-led research groups through six Research Groupings (RGs). RGs bring together teams of between four and twelve PIs, from different traditional I/O/P subdisciplines, who can tackle research projects collaboratively through either aligned (for scale) or complementary skills. The constituency of the RGs, their areas of scientific focus and their 2020–25 aims are summarised in Table 1.

RG activities are underpinned by two additional cross-grouping focus areas: “Analytical and spectroscopy” and “Education and training”. The first of these enable 12 analytical research support staff to work closely with PIs to develop new techniques and maintain infrastructure to underpin our research portfolio. The Education focus guides pedagogy in the Department, helps link research to our undergraduate curricula and helps us develop and deliver effective research training to our CDT and other PhD students.

We have a strong focus on interdisciplinary research (expanded later) and intra-Departmental structures mesh with larger research Centres and Institutes within the University (Figure 1). We also interact closely with many external partners such as industry,

Northern 8 (N8) University partners and catapult centres such as the Centre for Process Innovation (CPI). As a specific example, our Bioactive Chemistry Research Grouping comprises seven PI-led groups who work alongside staff from other Departments under the umbrella of Durham's Biophysical Science Institute (BSI); they lead a multi-partner international GCRF Network in Neglected Tropical Diseases as part of the activities of the Centre for Infectious Diseases, which is part of the cross-faculty Wolfson Research Institute for Health and Wellbeing.

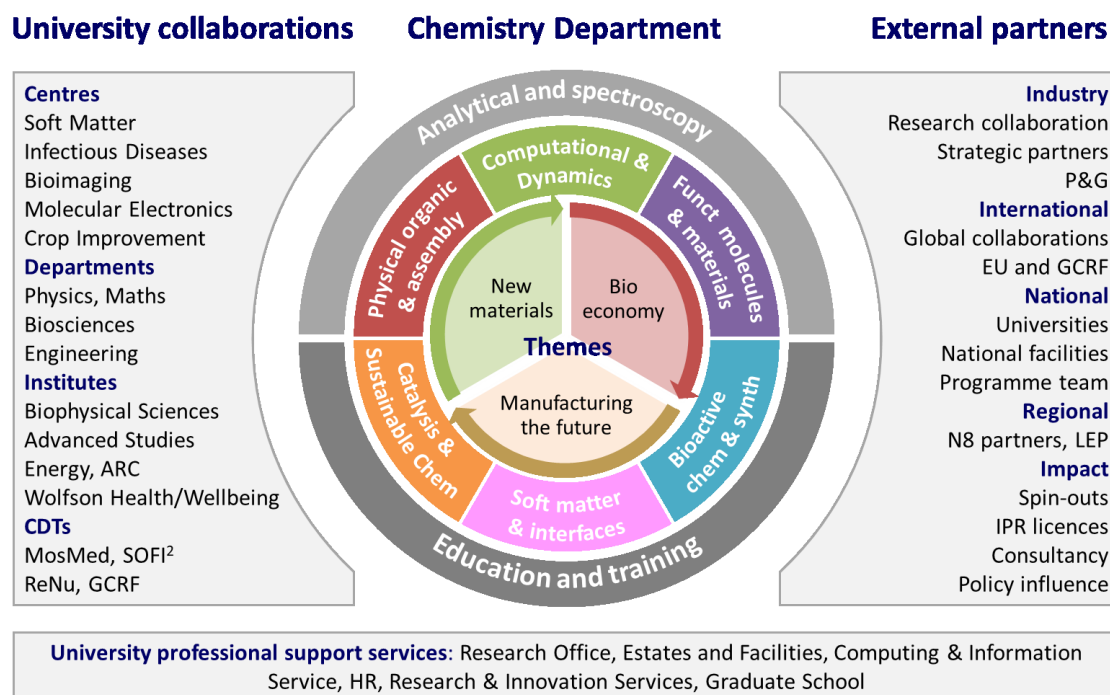


Figure 1: Research organisation at DU Chemistry

Research focus and research objectives (2020–2025): The focus areas of each RG is summarised in Table 1 which also contains the overarching aims of the grouping for the next five-year period. These are reviewed and agreed annually by Research Committee.

Table 1: Research Groupings (RGs); RG leader	Research focus areas
	2020–25 specific aims
Soft Matter and Interfaces <i>Badyal, Bain, Cooper, Hutchings, Katakay, Miller, Thompson, Wilson</i>	<p>We adopt an integrated, interdisciplinary approach across soft matter and soft interface research from fundamental aspects to fully realised industrial and societal applications, and from development of computational methodology to experimental innovation. We combine expertise across disciplines in chemistry at key interfaces with physics and biology.</p> <p>1. Further expand portfolio of industry-aligned research enabled by Soft Matter and Functional Interfaces 2 CDT (SOFI) renewal and continue strategic partnership research with P&G; 2. Develop predictive tools for design and optimisation of industrial formulations; 3. Translate bio-inspired surface technology into societal benefits in</p>

	water harvesting, water purification, and antimicrobial protection.
Bioactive Chemistry and Synthesis <i>Cobb, Kadri*, Karunakaran*, Mahon, Mackenzie*, Pohl, Sanderson, Steel</i>	<p>The grouping applies its expertise in physical, bioinorganic and organic chemistry, integrated structural biology, spectroscopy and imaging of biological matter to solve fundamental problems at the interface between chemistry and biosciences. We place particular emphasis on designing and synthesising chemical probes to address neglected tropical diseases and wider therapeutics.</p> <p>1. Expand our research portfolio and strategic partnerships with companies in the bio-economy and international research organisations of the Molecular Science for Medicine CDT (MosMed). 2. Establish a sustainable research program on Neglected Tropical Diseases (NTD) with our overseas partners building on the success of the GCRF NTD Network; 3. Develop new chemical compounds and tools for drug discovery and diagnostics.</p>
Computational and Dynamics <i>Curchod*, Hutson, Tozer, Verlet, Wrede</i>	<p>Develop the fundamental scientific understanding that underpins chemical and physical processes through the development and use of computational quantum and classical mechanics, and by applying laser manipulation and innovative spectroscopic methods.</p> <p>1. Develop and apply novel methods at ultra-cold temperatures to enable new quantum technologies enabled by £6.7M Quantum Science with Ultracold Molecules (QSUM) grant; 2. Exploit sensitive new spectroscopic methods to advance health-care technologies. 3. Design and use methods to understand photon and electron driven chemistry in materials, the atmosphere and the interstellar medium.</p>
Functional Molecules and Materials <i>Beeby, Bryce, Coleman, I Evans, J Evans, Hodgkinson, Howard, Johnston*, McGonigal*, Pal^s, Palsson, Parker, Williams</i>	<p>Preparation, analysis, understanding and exploitation of functional molecules and materials with applications from materials science to the life sciences. Our focus areas include energy generation, storage and conversion, imaging, sensing and detection, electronic, magnetic and photoresponsive properties, bioactive and pharmaceutical behaviour.</p> <p>1. Further develop strengths in photo active materials and molecules for sensing and therapeutics; 2. Develop new research strengths in switchable molecular materials and their applications. 3. Strengthen energy materials research strands including enhanced training through the Renewable Energy CDT (ReNu).</p>
Catalysis and Sustainable Chemical Processes <i>Baxendale, Beaumont, Dyer, Fox, Sandford, Taylor*, Walton, Whiting</i>	<p>Demonstrate new clean & sustainable routes for the production of feedstock chemicals from biomass and waste materials. Identify step-change improvements in established chemical manufacturing routes by efficiency of both chemistries and processes. Use insight from</p>

	cutting-edge characterisation and mechanistic science to deliver improved catalyst systems for industry.
	1. Exploit and develop IPR around flow-catalysis and microprocess chemistry; 2. Develop efficient methane activation/oxidation catalysts for resource-efficient chemical processes with industry partners; 3. Continue to grow existing external partnerships spanning industry, global academia and the EPSRC UK Catalysis Hub and the N8.
Physical Organic & Assembly <i>Hodgson, Kitching[§], O'Donoghue, Steed</i>	Molecular assembly and function in organic molecules and materials. Molecular properties and reactivities are tailored through gaining fundamental (quantitative) understanding using photophysical, computational, kinetic, supramolecular and crystallographic techniques to inform synthesis of new molecules, materials and processes.
	1. Exploit cutting edge kinetic analysis for <i>operando</i> delineation of mechanisms and predicting reactivity patterns in areas including chiral quaternary ammonium salts, reactivity scales of carbenes and phosphorylation reactions; 2. Deliver quantitative understanding of the intermolecular interactions underpinning self-assembly processes; 3. Apply our understanding to new chemistries including enzyme cofactors, industrial biocatalysts and designer crystallisations.

