Institution: University of Liverpool

Unit of Assessment: Chemistry

1. Unit Context and Structure, Research and Impact Strategies

Our vision is to advance the chemical sciences though intellectual leadership delivering positive changes to society and the economy.

The progress toward the realisation of our vision since REF2014 is evidenced by the 121% increase in research income (§3.1), improved academic impact of our research (52% increase in citations per paper, SciVal report) and a substantial increase in staff (26% Category A, 4% PDRA), students (66% PGR, 28% UG) and support staff (270%) (§2.3) (**Table 1**). We have expanded and broadened impact generation activities (§1.3) and improved the quality of our infrastructure (§3.3-3.4) and embedded our commitment to equality, diversity and inclusivity in our policies (§2.1).

Table 1 Summary of Achievements

	Chemistry	**REF2014**	**REF2021**
	Research income	£33M	£73M
People	Staff returned, Teaching & Research (FTE)	34	43
	PDRAs	112	116
	PGR student body	123	208
	UG student body	364	465
	Support staff (Analytical, Technical)	7	26
	Fellowships	13	20
Outputs	Papers	>800	>900
	Citations	>12000	>20500

1.1 Overview of Unit Structure

The University of Liverpool's Chemistry Department comprises of 53 academic staff (43 category A), 116 PDRAs, 208 PGR and MSc students, 465 undergraduate students and 26 technical and professional services staff. It is part of the School of Physical Sciences, along with the Departments of Mathematical Sciences and Physics, and sits within the Faculty of Science and Engineering.

Our research activities are organised into 5 research clusters while the cross disciplinary research takes place within research centres and institutes (**Figure 1**). The principal aim of the clusters is to bring together common expertise from a range of sub-disciplines that can address central societal research challenges. Most members of staff are in more than one cluster. Clusters evolve and develop as new challenges emerge and research priorities change, for example co-locating computer scientists with chemists to address materials research. This allows us to be innovative and responsive while ensuring a coherent research direction.