ECR; [§]Royal Society URF, now permanent; [†]GCRF Fellow; ^{}BBSRC Fellow

The Department as a whole has set five overarching focus areas for 2020–2025:

- **Funding/building on strengths:** We plan a number of collaborative multi-disciplinary, multi-investigator research activities based on the strength areas of our Research Groupings and our links to University research centres and other partners. These include: photo active materials and molecules for sensing, therapeutic and emission-dependent applications; exploitation of first-principles soft-matter modelling to societally important formulation challenges; application of biochemical expertise to treat neglected tropical diseases; improved understanding of photon and electron driven chemistry in materials, the atmosphere and the interstellar medium; improved industrial sustainability via application of novel chemical processes, mechanistic insight and enhanced catalysts.
- **Partnerships:** One of Durham's strengths has been our ability to assemble dynamic PI teams to tackle interdisciplinary research challenges, often in partnership with other Durham Departments or external bodies. Partnership-working remains a high priority. We will continue to focus on key industry-facing research partnerships. We will exploit links developed through recent ERDF Collaborative Outreach to SME's in Applied Surface Engineering Technologies (COAST) funding to continue collaborative research with local SMEs. We will follow through on a number of initiatives in collaboration with our local LEP, the N8 and the Centre for Process and Innovation (CPI). We will continue to develop our research partnership with P&G, with particular focus on soft matter chemistry and challenges at the chemistry-life sciences boundary. We will develop new industrial partnerships.
- **Studentships and community:** We will continue to attract the best staff and students to Durham University. Sustain our research community by identifying internal and external funding streams to keep PhD student enrolment at ca. 35 pa. We will support our current

CDTs in delivering high-quality PhD training, and plan for their renewal. Our EDI strategy aims to foster an inclusive, supportive, collaborative and collegiate culture at all levels of the Department. Our planned activities should allow us to obtain Athena Swan silver recognition within five years. We will ensure that staff working across the research spectrum from blue-skies to applied are appropriately supported, recognised and rewarded, and will continue to encourage student enterprise, using Plastech (see below) as an exemplar.

- *Internationalisation*: We will grow our international links through Erasmus/Turing, industry and academic research collaborations. We will exploit research collaborations built up through recent GCRF funding in the area of neglected tropical diseases and are building research links to a number of international companies through research interactions detailed elsewhere.
- *Infrastructure*: A successful chemistry department needs a fit-for-purpose building and state-of-the-art analytical facilities. By 2025 we will have implemented the laboratory and infrastructure refurbishment with a £15M investment from the University. In parallel, we are working towards a new Chemistry building with a target build date of 2030.

Research management: Monitoring and reviewing our research strategy are the responsibilities of our Research Committee (ResCom) (Table 2). ResCom reports directly to the Board of Studies (BOSIC), which administrates, supports and monitors all Departmental activities. Cross-committee representation means that key aspects of EDI, safety, staff progression, outreach and postgraduate training are integral to ResCom operations. We ensure each committee membership has an appropriate balance of gender and career stage and reflect this in our workload model. Research Centres and Institutes (Figure 1) are assessed annually by the Faculty and University Research Committee, on which the Department has representation (Bain is DU Vice Provost Research; Cobb is BSI Director). DU Professional support personnel provide legal, financial, technology transfer, research support, HR and IT services.

Table 2: Committees – Members	Committee remit
Research Committee (ResCom) – DoR, Director of Impact (DoI), HoD, RG leaders underlined in Table 1, Research Admin. (8 male/2 female)	Formulates/implements research and impact strategy, PGR funding, grant applications, awards, impact activities and research leave. Oversees analytical facilities and workshops.
Management Advisory Board (MAB) – HoD, DoR, DoE, Dir. Graduate Studies (DGS), EDI Chair, BOSIC member, Dept. manager. (5 male/2 female)	Advises HoD on education and research strategy and implementation, budgetary, appointments, infrastructure, operational and personnel issues.
Equality, Diversity and Inclusion Committee (EDI) – Chair, Secretary, HoD, 7 staff: 3 PDRA, 2 PGR, 2 UG. (11 male/9 female)	Develops EDI culture within the Department, implements the Race Equality Charter, Athena Swan strategy; advises upon transparency and equality of all Departmental procedures.
Safety Committee – Chair, Secretary, DU safety advisor, Technical safety coordinator, 6 staff, 1 PDRA, 1 PG, Biosciences rep. (9 male/3 female)	Implements DU Health and Safety policies, engender a safe working environment; prevention of injury; oversees good lab practice; monitors safety protocols for the use of radiation, laser, chemical and biological materials.
Department Promotion and Progression Committee (DPPC) –	Appraisal of staff through published University promotion and progression criteria;

<i>HoD, DoR, DoE, 2 BOSIC, external academic, Faculty rep., Dept manager. (6 male/2 female)</i>	recommendations for promotion and discretionary awards, individual feedback on career progress.
<i>Outreach Committee – Chair, 6 staff. (4 male/2 female)</i>	Promotion of activities to enthuse and inform the public in the chemical sciences by targeted visits to schools or festivals.
<i>Graduate Studies Committee (GSC) – DGS, 3 Academics, Postgrad. Admin., 3 PG. (5 male/3 female)</i>	All aspects of recruitment, training, monitoring and welfare of graduate students.

Review of achievements against plans from REF2014: specific plans described in REF 2014 included:

- *Partnerships:* Our strategic partnership with P&G has continued and ICS 3 describes effects on the products and practices within the company. This collaboration has grown to a £26M grant portfolio across the University. The Integrated Chemical Research Facility (ICRF) (£1.4M investment 2013) allowed seven companies and SMEs to complete 18 proof-of-concept studies (e.g. Sterling Pharma, Romag, Chemoxy, Sinopec) contributing £90K income to the Department and initiating longer term research projects (e.g. Thomas Swan, Sinopec). Individual PI-industry collaborations continue to flourish both with UK-based (e.g. GSK, Johnson Matthey, Afton, Syngenta, AstraZeneca, Evonetix) and international companies (e.g. SONY–Germany, Murata–Japan, Shell–USA, Abbvie–USA) via CASE-type and fully funded PhD/PDRA routes.
- *Doctoral training:* We successfully targeted industry-academia training of student cohorts through initiatives with industry, UKRI and EU funders. Our CDT in Soft Matter and Interfaces (SOFI, 2014–2022) recruited 81 PhD students (40 at Durham) over 5 cohorts involving 25 industrial partners including Croda, Mondelez, Nestlé, Synthomer, GSK & Schlumberger. In 2019, several CDTs involving Durham Chemistry were supported: the enhanced SOFI programme (SOFI², 2019–28, £5.4M, Durham-led with Leeds and Edinburgh, 40 students to Durham) collaborates with a larger industrial base including new partners Bayer, IBM and Syngenta; CDT Renewable Energy NE Universities (ReNu led by Northumbria); Durham BBSRC DTP; Durham GCRF internal CDT and MosMed CDT (£7.5M, co-led with Newcastle, 35 PGs to Durham, 2019–28). We led (2014–18) three Marie Curie EU ITN networks: Molesco (£4.5M, 14 partners), MICSED (£1.4M, P&G strategic partner) and Fluor21 (£3M, 11 partners).
- *Future focus 2014–2020:* We responded rapidly to staff changes and new funding opportunities. Research in nano-carbon chemistry led to the flotation of Applied Graphene Materials (AGM) plc (ICS 1) and the ERDF funded COAST project (£4.5M, £810K to Durham) which provided labspace to handle nanomaterials (£580K DU investment) and interface with 19 SME industrial partners. The Bioactive RG targeted neglected tropical diseases leading to a GCRF-funded Network (£8M, 14 partners in South Asia, South America) and led the EU Horizon2020 Virus-X consortium (£7M, 2016–20). Sustainable chemistry research with Sasol and Saudi Aramco and fluorination methodology with Sanofi led to exploitable IPR.
- *Internationalisation:* We have a diverse approach to developing international partnerships. We maintain close international links with our 8 strategically-focused Erasmus partners such as FU Berlin, JMH Wurzburg, CU Leuven (39 students research placements 2015–present; 27 hosted). Our three Durham-led EU ITN networks and GCRF NTD network and many best-with-best individual collaborations with academia and industry further expanded our international reach. For example, strength in sensing at the Bioactive/Functional Molecules RG boundary led to collaborations between Pal

and Tour (Rice, USA) and the POA-RG hosted the prestigious European Symposium on Organic Reactivity (ESOR 2018) conference.

- *Infrastructure and equipment:* We maintained our research analytical equipment portfolio with investment of £1.6M from DU over the period (Section 3).

Investment in people and infrastructure (2020 onwards): Plans include:

- *Equipment and building:* The University has committed funding for a £15M investment programme over 5 years involving refurbishment of research and teaching space and general infrastructure renewal (see Section 3). A new Chemistry building is at the scoping stage for implementation in phase three of the 2017–2027 University strategy with plans to allow a 2030 build start date.
- *Staff appointments:* We plan a relatively stable staffing profile for 2020–2027, and four Cat. A staff have discussed their retirement plans over the next five years with the Department. We are currently advertising externally for a new Head of Department and for two Grade 10 Professor appointments, whose research has a particular emphasis on synthesis to strengthen our activities in our Functional Materials, Soft Matter and/or Biological Chemistry research groupings.

Impact – strategy, context and implementation: Our strategic approach to impact has evolved over decades of working closely with many stakeholders. Our research outputs affect all six main impact areas: *economic* (e.g. creating and hosting businesses, licensing IPR, transferring research to industry), *environmental* (energy-reducing, cleaner processes), *healthcare* (drug syntheses, medical devices), *societal* (outreach activities, historic manuscript analysis), *policy* (drug-regulatory changes) and *professional services* (expert witness consultancy, affirming and changing company strategy and operations). The Durham-P&G team (ICS 3) were awarded the RSC's 2015 "Teamwork in Innovation" award for "multidisciplinary, collaborative and high-impact research leading to product innovation".

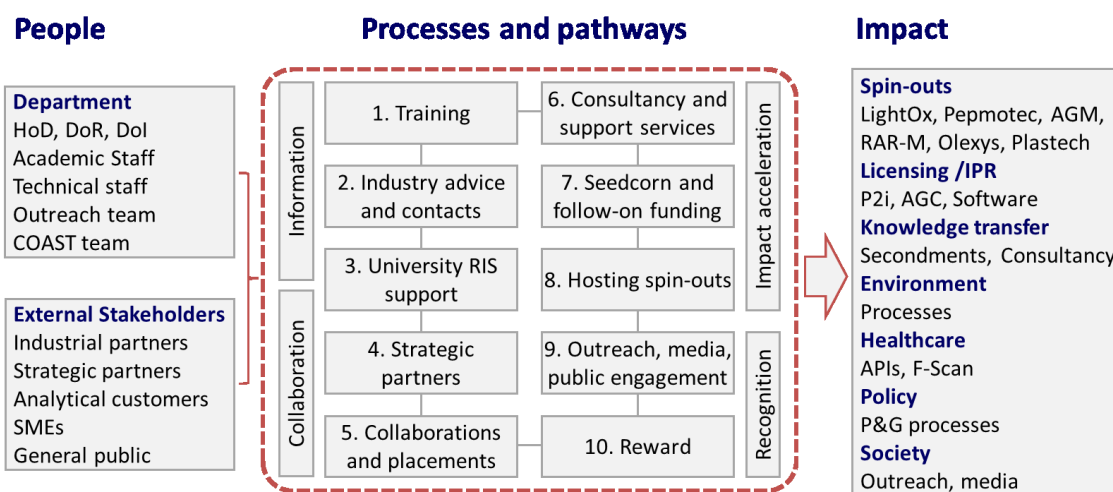


Figure 2: Impact strategy and processes

Our underlying strategy (Figure 2) for developing impact is based on four key enabling functions: *information*, *collaboration*, *acceleration* and *recognition* and activities are run through the well-established processes 1–10 shown in Figure 2, managed by the HoD, DoR and Director of Impact. Examples of each process include:

1. *Impact training*: We have regular (~3 annual) Departmental briefings on areas such as entrepreneurship, InnovateUK funding and outreach via awayday/training sessions (e.g. Industry-Academia linking schemes; outreach activities; Responsible Research and Innovation training for PIs).
2. *Industrial advisory boards*: Several RGs have industrial advisory boards to counsel on research. For example, the Centre for Sustainable Chemical Processes' board has 12 industrial members and meets annually. Our ERDF COAST funding (£4.5M, see above) has allowed interaction with 63 SMEs (including partner CPI interactions).
3. *University Research & Innovation Services (RIS) support*: RIS provides support for developing impact particularly in IPR processes including filing, licensing, registration and protection, spin-out company registration, business plan formulation and venture capital applications. DU holds a portfolio of 20 patents arising from Chemistry research in areas such as liquid movement, nanoparticle switching, peptide science and devices for breath analysis. This portfolio enabled 4 new company spin-outs within period (LightOx, Pepmotec, Nevragenics, PlasTech).
4. *Strategic partners*: We continue to build our strong partnership with Procter and Gamble (P&G, ICS 3). Research funding since the beginning of this collaboration includes the Regional Growth Fund project on surface modification (£1.4M), EU-funded ITN industrial doctorate programme MICSED (2014–2018, £1M) and EPSRC/Industry funded Molecular Migration (£2M). The overall partnership has won the P&G Global Partnership award, the 2015 RSC Teamwork Award, been cited in US Congress and described in letters from P&G's Global Vice President to 10 Downing Street. Our relationship means we can move quickly to co-support new interdisciplinary research opportunities with the company.
5. *Collaborations and placements*: We have built a large network of industrial partners involved in collaborative research through interactions at many levels. Annually, we place ca. 20 4th year MChem students into industry. Industrial chemists present seminars at our fortnightly synthetic seminar series. We host researchers from industry in the ICRF facility and the industrially-linked SOFI CDTs recruited 41 PhD students who spent significant time with their collaborating industrial partner. Our industrial collaborative research portfolio is 17% of our total research income (£36.6M). 28 PhD students have been part or fully funded by industrial partners and Innovate UK.
6. *Consultancy/analytical services*: Departmental expertise and infrastructure has provided impact to external organisations. 18 staff have individual consultancy contracts with 26 global companies. Our analytical services provide data and interpretation to many organisations (typically £100K income pa): solution state NMR has provided spectra and analysis for 16 companies; solid state NMR has supported 12 Universities and 58 companies (income £408K in period); DU spin-out OlexSys provides software for many X-ray crystallography analyses performed world-wide.
7. *Impact acceleration funding*: We use various support mechanisms to translate research ideas (TRL 1–3) to prototype and business cases (TRL 4–6). N8 funding with Thomas Swan enabled IPR that was subsequently developed to the manufacturing scale. EPSRC Impact Acceleration Account (IAA) funding enabled ten projects (£340K plus £180K in-kind contributions) including new antimicrobial applications (Kataky/Coleman, CPI, Smith + Nephew) and custom lipid synthesis (Sanderson, HighForceResearch). The iCURE and Northern Accelerator programmes funded business case development and a business manager for spin-out Pepmotec. The University has secured two tranches of MRC Confidence in Concept funding (led by Cobb, £600K) for 4 PDRAs in Chemistry to develop new IPR (Sanderson, screening technology for cell membranes) and prototype devices (Carty/Wrede, breath acetone sensor device).
8. *Hosting start-ups*: The Department provides space and infrastructure access to spin-out companies in their early years (e.g., LightOx, RAR-M, AGM, OlexSys, PB

Spectroscopy, Plastech and Pepmotec). Beyond the start-up phase, businesses can relocate to incubator space at University-partner Netpark (Reinnervate/Reprocell) or the nearby Wilton Centre, a 75-acre science park (AGM).

9. *Outreach, media and public engagement*: Our outreach team contributes to annual events such as School Science Festival, (3 days, 600 Year 9/10 pupils), NESIP (6th form research project week, 30 students and 5 teachers), Sutton Trust summer school (4 days, 40 Y12 students), Celebrate Science festival (3 days, 7000 visitors) and many smaller scale school visits and public lectures. Media appearances are listed in Section 4.
10. *Reward*: Impact activities are encouraged and recognised in promotion procedures, and discussed during annual staff reviews by DPPC. Staff benefit from a share of any licensing fees arising from IPR and maintain equity in spin-out companies. Coleman (AGM) and Whiting (LightOx/RAR-M) received teaching relief funded by the companies involved to drive growth in the crucial venture capital funding phase.

Impact strategy relationship to case studies: our established mechanisms to support impact are apparent in the development of our case studies:

ICS 1, Graphene: Research was patented and a business case developed with RIS support (Impact process and pathway 3, Figure 2) for the establishment of Durham Graphene Science hosted within the Department (8). Following VC funding, the renamed Applied Graphene Materials, was listed on the AIM stock market with support from staff secondment (10) providing scientific advice (6) and RIS (3). Media coverage appeared in the Sunday Times and Financial Times (9).