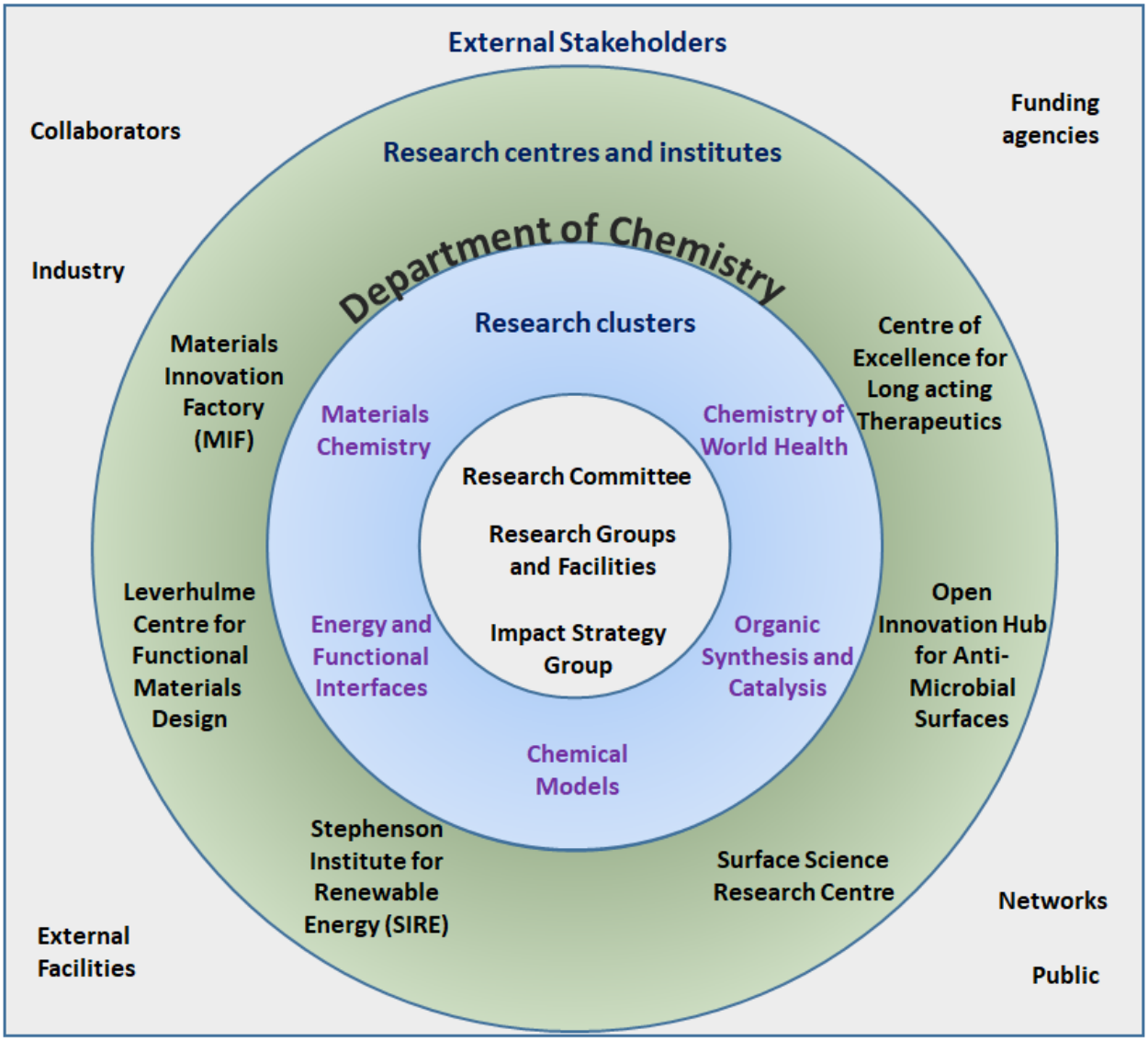

Figure 1 Overview of Department's Research and Impact Organisational Structure

Our current research clusters comprise:

- **Materials Chemistry** (Leader: **Claridge**) spanning organic, inorganic, hybrid, and nanostructured materials, including their applications, and defining innovative ways to discover new materials.
- **Chemistry of World Health** (Leader: **O'Neill**) focusing on the medicinal chemistry and drug development of anti-infectives, chemical biology, drug delivery via nanomedicine, bio-organic chemistry, anti-microbial surfaces and medical diagnostics.
- **Energy and Functional Interfaces** (Leader: **Brust**) covers biomass to fuels and chemicals, thermo-materials, electrochemical energy storage alongside interface and nanoscale science, catalysis, single molecule electronics, fluid processing and anti-microbial surfaces.
- **Organic Synthesis and Catalysis** (Leader: **Bower**) includes organic synthesis, homogeneous, heterogeneous, photo, electrochemical and bio-catalysis encompassing the construction of complex molecular entities.
- **Chemical Models** (Leader: **Troisi**) innovates all aspects of modelling chemical systems (quantum, classical, data-based and novel combinations thereof) with special focus on applications relevant to our research clusters in materials, energy and health.

Many of our greatest successes in research and impact are associated with multidisciplinary research centres or institutes where Chemistry is a founding member: (Materials Innovation Factory (MIF), Stephenson Institute for Renewable Energy (SIRE), Open Innovation Hub for Antimicrobial Surfaces, Surface Science Research Centre, Leverhulme Centre for Materials Design and Centre of Excellence for Long Acting Therapeutics (CELT)) (§1.4).

1.2 Research Strategy

Our goal is to produce research at the highest international level by

- Extending the frontiers of knowledge within and beyond existing research disciplines
- Combining expertise within and beyond the University to address current and future challenges, particularly in Materials, Health and Energy
- Fostering an exciting, creative and supportive environment

Our research strategy is defined by the Department's Research Committee composed of the chairperson, the 5 cluster leaders, the Director of Post-Graduate Research, 2 Early Career Academics (ECA) the Equality, Diversity and Inclusivity lead, and Head of Department (HoD). This committee allocates resources, such as EPSRC and University studentships, on a competitive basis, in alignment with our research strategy, while giving priority to ECA staff and interdisciplinary projects (§1.4).

Research strategy is developed with the primary goal of addressing global challenges through the intellectual leadership of the Department in the relevant areas, including the Regius appointment (§1.2.1). Information, emerging opportunities and good practice are disseminated across all staff, and ideas from individuals and groups are collated, discussed and developed at the cluster and the departmental level. Key elements of our strategy are co-developed within the interdisciplinary centres and institutes that Chemistry is part of (§1.4). We are key contributors to the University Strategic Research Themes of Advanced Materials, Digital, Infectious Diseases and Climate Futures.

1.2.1 Achievement of Strategic Research Aims

In REF2014 the Department identified 4 broad Strategic Aims (2014 SA1-4) and we demonstrate below how these have been met.

2014 SA1) Expanding research activity aligned with strategic themes

The achievements of our Department were acknowledged through the award of a Regius Chair in Chemistry in 2016 (only 3 in the UK). We have strengthened the area of Synthesis and Catalysis through the appointment of **Bower** to the Regius Chair combined with a £5.2M refurbishment of synthetic organic chemistry laboratories. We have built on the success of the Centre for Materials Discovery (2007-2017) by establishing the MIF (2017-, total setup £81M funded by University of Liverpool, Unilever & UK Research Partnerships Infrastructure Fund) and appointing 5.5 FTE new academic staff (**Crick**, **Chong**, **Clark**, **Slater**, **Dyer**), including a leadership position in theoretical chemistry allied to MIF and SIRE research (**Troisi**). Medicinal Chemistry has been bolstered with 2 new appointments (**Hong**, **Singh**) joint with Pharmacology, to support the development of new candidate anti-infective and anti-microbial drugs. In Energy and Functional Interfaces, we have made 2 new academic appointments (**Hasell**, **Vezzoli**), maintaining the balance across our strategic areas of strength. We have grown the area of biomass conversion to generate chemicals and polymers through our MicroBioRefinery facility (£2.6M), a collaboration with Unilever and ABSugar. We have enhanced our excellent facilities including >£20M of open-access equipment (§3.3-3.4) and expanded our technical support to >20 FTE.

2014 SA2) Seeking new funding opportunities

We have increased our research income dramatically from £33M (REF2014) to £73M allowing investment in core research infrastructure including leveraging University support to target external capital funding as detailed in §3.3. This was made possible by a successful diversification of our funding sources detailed in §3.1.

2014 SA3) Tackling RCUK challenge areas

We have established two new centres linking Chemistry of World Health, Energy and Functional Interfaces and Synthesis and Catalysis clusters to tackle challenges relevant to industry (§1.3, §4.1-4.3): (i) the Open Innovation Hub for Antimicrobial Surfaces (**Raval**), a multi-disciplinary initiative to develop new technologies to tackle biofilms and anti-microbial resistance; (ii) the Centre of Excellence for Long Acting Therapeutics (**Rannard**), a knowledge hub and dedicated laboratory to accelerate product development.

2014 SA4) Influencing policy

We have influenced policy through advisory roles for government (**Rosseinsky**, **Cowan**, **Rannard**), and in a range of national or international institutions as detailed in §4.5 and §4.6.

1.2.2 Strategic Research Aims for the Next 5 Years
The Department will expand its research activity through the 7 Strategic Aims (SA) below, aligned with our vision:

SA1) Build on investment in the MIF in 3 strategic research areas: net-zero materials and sustainability (aligned with government's "Net Zero" 2050 goal), smart mobile robotics, and artificial intelligence led materials discovery.

SA2) Grow and enhance methodologies for the construction of complex molecules building on the Regius Chair appointment and renovated synthetic chemistry laboratory, also harnessing the MIF's existing and emerging platforms in automation.

SA3) Extend the reach of Nanomedicine by broadening the scope of long acting therapeutics including implants, injections or oral dose, also increasing current engagement with pharmacologists, clinical scientists and pharmaceutical industry.

SA4) Build on the Open Innovation Hub for Anti-microbial Surfaces by expanding capability into anti-viral and antimalarial products relating to SA3, combining our strengths in anti-microbial surfaces with the Chemistry of World Health cluster and co-working with industry.