ICS 2, Structural Science: collaborative research (5) led to cryogen cooler manufacture and a spin-out company developed with RIS (3) is hosted within the Department (8). New crystallisation techniques were licenced via RIS (3).

ICS 3, Procter and Gamble: following RIS and Department information events (1) a University level strategic partnership (4) was developed. Many collaborations and placements (5) led to technology adoption in-house by P&G. Media coverage (9) included statements to US Governors and the UK Prime Minister's office.

ICS 4, LightOx: collaborative research between Whiting, Pohl and Ambler/Biosciences led to IPR filed by RIS (3). Seedcorn, IAA and Confidence in Concept funding (7) helped develop the science business case and formation of LightOx, initially hosted within the Department (8) and then externally. Staff buy-out for Whiting (10) gave time for developing the business in the early stages when raising VC funding.

Supporting interdisciplinary research: Our research structure (Figure 1) was specifically designed to promote interdisciplinary research. We have strong interdepartmental research collaborations with colleagues in Biosciences, Physics, Engineering, Mathematics and Earth Sciences. Much of this activity is inspired and enabled by our research Centres and Institutes (Figure 1), several managed by Departmental staff (e.g. Cobb and Pohl Direct and co-direct the Biophysical Sciences Institute; Johnson and I Evans are on the Energy Institute board). The integration of 7 groups from Biosciences in Chemistry (each of which shares office space with a Chemistry group) helps foster collaborations. Three staff are 50% appointments with other Departments (Carty, Hutson with Physics; Pohl with Biosciences). Our Natural Sciences undergraduate degree programme encourages collaborations to develop from the 4th year research project stage; typically 15 students per year co-supervised by Chemistry and Biosciences/Physics staff

members, enabling new research activities funded by the Faculty MChem/MSc programmes.

Chemistry staff are also involved in inter-faculty research. Beeby and I Evans are part of multidisciplinary collaborative projects on cultural heritage involving high-profile artefacts from UNESCO World Heritage Sites. Expertise in analytical methods helps elucidate provenance and production methods influencing conservation techniques. Beeby's extensive work on manuscript imaging described in ICS 4. CoFUND/EU funding has brought four Institute for Advanced Study Fellows to the Department. Vogt, for example, worked jointly between Chemistry and History, lecturing on advanced catalyst characterisation, Greek philosophy and the development of models in the physical sciences during his fellowship.

Open research environment: Staff have embraced the open research environment with ca. 95% of our 1413 outputs (2014-2020) outputs fulfilling REF and UKRI OA policy requirements. Publications submitted by international collaborators are the only exceptions. Accepted manuscripts are all deposited on Durham Research Online (DRO) following publisher guidelines within one month of acceptance and research data is deposited within an open access DRO database (a new 5.6PB data storage system for experimental results has just been commissioned). We have made full use of RSC Gold standard open access voucher systems managed by library staff (168 APCs for Gold OA including 68 RSC Gold 4 Gold vouchers) over the REF period. We regularly interact with library staff to incorporate Open Research ideas into the Department (e.g. PlanS). Staff leadership activity in this area includes Howard's role on the Royal Society Open Science committee and Baxendale's role on the Beilstein scientific advisory board. The RS provide national advice on this topic and Beilstein offers platinum open access for all publications and associated data.

Culture of research integrity: The Department performs its research activities with strict adherence to the University's Ethics Policy. Reference to ethical guidelines published by UKRI or Wellcome are made when required.

- Ethical review of all research projects requiring human or animal subjects, whether within the University or with collaborating institutes, is required before research begins and is managed by our Ethics representatives (Pal, Mahon and a lay member from the local community). A report covering projects that required ethical review is tabled at BoSiC and DU Science Faculty Board each October.
- All research collaborations are performed under agreements developed with Legal Services covering legal obligations, financial management, IPR, liability, material transfer, data management, insurance, negligence and termination clauses.
- Regular training is given to all staff in: Data protection laws (GDPR) for both the UK and EU, avoiding unconscious bias, diversity and inclusivity, and collegiate research practices.
- Research ethics is included in Departmental and CDT postgraduate training.

COVID-19 Impact: COVID-19 has had significant impact on Departmental research in 2020. We undertook a number of measures to keep staff and researchers engaged and supported during initial lockdown. Through significant efforts from our technical team, we were able to restart lab-based research from late June, with wider access from September. We have an electronic booking system to enable lab access and contact tracing, have established group- and research-zone bubbles and have implemented procedures for safe

access to analytical facilities and other infrastructure. COVID has not changed our long-term research strategy, just delayed implementation.

Section 2. People

Current staff: our 46 returned research/impact staff (Cat. A) are listed earlier in Table 1 according to their primary Research Grouping.

Staffing recruitment strategy: Our staffing strategy is to continue to develop areas of research strength following DU EDI/Athena Swan principles whilst maintaining an appropriate breadth of chemical knowledge to deliver a world-class, broadly-based, research-led UG programme. Overall, our REF2021 Cat. A return cohort is four more than REF2014 and includes 5 Fellowship holders on fixed-term contracts. Six of our returned staff are ECRs.

- **Leavers:** Seven members of staff (Cat. A) relocated in the REF period: Cameron to Monash (Australia) and Prassides to Osaka (Japan), Engelskirchen to a career in patent law in her native Germany, Hess to TUM Munich, Moseley to Teesside and Kenwright and Khosravi to retirement.
- **Appointments:** Seven staff have been appointed at the Assistant Professor level within the period (replacing the 2 full, 2 associate and 3 assistant Profs listed above). This followed our policy of non-biased appointment of the best candidates available within our broad research areas and growing their careers within the Department: Walton (catalysis), Taylor (catalysis), Johnston (battery technology), McGonigal (supramolecular), Kitching (organic methodology), Mahon (chemical biology/polymer synthesis), Curchod (theory) and Pal (microscopy). Each appointment strengthens a Research Grouping. Each new appointee has rapidly established their research groups and attracted funding (first grant awards to Walton, McGonigal; Taylor, EPSRC Industrial Fellowship; Curchod, ERC).
- **Fellowships:** we have hosted URF (Kitching, Pal), EPSRC (Degiacomi: theory), ERC (Curchod: theory), 1851 (Avestro: synthesis), Newton (Auckett: materials; Das: surface science; Wu: synthesis), CoFund (Porta: chemical biology), GCRF-funded (Kadri, Karunakaran: biochemistry) and BBSRC (Mackenzie) fellows within the REF period who participate in RG activities (Table 1). All potential fellowship candidates are reviewed by MAB for scientific quality and strategic fit. A mentor is assigned to help them develop the strongest possible research application. Most fellows are supported within the laboratories of established PIs and are allocated 4th year MChem students to support their research. Pal & Kitching were appointed to permanent positions in Chemistry, Avestro to Chemistry at York and Degiacomi to Durham Physics following open advertisements exemplifying the career development opportunities we provide.

Staff development strategy: We have a strong commitment to support staff at all levels following our EDI/Athena Swan plans including:

- **Mentorship:** Mentorship is provided at all career stages following the University "Building a Mentorship Culture" programme, and explicitly recognised in promotion processes.
- **Training:** We work with the Durham Centre for Academic Development (DCAD) to support all researchers in the Department. Bespoke courses delivered through their "Researcher Development Programme" are used to train staff in best research practice, ethics and to ensure adherence to the implemented Concordat to Support the Career Development of Researchers.

- *Probation, appraisal and promotion:* We follow University DPPC processes and fifteen staff (10 M, 5 F) have been promoted within the first 3 years of this new scheme. Academic staff and independent fellows develop Personal Research Plans (PRPs) annually with a mentor to discuss research goals and ambitions/opportunities for the future.
- *Research leave:* All staff are encouraged to take 2 or 3 terms of contiguous research leave to enable sufficient time to concentrate on stated key research objectives such as skills development, publications, impact development and grant capture. Applications for research leave are assessed by ResCom to ensure 6–9 staff take research leave each academic year.
- *Technical staff:* We have supported staff to take part-time degrees and the University follows the Technicians Commitment. Chemistry technical achievements have been highlighted and celebrated at University-wide events.