SA5) Grow SIRE in core areas of research in energy storage and functional interfaces whilst developing advanced surface sensitive *in operando* spectroscopic tools to probe catalytic reactions and electrochemical interfaces.

SA6) Capitalise on appointments in Medicinal Chemistry through developing new candidate anti-infective drugs, especially those tackling anti-microbial resistance, coordinating transition of molecules into Phase 1 clinical trials and identifying biological targets.

SA7) Reinforce the central role of Chemical Models in our materials, energy and health research, integrating all branches modelling with experimental characterisation and exploiting novel interactions with Computer Science and robotics.

1.3 Impact Strategy

To realise knowledge transfer and commercial exploitation from our research through industrial and public engagement, maximising possible traction with the private sector based on common scientific problems and complementary expertise.

Our Department prides itself on translating science into significant real-world impact, often via long term partnerships with major companies, where we act as a facilitator of growth of the regional economy: the primary exemplar here is the MIF partnership with Unilever. Three staff members act as *impact leads* (**Cowan, Rannard, McDonald**) and are supported by a new Impact Strategy Group (with representation from all research clusters and colleagues with experience in translational science) to establish major enduring external collaborations enhancing our impact in the UK and internationally. Our impact strategy is implemented at three levels through departmental policy, support and promotion.

Policy

Impact is embedded in our activities: resource is allocated for all staff leading major impact activities which could either be a PGR studentship or sabbatical support (§2.6). Impact is also an important factor in promotions (§2.6) and in recruitment (§2.3). All impact-generation activities are now accounted for in our departmental workload model (§2.6) and impact is a standing agenda item for all staff meetings.

Support

We support researchers in all aspects of translation (financial, legal and technological) and facilitate impact-generation activities from identification of the initial opportunity to the provision of additional resources. Potential impact activities are discussed with all staff members in their annual appraisal (§2.6) and a suitable mentor is identified. The researcher and their mentor will identify a broader network of support needed including working with the Knowledge Centre for Materials Chemistry to identify potential partners (§1.3, §4.2). We have initiated an annual "business and impact development camp" including introductions to IP and securing investment. Financial resources, awarded in line with our strategy, include departmental funded summer student bursaries, EPSRC Impact Acceleration Account (£572k across 22 projects with collaborators including Johnson Matthey, Liverpool ChiroChem and RDGraphene), and Faculty enterprise awards (£894k across 13 projects leading to spin-out companies CageCapture and TandemNano). We have been successful in 3 Innovate UK ICURe Innovation to Commercialisation awards (**A. Cooper**, **McDonald** and PGR Zhang) with our IP exploitation accelerated by external entrepreneurs.

Promoting our Department

We aim to promote our facilities (§3.4) and expertise in dedicated engagement events (detailed in §4.2) and to disseminate the main achievements through high profile press and media outlets (detailed in §4.4).

The success of our impact strategy is exemplified by all the submitted case studies. Three of them – "Enabling the Lucite ALPHA Process for the sustainable production of methyl methacrylate" (**Iggo**), "Laboratory study of asymmetric catalysis leads to a spin out" (**Xiao**) and "Catalysing Innovation through the Centre for Materials Discovery" (**A. Cooper**, **Rannard**) - relate to commercialisation directly from our research. Our emphasis on public engagement is exemplified through "ChemTube3D: an internationally renowned Open Educational Resource" (**Greeves**).

1.3.1 Achievement of Impact Strategy Aims

In REF2014, the Department identified 6 Impact Aims (2014 IA1-6):

2014 IA1 & IA4) Exploited academic-industrial collaboration and Marketed our skills and expertise to industry

We collaborate with >100 companies across Materials, Health, Functional Interfaces, Synthesis, Catalysis and Energy research including AstraZeneca, Ansell, BP, Croda, DePuy Synthes, Eisai, ExxonMobil, GSK, IBM, Johnson Matthey, Lucite, NSG Pilkington, Pfizer and Unilever. We have secured £6M of income from UK Industries (119% increase since REF2014) and industry has supported >30 studentships.