Supporting ECRs and PDRA: The management team and appointed mentors help new staff by:

- *Induction:* All staff receive Departmental introductions and attend a University-wide induction day which introduces the University career progression processes and has a training session on tackling unconscious bias.
- *ECR training:* ECRs engage in training programmes within Chemistry (library resources, IT, HSE, financial processes) and University-wide (first aid, grant writing workshops, leading research programmes). We support ECRs in completion of the PG Certificate in Learning and Teaching in HE, managing research projects, building research funding portfolios and developing research group culture.
- *Post-doctoral researchers:* We have hosted 60 PDRA researchers over the REF period and recognise the vital contribution they make to our research output. Progress in research and wider career advice is provided and developed in annual DPPC review. Mentorship in developing CVs, fellowship applications and career progression is managed by the supervisor and independent mentors appointed at the start of the PDRA contract. Many PDRAs contribute to UG teaching provision, leading tutorial and workshop classes and all PDRAs are able to access University-wide transferable skills training courses. The PDRA community is supported by a Departmental PDRA Forum (social and career-advice events) and a University-wide forum and a PDRA representative is a member of BOSIC to enhance cohort integration.

Facilitating collaborations with industry: we operate a variety of procedures to stimulate and facilitate staff exchanges with industry which often lead to research or impact generation:

- *Research collaboration with industry:* The Department has a well-established track record of collaborating with industry. Over the REF period 57 PhD studentships have been fully or part funded by international industries (including GSK, Johnson Matthey, Murata, P&G, Syngenta, AstraZeneca, Xaar, FFEI, Lynx, Life Arc, High Force Research, Inca Digital Printers, Merck, Unilever, Bristol Myers Squibb, Croda, Akzo Nobel, Sun Chemical, Danone Nutricia, Nestlé, Flotek, Sinopec, Screen, Chiesi, Aptuit). 114 of our publications (8%) list an industrial collaborator as a co-author.
- *Secondments:* The Department has hosted researchers from several companies (e.g. Sinopec, Johnson Matthey, Thomas Swan, Lomox) for periods of between 1-12 months to provide access to specialist expertise and skill bases. Staff secondments to industry include Coleman to AGM and Whiting to LightOx.

- *Industry/Entrepreneur Fellowships:* Taylor, recruited to a lectureship from BP, holds an EPSRC Industrial Manufacturing Fellowship. David King, following a long and successful career in the chemical industry, is employed part-time within Chemistry as a Royal Society Entrepreneur in Residence to develop entrepreneurship and industrial links across research and undergraduate portfolios.

Recognition and reward: The principal methods of rewarding all staff for research and impact is by the DPPC promotion process. Exceptional Contribution points or Merit Awards are used for different staff grades. Staff receive a 10% return of net overheads raised on external research grants as unrestricted research group funding to stimulate new activities. Departmental returns are spent on PG funding and supporting projects. Royalties and license fees arising from DU IPR are shared between the inventors and DU.

Research students: The research interests and collaborative nature of the Department are such that individual research groups are small-to-medium in size; the largest group in the Department has typically been *ca.*10 members, though our CDTs involve larger cohorts. Despite external funding challenges, our PhD student cohorts over the REF period (Table 3) remain around 33 pa normally on 39-month PhD tuition programmes. We maintain a reasonable PG gender balance (typically ~43% female).

Table 3: PhD student cohorts	2013 /14	2014 /15	2015 /16	2016 /17	2017 /18	2018 /19	2019 /20	Totals
PhD Students starting	41	32	34	31	24	34	35	231
PhD completions (REF4a)	21.1	23.5	27.6	39.6	37.2	30.5	23.0	202.5

- *PG recruitment:* GSC oversees on-line applications, site visits, interviews and offers. We recruit globally via the DU website, personal, national and international contacts, *findaphd.ac.uk* and related portals, the chemical press and the EU study portal (CORDIS).
- *PG funding sources:* Our supervision, review and feedback mechanisms over the REF period have allowed 231 PhD students to start their studies funded from a variety of sources (Durham funded 69; CDTs 40; industry 48; others inc. EDRF/EU/GCRF/self-funded 74).
- *PG support mechanisms:* GSC is responsible for representing and communicating training, research, EDI and pastoral matters important to PGs; disputes are overseen and managed by the GSC Chair with support from University services including Legal, Disability Support and the International Office. Each PhD student is assigned a supervisory team comprising of a principal and secondary supervisor who monitor progress and advise on research aims, experiment design and results interpretation on a daily basis. Regular research group meetings and quarterly reports help maintain focus on research objectives, identify problems and solutions while enhancing communication skills. Our PhD cohort has a representative on BOSIC, GSC, EDI and Safety Committees, detailed in Table 2.
- *Scientific and skills development:* Since 2009, our graduate training programme has provided a flexible model for cohort-based training which emphasises the importance of continued in-depth learning throughout the PhD programme. Students undertake a training skills analysis using PebblePad. A portfolio of lecture modules allows PhD students and supervisors to create a tailor-made training package by selecting from a menu of *ca.* 40 courses, both internal and external, ranging from traditional lecture

modules to small group tutorials and guided reading. Seminars, research colloquia and our Annual PhD Gala Symposium, where graduating students present their research to the Department and penultimate year students engage in poster presentations, supplemented by activities organised by the University Research Institutes (BSI, Energy, IAS), provide communication skill enhancement. Progress is monitored by DU GradSchool via formal reports (after 8 and 20 months of full-time research) and student-led blogs of project meetings. EDI considerations are integrated into postgraduate training.

- *Transferable skill development:* We develop novel PhD training mechanisms to build strong interdisciplinary graduate-student cohorts which are embedded in Durham's Doctoral Training Centre strategy. Our CDTs (SoFI, MosMed, GCRF, ReNu, Energy) provide training in enterprise, communication, entrepreneurship and project management boosting employability. All modules are available to all Departmental PhD students. University level Researcher Development Programmes (online modules developed with Epigeum) are available for transferable skills training. The PG Events Committee were awarded an RSC Inclusion and Diversity Grant (2016) to fund a series of informal discussions on entering academia, research and career development and CV preparation.
- *PG development of impact:* PGs are encouraged to develop impact/entrepreneurial ideas even at this early stage of their career. A challenge exercise as part of the SOFI CDT mini-MBA module led to three PG students developing DU spin-out Plastech Innovation, which processes plastic waste into aggregate for concrete reducing incineration and landfill costs. Plastech was recognised by the Shell LiveWIRE April Smarter Future Award and by the CBI as one of the "20 companies to watch in 2020" within the NE.

Student and PDRA experience: An indication of the success of our PhD training is given by the career destination and achievements of our alumni from the REF period:

- We promote and encourage PhD travel, research exchanges and attendance at international training schools. 58 of our PhD students spent 1–3 month placements in the laboratories of their industrial sponsors. Academic collaborations allowed 12 PhD students to study in international institutions, including Harvard, California, Rennes, Ropar, Kyushu, Dresden, Tarragona and Rio de Janeiro. All PGs are supported financially to attend at least one international conference.
- Our PhD students are in high demand after completing their studies. Analysis of those graduating in period shows that all seeking employment were successful. Of known first-destinations, 49% continued research in academia as PDRA's, 6% entered secondary school teaching positions, 38% entered the chemical industry while 7% followed other careers.
- During the REF period, 18 of our PhDs/PDRA's took up academic positions world-wide within 3 years of completing their studies at Durham including posts in Vienna, Angers, Kent, Loughborough, Dublin, Victoria, Egypt, Malaysia, Finland, Iceland, Thailand, Northumbria, Newcastle and China.

Equality and diversity: The EDI Committee forms a core part of our management activities. Within the REF period EDI considerations have led to changes in Departmental activities: all meetings and seminars are held 9.30–16.00; working-from-home was encouraged pre-Covid; teaching timetabling takes into account care responsibilities; all search, interview and appointment committees follow EDI principles; our workload model balances teaching/admin load; all staff have completed workshops run by HR professionals on Equality and Diversity, Collegiate Working and Unconscious Bias; appointments are

made on an equal opportunity basis. The Department was awarded Athena Swan bronze status (2017) and is committed to apply for silver in 2021.

- *Staff profile:* We have eleven female members on our academic and teaching team and four BAME staff returned as Cat. A. Our 2019 undergraduate intake was 40% female and postgraduate 43%. Our staff profile includes individuals of different gender, ethnicity, with declared disabilities and with significant caring commitments, all of whom are recognised for their contributions to the Department. Our staff (both fixed-term and permanent) come from countries including Belgium, Germany, Spain, Hungary, India, Ireland, Russia, Serbia, Sweden and the UK. Our 2019 postgraduate population intake came from eight countries. We work with individual staff members to accommodate requests for part-time working to allow caring and other activities. Four of our category A returned staff work part-time.
- *Career pathways for fixed-term staff:* Fixed-term staff (Fellows, PDRAs) are assigned mentors to provide advice on career development and job applications. Fellowship holders are encouraged to apply for non-fixed term positions in open competition within the Department if a suitable post becomes available. This follows our policy of appointing the best candidate following a global recruitment process. Retention cases for outstanding fellowship holders are made to the Faculty.
- *Staff support:* The Department offers staff returning to work a reduced workload (50%) and flexible working hours. Research leave is offered after parental leave, and we have space and facilities in the Department for breastfeeding. University policy provides funding to cover care costs/responsibilities when travelling on business.
- *Staff and PGR well-being:* Informal contact, the mentor system and ADR process act as early warning signals for problems with staff well-being. Occupational Health (OH) within the University is contacted and confidential courses of action are taken after discussions with the staff member affected and line manager. Five staff have completed mental health 'first aid' training in conjunction with OH office. Staff and PGs are encouraged to report instances of ill-health, bullying or mental health issues first to their line manager/supervisor and then to HR/DGS. An action plan involving appropriate University support services is initiated. Leave of absence from the Department is supported by extension of the tuition period.
- *Role models:* We celebrate the success of all individuals to provide role models for ECRs and students. We include a diverse range of speakers from academic and industrial backgrounds in our seminar series and flagship "Durham Lectures" programme; two of the last five annual lecturers have been female.
- *EDI for REF:* The submission was managed by the HoD, DoR and DoI with support from Research Committee – a team of ten including two female staff across Associate/Full Professor levels, and followed the procedures articulated in the institutional REF Code of Practice. Two female and one BAME staff member (from a team of eight) graded outputs as part of our REF papers selection process and one female of four external readers helped calibrate our own assessments. Outputs were selected from all RGs (Cat A and B staff) focusing on scientific excellence and originality to give an accurate representation of the Department's research strengths.

Section 3. Income, infrastructure and facilities

Research income: Our aim has been to diversify income streams to include industry, InnovateUK, GCRF and EU funding programmes, self-funded overseas students with scholarships, and to target larger collaborative grants. Research income over the period totals £37.4M (REF4b) and a comparison with REF2014 data (Table 4) shows the

continuation of a broad-based research funding portfolio with a particular increase in EU funding over the period.

Table 4. Funding	REF 2014 (£M)	REF2014 (%)	REF2020 (£M)	REF2020 (%)
RCUK/UKRI	20.3	69	21.1	56
Industry	3.4	12	6.2	16
EU	3.7	13	8.9	24
Others	1.8	6	1.2	4
Total	29.2	100	37.4	100

- *EDI support for acquiring research funding:* All staff are encouraged to lead major, multi-PI grant applications (e.g. O'Donoghue led a CDT bid) and this is monitored by ResCom and EDI committees. All staff receive individual advice, internal peer review and support from Research Office staff. All staff have equal access to resources and free-at-point-of-access analytical facilities.
- *Large research consortia and major grant awards (>£1m):* Examples of Durham-led major multi-partner collaborative grants are shown in Table 5.

Table 5	Funding	Title and Collaborators
Cobb, Sandford	EU ITN, £3.3M (2014–18)	Fluor21: Organofluorine Chemistry 7 academic and 4 industrial partners in EU
Bryce	EU ITN, £4.5M (2014–18)	MOLESCO: Molecular Scale Electronics 10 academic and 9 industrial partners in EU
J Evans	EU ITN, £1M (2014–18)	MICSED: Molecular Interactions in Complex Systems P&G Belgium and Germany innovation centres
Bain	EPSRC, £2.3M (2016–20)	Evaporative drying of droplets and the formation of microstructured and functional particles and films DU Engineering, Bristol, 14 industrial partners
Cobb, Steel, Pohl, Sandford	GCRF, £8M (2017–21)	A Global Network for Neglected Tropical Diseases 14 partners in Asia, South America and York, UK
Pohl	Horizon2020, £7M (2016–20)	Virus-X: Viral Metagenomics for Innovation value 15 participants from 8 EU countries
Hutson	EPSRC, £6.7M (2017–22)	QSUM: Quantum Science with Ultracold Molecules DU Physics, Imperial London, Oxford
Bain, Hutchings	EPSRC, £5.4M (2019–28)	CDT: Soft Matter for Formulation and Industrial Innovation (SOFI ²) Edinburgh, Leeds and >25 industry partners
Pohl, Cobb	EPSRC, £7.5M (2019–28)	CDT: Molecular Sciences for Medicine Newcastle, Medical School
Wilson Thompson	EPSRC+Industry, £2M (2017–21)	Molecular Migration Durham, Sheffield, B'ham, P&G, Akzo, Modelez
Coleman	ERDF, £4.5M (2017–20)	COAST: Collaborative Outreach in Applied Surface Technologies CPI and 19 industrial partners

Infrastructure and facilities: The University has continued to invest in Chemistry infrastructure (buildings and equipment) and technical support to support the needs of our Research Groupings and PI groups. ResCom oversees investment of Departmental and University research funds.

- *Technical and support staff:* Analytical services are free-at-point-of-access for all researchers; this is of particular importance in supporting ECRs. Our major Research Services (NMR, Mass Spectrometry, Crystallography and Separation Science) are managed and supported by 8.2 FTE staff. Other analytical services are supported by 3 FTE additional technical staff. Services are given an annual operating budget by the Department. Other services operate as "Facilities" and are funded collaboratively by individual research groups/groupings. We have dedicated mechanical (2 FTE), glassblowing (2 FTE) and electronics (2 FTE) workshops. A further 7 FTE of our technical team provide support in purchasing, safety, waste-disposal and building management. Administrative/secretarial support for education and research is provided by a team of 7.2 FTE and we have 5 FTE teaching laboratory staff and 5.4 FTE lab attendants.
- *External income:* Analytical service staff (Category C) engage with external users to raise income and build links with industry. For example, the solid-state NMR service has provided analyses to 58 industrial customers raising £408K while solution state NMR spectra and analyses were supplied to 16 companies within the UK.
- *Investment in estate:* Through University support, £15M is allocated (2020–25) for teaching and research laboratory upgrades including heating/air handling infrastructure and IT cabling upgrades. £2M has been invested in new gas pipework throughout the Chemistry building; £1.8M in new fire alarm and protection systems.
- *Faculty/Library/IT facilities:* We have access to high-end electron microscopes operated as a DU Science Faculty facility and to excellent library facilities with a 2–4% annual increase on Chemistry resource between 2014 and 2019 to £283K (2019–20) for books, journals and other publications that are freely available to all staff. Estates and Facilities, financial management and IT support are provided by centralised resource.
- *Specialist research infrastructure and facilities:* In the REF period we have invested a further £2M in research equipment including solution state NMR (£400K), mass spectrometry (£120K), crystallography (£440K), microscopies (£365K), chemical analysis (£170K), thermal analysis (£200K), floating zone furnace (£440K) and separation science (£315K) supported by DU funding. This has allowed us to significantly enhance the capabilities our analytical equipment base (Table 6).
- *Collaborative use of research infrastructure:* We work with partners in the N8 Universities to implement best-practice for infrastructure sharing. High Performance Computing facilities located at Leeds augment local facilities and members of the ResoN8 network of NMR facility managers were nominated for a Papin Prize in 2019. recognising sharing of equipment and training within N8 Universities.
- *Major research facilities:* 9 staff have accessed major research facilities (e.g. Diamond, ISIS, ILL) (total £ 4.2M in-kind, REF4c). For example, Thompson has utilised ISIS (£1.6M value) for projects in collaboration with P&G (Belgium and Germany), Akzo and Mondelez International Microstar as part of the Stability project investigating behaviour of lubricants under shear.