We have capitalised on MIF through a strategic partnership with Unilever R&D that emerged from a shared vision to transform how chemistry is done. The MIF creates digital discovery tools and high-value materials IP through partnership in a unique translational research facility built on knowledge leadership in Materials Chemistry. The combination of leading academics, open access equipment, lab automation, and digital chemistry creates seminal academic publications. MIF has become a "beacon" activity for companies, large and small, and academics in the UK and beyond, focusing on advanced materials, chemistry, and formulation (§3.4). Commercial outcomes include: new materials, faster de-risking of innovation, new business models and start-ups, and digitally transformed innovation. There are >100 Unilever staff co-located in the MIF, a further 15 companies used MIF facilities, resulting in the acceleration of >50 new product developments and >250 staff from external organisations received training and accessed experimental facilities in the MIF laboratories. Knowledge Exchange partnerships, set up as part of the Knowledge Centre for Materials Chemistry (KCMC), have delivered >100 projects and >£12M in research income for the University of Liverpool.

Collaborative projects with commercial partners are exemplified by Innovate UK funding with 17 new projects commenced in the REF period (>£3.2M) including Smart Responsive Antimicrobial Implants (**Raval**, Smith & Nephew) and Scale-up and commercial evaluation of the manufacture of bio-based precursor for polymers (**Carnell**, Biome Technologies and University of Leeds).

2014 IA2) Addressed societal needs in energy

SIRE is developing efficient generation of hydrogen as a fuel for local transportation for island communities and electrochemical energy in liquid and solid-state batteries extending lifetimes and durability (as part of EU and Faraday Institution projects). SIRE, working with industries including Jotun, has delivered coatings based upon nano-encapsulation which has been translated to a wide variety of applications, including coatings that prevent marine biofilms that could reduce the CO_2 footprints in shipping.

2014 IA3) Strengthened Medicinal Chemistry and Nanomedicine

We have developed, with Eisai, a new drug candidate now entering a Phase 1 clinical trial for river blindness and elephantiasis. Alongside Eisai, GSK and the Medicines for Malaria Venture we have candidate selected a novel peroxide antimalarial E209 with efficacy against artemisinin resistant strains.

A cross-Faculty partnership has co-located Materials Chemists and Pharmacologists in the MIF and we have developed the first ever long-acting prophylaxis for malaria which led to a $32M grant (Unitaid, $20M to Liverpool) to extend this for Hepatitis C and latent TB. We are partners in the first EU Nano-Characterisation Lab for commercialising nanomedicines, collaborators in optimisation of dosing of HIV therapies (USAID £50M, £4.2M to Liverpool) and have had candidate therapies added to the US Department of State Formulation Prioritisation List. We are collaborating in the first human trial of an orally dosed nanomedicine for HIV therapy and have agreement with Medicines Patent Pool to develop HIV nanomedicines.

2014 IA5) Exploited IP

Since 2014, 55 patent applications were filed and this portfolio of patent families has resulted in 166 regional/national filings which have generated 65 national grants. 20 of the patent families have been licensed to commercial entities or constituted the basis for 6 spin-out companies (§4.3). Commercial beneficiaries include Liverpool Chirochem, CageCapture, Ceres Power, Polymer Mimetics, Porous Liquid Technologies and Tandem Nano. In addition, IP has been licensed to: Micromeritics Instruments to establish new gas sorption technologies, Mobotics on mobile robots for chemical research and Polymer Mimetics, a joint venture with Scott Bader.

2014 IA6) Strengthened outreach

We have engaged >4000 school pupils per year with Chemistry. Specific initiatives target students from underprivileged backgrounds and local areas of deprivation, such as the RSC funded project 'Wirral Microplastics' which supports sessions for Y12 and Y8/9 students in Birkenhead. In this REF period there have been more than 5 million users worldwide of Chemtube3D developed by **Greeves** (one of our impact case studies). Additional exemplars of our public engagement activities are given in §4.4.