Table 6: Equipment

Major Services	Solution-State NMR	Agilent 700, 600, 500 MHz; Bruker 400 MHz (×3)
	Mass Spectrometry	GCMS-QP2010; Autoflex II ToF/ToF; QToF Premier; LCT Premier XE; TQD; Xevo QToF; Synapt G2s HDMS
	X-ray Crystallography	2 Bruker small-molecule single crystal diffractometers; X-ray reflectometry; small angle X-ray scattering; Bruker Microstar rotating anode; Innovadyne nanolitre crystallisation robot
Other Services	Separation Science	3 HPLCs (diode-array, UV-vis and RI detectors); Mass Directed AutoPurification System; GC-FID, GC-TCD; 2 ion chromatographs; Viscotek Trisec SEC (×2)
	Thermal Analysis	2 PE TGAs with Hiden evolved gas MS; PE simultaneous thermal analyser (STA); PE TGA/IR/GC-MS system
	Probe Microscopy	2 Leica SP5 confocal microscopes; Bruker and AIST-NT scanning probe microscopes for: semi/non/contact, conductive, tuning fork and peak force AFM, LFM, advanced MFM, Kelvin probe, capacitance and EFM, STM, SNOM and 3D scanning imaging; nanolithography/manipulation capabilities and tip enhanced Raman spectroscopy (TERS); fluid cell and hot stage microscopy
Facilities/Other	Solid State NMR	Bruker: 500 MHz, 400 MHz; Varian: 300 MHz; ultra-fast MAS
	Ion Beam Accelerator	NEC Pelletron accelerator: forward recoil scattering, Rutherford & non-Rutherford backscattering, nuclear reaction analysis, PIXE
	Materials Characterisation	3 Bruker high and low T powder X-ray diffractometers; QD SQUID magnetometer and PPMS (physical properties measurement system shared with Physics); XPS; environmental SEM; impedance rig; diffuse reflectance; IR spectroscopy; Faculty-run transmission and scanning electron microscopes
	Spectroscopy	Circular dichroism; CPL; spectro-electrochemistry; time-resolved luminescence IR and Raman microscopy; light scattering; multi-cuvette UV-vis spectrophotometry
	Miscellaneous/Other	Quartz crystal microbalance; elemental fluorine and gas handling facility; flow/process equipment including GCMS on-line analysis; high-pressure research laboratory; nano-materials laboratory; catalytic pyrolysis and test facility; protein production facility consisting of Harbiger Bioreactor, AktaPure FPLC, Biacore T100 surface plasmon resonance and Micocal ITC; floating furnace
	High Performance Computing	HPC is provided via Hamilton, the University's 4800-processor core parallel supercomputer

Links between impact and infrastructure, facilities and expertise: Our infrastructure and expertise directly enables research impact by a variety of methods.

- *Relation to case studies:* ICS 1 Graphene relied upon Faculty SEM/TEM facilities; ICS 2 Structural Science utilises the extensive X-ray and powder diffraction facilities; ICS 3

P&G utilises analytical facilities, surface characterisation, computational modelling infrastructure; and ICS 4 LightOx required spectroscopic characterisation of small molecule probes using NMR and Mass spectroscopy facilities.

- *Consultancy and professional services:* our expertise and infrastructure are used to engage with stakeholders via consultancies as detailed earlier. Four staff have contracts to provide expert witness advice for (confidential) legal matters.
- *Training and staff secondment:* Sterling Pharma Solutions and Thomas Swan have carried out consultative research projects to meet customer requirements using our industry-facing high pressure and fluorine labs. Chemists from Sterling Pharmaceutical Solutions were seconded to DU to complete a contract for a Japanese pharmaceutical customer.
- *Benefits in-kind:* Our strategic partnership with P&G has led to the provision of equipment from the company into the Department to carry out collaborative research experiments and equipment developed at Durham has been purchased and adopted by P&G in-house (see ICS 3).

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

Collaborative research lies at the core of many of our activities, and all our academic staff make significant contributions to the chemical science and wider communities. Our outputs are the result of strong collaborative research programmes: 60% of papers involve international co-authors, 18% national, 19% institutional and 3% single authorship (SciVal). Tables 7 & 8 summarises some key data (source: SciVal), and we highlight selected activities below.

Table 7: Collaborations		Table 8: Leadership & Community	
Staff with collaborative publications Durham/national/international	28/34/37	National/international awards and named lectureships	11/13
Staff collaborating with DU Biology/Physics/other subjects	12/8/8	Staff elected to Royal Society FRS	4
Number of company interactions	>100	International advisory boards	18
Publications in period	1413	Keynote/plenary int'l lectures	>250
Number of UK academic collaborating authors	111	Editorial boards	19
Number of international coauthors	>1000	Staff as EPSRC College members	18
Number of international visitors	>250	Staff on RSC/IOP/etc. committees	15

Collaborations: Areas which exemplify our collaborative research and build specifically on our strategic aims (Section 1) of academic partnerships, interdisciplinarity and internationalisation are:

- *Other DU Departments:* Highlight examples of interdisciplinary research within DU include: Hutson, Cornish (Physics) on ultracold molecules, EPSRC, £6.7M; Bryce, Fox, McGonigal, Monkman (Physics): High-Efficiency Phosphorescent OLEDs; Hodgson, Cann (Biosciences) concerning molecular events in the global carbon cycle, BBSRC £700K; Miller, Steed, Sutcliffe (Maths), Jackson (Cambridge) Knot theory in modern chemistry, Leverhulme, £1.7M.

- *UK collaborations:* 34 staff collaborated with colleagues in 38 UK University Departments to produce 258 publications. Notable examples include: Beaumont, Kyriakou (Aston) silver surface catalysts for energy applications partner in EU MSCA – BIKE ITN, £247K; Cooper, Cucinotta (Newcastle) on light-harvesting antennae; Hodgkinson, Brown (Warwick), Yates (Oxford), Ashbrook (St Andrews) Collaborative Computational Projects 1 & 2 on NMR Crystallography, EPSRC £495K; Johnston, Islam (Bath) on anti-perovskites; O'Donoghue, Smith (St Andrews) mechanistic studies of *N*-heterocyclic carbenes, EPSRC £1M; Parker, Kuprov (Southampton), McInnes and Chilton (Manchester) examining non-classical paramagnetic susceptibility in rare earth complexes, EPSRC, £1M; Sanderson, Beales and Connell (Leeds) integrated biophysics approach towards membrane-active anticancer therapies, EPSRC, £906K; Williams, Kozhevnikov (Northumbria) photophysical examination of materials, EPSRC £800K; Dyer, Greenwell (Geology), Theodorou (Harper Adams), Wells (York), Gallagher (Aberystwyth), Flynn (Swansea), McEvoy (Highlands and Islands) and Fraunhofer-Institut (UMSICHT, Germany) on methods for generation of energy from seaweed and other readily available biomass materials, EPSRC £1.6M. Steed, Day (Southampton) on supramolecular gel phase crystallisation strategies, EPSRC, £647K
- *International collaborations:* 37 staff collaborate with colleagues in 26 countries worldwide which has resulted in 849 joint publications (60% of publications). In addition to the EU and GCRF funded networks described above, other major funded international collaborations include: Badyal, Çelebi-Newton (Selçuk, Turkey) antibacterial nanocoating technologies for on-site water decontamination, RS+UK-Turkey Hub £550K; Baxendale, Jensen (MIT) on flow processes; Cobb, Wong (Hong Kong Baptist) on chemical biology; Curchod, Agostini (Paris-Sud) on the fundamental theory of coupled electron/nuclear dynamics in molecules; I Evans, McIntyre (ANSTO Sydney) co-supervision of PhD students; J Evans, Campbell (Brigham Young) Fullbright award on group theory, Pal, Tour (Rice, Texas) on molecular machines; Steel, Rossi-Bergmann (UFRJ Brazil) on patented antileishmanial chemotherapies; Steel on antileishmanial drug delivery with Nangia (Hyderabad), Ali (Kolkata), Sundar(BHU); Tozer, Levy (Tulane), De Proft (Brussels), Helgaker and Borgoo (Oslo) on DFT theory; Verlet via H2020 network; Walton, Verma (IIT Kanpur, India) on copper complexes as antibacterial resistance breakers; Wrede, Momose (Vancouver) on cold molecular collisions; Hutson, Julianne (Joint Quantum Institute, Maryland), Schreck (Amsterdam), Aldegunde (Salamanca) and Nägerl (Innsbruck) on computational chemistry.

Chemistry community contributions: Durham staff contribute to the national and international chemistry community in many ways. Examples include:

- *Publications:* Durham publications (1413) are highly cited with over 22,000 citations in period.
- *Editorships:* 16 staff serve on 19 international journal editorial boards including Baxendale: Executive Editorial Board for *Beilstein Institute Publishing*; Steed: Co-Editor-in-Chief, *Monographs in Supramolecular Chemistry*, RSC; Editor, *Crystal Growth and Design*; Hutson and Verlet: Co-Editors of *Int. Rev. Phys. Chem*; Coleman: Editor *FlatChem: Chemistry of 2D Materials*; Hodgson: Guest Editor, *Molecules*; Curchod section editor *Molecules*; O'Donoghue: invited Editor for *Org. Biomol. Chem.*, *Curr. Opin. Chem. Biol.*; Hodgkinson: *RSC Specialist Periodical Report in NMR*.
- *Publication review:* Collectively staff referee publications for all the major RSC, ACS, Wiley and Elsevier journals and other publishing houses (Taylor and Francis, Beilstein); all staff review research proposals submitted to UKRI (EPSRC, BBSRC, STFC), Wellcome and Leverhulme, serve on the EPSRC/BBSRC colleges/committees and

review research proposals for countries including Singapore, Canada, South Africa, Russia, Netherlands, Finland, Portugal, Cyprus, USA and Switzerland.