1.3.2 Strategic Impact Aims for the Next 5 Years

In line with our impact strategy, we have developed the following 7 Impact Aims (IA) responding to societal, industrial, health and economic demands:

IA1) Establishing MIF as the main national academic reference point for data-enabled and automation-enabled innovation in materials discovery. As many companies are transitioning toward an Industry 4.0 model of innovation, MIF will provide specialist training, access to unique facilities and distinctive knowledge-leadership, exploiting our close collaboration with Computer Science at Liverpool. Our unparalleled knowledge-base at the interface between chemistry and computer science will benefit Liverpool, North-West and the UK. We will develop a focused number of strategic partnerships with large R&D intensive manufacturing companies (~FTSE 350) with substantial UK presence. We will extend the concept of open access to include incubation and deployment of seed capital, making the skills and resources within the MIF more available and accessible for example through links with the UK's Centre for Process Innovation to provide access to support through the technology readiness levels towards commercialisation.

IA2) Addressing future societal needs in energy through the SIRE, further developing nano-encapsulation coatings for chemical energy storage, strengthening industrial collaborations and developing next generation energy storage technologies including metal-air, solid-state batteries and electrochemical capacitors, aligned with the UK Government's "Net Zero" Challenge.

IA3) Building on strengths in Medicinal Chemistry, working with the Liverpool School of Tropical Medicine, to develop lead molecules against river blindness and elephantiasis affecting >120 million people, including clinical trials of AWZ1066 in the UK and in Africa. We aim to candidate select a novel antimalarial and will pursue a new salt form of tizoxanide to enter clinical trials.

IA4) Capitalising on investment in Nanomedicine by exploiting the materials/pharmacology collaboration more broadly, translating to "good manufacturing practice" production, performing human evaluations of long acting therapeutics, including for HCV and latent TB, and expanding our work with industry.

IA5) We will develop, with pharmaceutical and agrochemical companies, complex molecule syntheses and catalytic methods easily adaptable to scale-up and devise semi-autonomous route optimisation, building on our recent successes in similar activities (§4.3).

IA6) Extending the Open Innovation Hub for Antimicrobial Surfaces through its research and innovation ecosystems working with multinationals, SMEs, academia and the NHS. We will address societal needs through, for example, the recent £6.6M ERDF programme on 'Formulated Materials for Infectious Disease Prevention'.

IA7) Outreach delivered in the Central Teaching Labs will continue to support educational attainment in the Liverpool City Region. Support for teachers will be extended providing much-needed hands-on workshops for primary teachers. In response to COVID-19 we are developing new material for remote delivery, that will expand the geographical reach of our outreach activities.

1.4 Interdisciplinary Research

Our major impacts are increasingly rooted in interdisciplinary science which is promoted by our research and impact strategies (§1.2, §1.3). The Chemistry Department has spearheaded a number of interdisciplinary centres focused on driving collaborative research and impact across the University. Staff in Chemistry lead interdisciplinary research centres (**Figure 1**) including the MIF (**A. Cooper** (Director), **Rosseinsky**, **Rannard**, **Lopez-Sanchez**, **Troisi**, **Dyer**, **Chong**, **Slater**), SIRE (**Hardwick** (Director), **Blanc**, **Cowan**, **Hasell**, **Lopez-Sanchez**, **Sergeev**, **Shchukin**), Surface Science Research Centre (**Raval** (Director), **Arnolds**, **Darling**, **Dyer**, **Hodgson**, **Volk**), Leverhulme Research Centre for Functional Materials Design (**A. Cooper** (Director), **Rosseinsky**, **Berry**, **Blanc**, **Cowan**, **Darling**, **Hardwick**, **Dyer**, **Chong**, **Troisi**, **Slater**), Open Innovation Hub for Antimicrobial Surfaces (**Raval** (Director)) and Centre of Excellence for Long Acting Therapeutics (**Rannard** (co-Director), **McDonald**). Success is indicated through our increase in research income (§3.1), outputs (§1.1 and **Table 1**) our engagement with key research users (§4.2), contributions to the economy and society (§4.3) and engagement with communities and the public (§4.4).

Interdisciplinary research in our Department exploits synergies with other departments measurable from the large grant value (>£35M) with investigators from other units (§3.1). Outside those originating from interdisciplinary research centres, 12% of our publications were co-authored with colleagues from other Liverpool departments including Electrical Engineering, Physics and Pharmacology. Drug development activities (**O'Neill**, **Berry**, **Hong**, **Nixon**) with Liverpool School of Tropical Medicine contributed to a Queen's Anniversary award for Pharmacology.

We further promote interdisciplinarity through joint appointments with other departments (§1.2) and including interdisciplinarity as a criterion to award PGR studentships.

1.5 Progress Towards an Open Research Environment

The Department develops a combination of dedicated policies, training, and facilities to enable an effortless adoption of Open Research Environment practice as defined in the Concordat on Open Research Data.

97% of our research outputs are available through the Liverpool repository and 63% of such outputs in this REF period are available "open access". All PGR students receive training in open research and data management. Liverpool Research Data offers perpetual storage suitable for raw research data and a yearly programme of training events for staff. We are developing integration of data acquisition and storage with an innovative scientific data management system ("ParaDIME") that securely stores data in a searchable environment and is currently active in MIF; it will be deployed across a range of characterisation facilities (§3.4) to enable data-driven research.

1.6 Research Integrity

We develop our policies in accordance with the Concordat to Support Research Integrity focusing on compulsory training on Ethics and Research integrity for PGR students and staff, with robust management of these matters initially by the HoD and, when independent adjudication is needed, by the University ethics committee.

2. People

2.1 Engendering Equality, Diversity and Inclusion (EDI)

For chemistry to prosper we must attract, develop and retain a diverse community of talented people (*e.g.* https://www.nature.com/articles/s41557-020-0529-x). Developing a vibrant and proactive culture to support EDI is a strategic objective for Chemistry at the University of Liverpool.

We adopt all the recommendations of the Royal Society of Chemistry's reports on "Diversity landscape of chemical sciences" and "Breaking the barriers – women's retention and progression in the chemical sciences". We have proactively addressed gender equality issues in particular (Silver Athena SWAN award (2017) and working towards Gold). Our policies are reviewed through regular meetings of diversity and equality groupings at School, Faculty and University levels.

2.1.1 Recruitment

Our recruitment strategy has a global reach - our researchers are truly international with 54% non-UK and 13% BAME academic staff. We are committed to the promotion of EDI in the recruitment process (highlighting Athena SWAN and flexible working), ensuring transparency and the presence of at least one female member in every academic interview panel. In this REF period we have succeeded in improving our gender balance year on year from 8% to 14% (national average 23%, RSC Diversity landscapes of chemical sciences). While this is a significant step, we recognise the need to improve this further across all protected characteristics.

2.1.2 Promotion, Retention and Recognition

We strive to provide a supportive environment for all through Professional Development Review (PDR, §2.6) and mentorship. Promotion criteria recognise an individual's contributions in all areas, including EDI (§2.6). Since REF2014, 4 women have been promoted: 1 to personal chair, 3 to senior lecturer, 1 of whom is a member of an ethnic minority group. We also recognise contributions through staff awards, such as **Clark** winning the Early Career Researcher (ECR) of the Year Award (2019).

Reliance on short-term contracts is partially mitigated through both PDRA and ECR awards (12 since REF2014) which extend employment and enhance PDRA's future prospects (§2.6). **Vezzoli** was a recipient of an ECR award and is now a permanent member of staff.

2.1.3 Environment (Physical Space and Culture)

EDI is central to our decision-making processes. Our departmental committees are representative in terms of gender and career stage and, from 2020, have a member responsible for EDI. We have a relatively small number of committees, each empowered to implement the policies of their action domain (*e.g.* Health and Safety, Teaching) and report directly to the HoD and at staff meetings. This arrangement ensures efficiency, transparency and ownership of the policies to be implemented. Examples of lead female roles include Head of Surface Science (**Raval**), Outreach Lead (**Aspinall**), EDI lead (**Slater**) and senior lecturers (**Nixon**, **Arnolds**, Teaching and Scholarship (T&S): **Sedghi**, **Johnson**). The promotion of female staff members to leadership

positions is complemented by dedicated training through the Aurora programme (**Slater**, **Clark**, **Sedghi**).