- *National/international advisory boards:* Many staff served on UK and international committees/advisory boards including Coleman: UK Govt group overseeing the National Measurement System, AMT/009 BSI committee, the UK national standards body, RSC CNN chair; O'Donoghue: Organic Chemistry Council of RSC Executive Committee, RSC Researcher Mobility Working Group; Bain: Harwell Research Complex, Chair of the Trustees of the RSC Pension Scheme; Dyer UK catalysis hub; I Evans: Scientific Council of Institut Laue Langevin, RSC Materials council; J Evans: Diamond Synchrotron Scientific Advisory Council, Oak Ridge National Laboratory (USA) advisory group; Parker: 'Commissione' for the Italian Government examining Chemistry Promotions in Italy, Chair, King's College London Chemistry Scientific Advisory Board, Departmental Review for Nottingham and Hong Kong City University; Pohl: Chair of Programme Advisory Committee at MAXIV (Sweden) and review committee of ALBA (Spain) synchrotron and Diamond MX working group; Sandford: Executive Committee ACS Fluorine Division, RSC Fluorine Group, Leicester Chemistry EAB; Steel: RSC Chemical Biology Division Council; Walton: RSC Research Fund and Dalton Division Council; Wilson: Chair, Physics Review Panel, Academy of Finland.
- *Royal Society:* our RS Fellows are very active within the RS committee panel structure: Badyal: Future Leaders African Independent Research (FLAIR) Fellowships, Theo Murphy Blue Skies Award, Science Industry and Translation Committee; Howard: Open Science, Awards & Medals, Wolfson Fellowships, Industry Fellowships, Grants Committee; Parker: SC3 (elects Chemistry FRS Fellows), Chair of Tier 1 VISA approvals, FLAIR Fellowships and International Newton Fellowship Panels.
- *UKRI and international grant committees:* 16 staff serve on national (UKRI) and international committees/advisory boards including I Evans: Member of the 10-person international panel advising UK Government on ~£1 billion investment in neutron science over the next two decades; Johnston: Science Board Supergen Energy SuperStore Research Hub; Johnston/Thompson ISIS Facility Access Panel; Parker: Flanders Research Council Panel, Senior Fellowship Panel, Institut Universitaire de France (IUF).
- *Conference organisation:* Many staff have served on national/international conference organising committees. Highlights include: Bain's initiation of both the Telluride Workshop on Complexity in the Chemistry and Physics of Lipid Membranes (2016, 2018, 2020) and Future Formulation I, II and III conference series; O'Donoghue/Hodgson's Chair/Co-Chair roles on the Durham-hosted European Symposium on Organic Chemistry, 2017.
- *Invited keynote/plenary lectures:* All returned staff have presented research at international conferences and the Department makes funds available to help staff attend. In period, staff have given >250 invited keynote and plenary lectures at major conferences world-wide.

Recognition: Awards and Fellowships for contributions to the discipline include:

Table 9	Fellowships, Prizes and Named lectureships
Badyal	Fellow of the Royal Society, 2016; Tilden Prize and Medal, RSC, 2017; CRSI International Medal, Chemical Research Society of India, 2018; Innovation and Technology Enterprise Lecture, CSIR- Pune, 2018; Fellow of National Academy of Sciences, India 2019; 2018 "100 most significant breakthroughs from UK university" listing.
Bain	Sir Eric Rideal Lecture and Prize, 2020
Baxendale	Zasshi-kai Lectureship, Tokyo, 2015
Beaumont	Leverhulme Fellowship, 2012–2017
Curchod	ERC Early Career Fellowship 2018–23
Coleman	Royal Society of Chemistry Derek Birchall Award 2017
I Evans	Royal Society Leverhulme Senior Research Fellowship, 2019
J Evans	Francis Lions Lecture, Sydney, 2015
Howard	Dewar Lecture, London, 2016
Hutson	Thomson Medal and Prize, Institute of Physics, 2016; R. B. Woodward Lecture, Harvard, 2014; Larmor Lecture, Belfast, 2018; Roger E. Miller Lecture, Waterloo, Canada, 2019
Johnston	2019 NMRDG/BRSG (RSC/IOP) Prize for Excellent Contribution to Magnetic Resonance by an Early Career Researcher
McGonigal	Molecules Young Investigator Prize, 2018
O'Donoghue	RSC Loschmidt Award for Physical Organic Chemistry 2014; Eli Lilly Lecture, Trinity College Dublin, 2016; Loschmidt Plenary Lecture, Syngenta, 2016
Parker	EPSRC Recognising Inspiration in Science and Engineering Fellow, 2014; ERC Advanced Fellow 2011–16; Frontiers of Science Lecture, Wayne State University, 2014; Kennedy Wong Visiting Professor Hong Kong Baptist University
Sandford	SCI Process Chemistry Award and Lecture, Cambridge, 2018; Irvine Review Lecture, St Andrews, 2019
Steed	Royal Society Wolfson Research Merit Award; L. F. Power Memorial Lecture, James Cook University, Australia, 2019
Taylor	EPSRC Manufacturing Fellowship
Tozer	Fellow of the Learned Society of Wales (FLSW), 2017; JILA Visiting Fellow, 2019
Verlet	ERC Consolidator Fellowship, 2012–17
Walton	RSC Inorganic Reaction Mechanisms Group Young Academic Award 2018

Wider contributions to the economy and society: examples of training, outreach and developing the impact of our research included:

- *Collaborative international PGR training:* We have organised/co-organised international PhD+ level training schools in: Powder Diffraction and Rietveld refinement and single

crystal diffraction methods (I Evans, J Evans, Howard) which have trained ~1000 students from around the world; Physical Organic chemistry techniques (O'Donoghue, Hodgson) STINT programme Uppsala, Sweden (four annual meetings, 50 PhD students, PGR training £200K funding from Swedish Govt); CCP5 International Simulation Summer Schools, Durham 2019–21 (Miller). Bespoke training packages were delivered to a total of 30 students across the EU on molecular electronics (Bryce), organofluorine (Cobb, Sandford) and soft matter (Evans) chemistry within EU ITN programmes. Steel has trained 50 students from 8 countries in the global south via GCRF funding.

- *Collaborative national PGR training:* Our CDT programmes offer bespoke scientific and transferable skills training programmes in Soft Matter (SOFI 1 & 2) and Medicinal Chemistry (MosMed). 81 students were enrolled on the SOFI CDT programme in 5 cohorts (28 graduated to date) and 12 students have started in the first year of the MosMed programme.
- *Outreach and public awareness activities:* Media appearances include Coleman: BBC Naked Scientist (2015); Howard: Radio 4 In our Time with Melvyn Bragg (2014, 2018, 2019), Radio 4 Christmas with Philip Ball on 'snowflakes' (2018–19), recordings for the Science Museum on Crystallography; Fox: developing international signs of chemistry words for deaf students with Edinburgh and Prague University; Kitching: Royal Society Summer Science Exhibitor (2018), Last Retort, article for Chemistry World (2017), ACS Live Stream C&EN News (2017); Pal: Royal Society Public Engagement ambassador, Scientific adviser BBC Horizon; Parker: Serbian TV to highlight conference in Belgrade, (2016); Sandford: Radio 4 In Their Element: Fluorine; Beeby and Evans BBC1 Inside Out, (2020). Badyal served on the 2020 Davos World Biodiversity Forum panel on Biomimicry to tackle biodiversity loss and public health challenges.

Developing and continuing economic and societal impact: In addition to the current impact case studies, we have many ongoing impact projects developing over the next REF period in flow chemistry, fluorination technology, anti-microbial wound dressings, phototherapeutics for cancer treatment, drugs for neurodegenerative diseases, atmosphere detection units, water-harvesting and water-oil separation developed through collaborations with industry, EU Networks and venture capital strategies.

Our impact is long term and case studies from REF2014 which are not eligible due to REF time limits still have important impact. Synthesis of a key fluorinated heterocycle using direct fluorination techniques by F2 Chemicals for Pfizer continues on the multi-tonne scale for the manufacture of anti-fungal Voriconazole (\$500M annual sales). The European Medicines Agency banned the use of linear Gd contrast agents (e.g. Magnevist) for use in clinical MRI (2017) following expert witness and research in lanthanide chemistry described in REF2014. Super-repellent surfaces formed by plasma techniques continue to be developed and marketed by P2i. Currently over 250 million devices including mobile phones, hearing aids and clothing items have been treated by plasmachemical techniques arising from a patent published in 1998.