We have compulsory EDI training for all staff and arrange additional training such as "Understanding Unconscious Bias" and "Making Better Decisions in Groups" for recruitment and REF panels.

Head of Department (HoD) has oversight of fair allocation of tasks and resources, recognising overall contribution and monitoring protected characteristics. This is managed through annual PDRs and a workload allocation model (§2.6), we adjust workload and expectations, for staff with health, social or family related circumstances to ensure continuation in their role. We are developing the workload model further, with staff input.

We have flexible working practices to support social/family circumstances, protecting time for carer and family responsibilities. All departmental meetings and seminars are held within core office hours and we provide free childcare for Open Days. The School has a flexible working adviser to help prepare for parental leave and a staff-led parents' network. The School provides funds for PDRAs and PGRs whose contracts do not include adequate maternity pay. Flexible working is no barrier to promotion into leadership roles including HoD (**Berry**).

Support is offered for returners to academic roles following a career break, with **Slater** being supported through a "returners fund" over 2 periods of maternity leave, 1 as PDRA and 1 as Royal Society Dorothy Hodgkin Fellow. A PDRA who supported the **Slater** research group during one period of maternity leave was recognised with an exceptional performance award.

Our culture of inclusivity is also reflected in the outreach activities directed to underprivileged communities (§4.4). Furthermore, we are constantly improving accessibility and practices across our building, most recently in the renovation of the Regius chair lab and meeting rooms.

In the 2017 School Staff Survey, results concerning "respecting people, diversity and equality" (93%) demonstrated a positive culture, which we will build on aspiring to 100%.

2.1.4 Equality and Diversity in Preparation of the REF Submission

Oversight of all aspects of REF was performed by a group with diverse membership, which undertook specialist training on EDI and ensured, as part of their brief, that EDI principles were followed with the University's Code of Practice.

2.2 Wellbeing

We have established a wellbeing group, with representation from all stakeholders, to proactively address improving the physical and social environment. Positive mental and physical health is promoted through mental first-aiders (training funded by our Department), establishing a "Wellbeing room" in our Department and through social events for the whole department, including fortnightly "coffee and cake" and "connect" events, and more widely through the "family barbeques". Our events include the Disabled Staff Network, support for charity fund-raising (many run by PGR students) and active engagement in institutional wide initiatives including the annual wellbeing week.

In the 2017 School staff survey 100% agreed with the statement that "Generally I enjoy my work" and we seek to ensure that this remains the case for everyone.

2.3 Staffing Strategy and Recruitment Strategy

To pursue excellence by
- Recruiting outstanding international researchers
- Nurturing their talent and enabling them to flourish

Our staffing and recruitment strategy form the basis of our vision (§1) and research and impact strategies (§1.2, §1.3). We recruit a balance of established senior academics (**Bower**, **Troisi**), to provide leadership in new research areas, as well as lecturers (8 FTE), PDRAs (116, 4% increase in REF period) and PGRs (208, 69% increase) to provide critical mass in strategic areas with an emphasis on impact.

In line with our research strategy (§1.2), strategic aims (§1.2.2) and impact aims (§1.3.2), new academic appointments have been made, including in the MIF **Crick**, **Chong**, **Clark** and **Slater** (Materials Chemistry cluster) and **Dyer** and **Troisi** (Chemical Models) and at the chemistry:life science interface **Nixon**, **Singh** and **Hong** (Chemistry of World Health). The appointments of **Hasell** and **Vezzoli** linked with the SIRE strengthened the activities around Energy and Functional Interfaces.

We have reduced the teaching load on research staff through 3 full time University Teaching Fellows, 2 (**Gaynor** and **Sedghi**, now a National Teaching Fellow) directly into the Department and the third (**Cropper**) to support Chemistry teaching in the Central Teaching Laboratory (CTL).

2.4 Supporting Fellowship Applications

We advertise research fellowships externally, interviewing promising candidates, with selected applicants given support in preparing their applications. We are proud hosts of 5 Royal Society University Research Fellows, 1 Dorothy Hodgkin Fellow, 1 UKRI Future Leader Fellow, 5 Newton Advanced Fellows, 5 Marie Curie Fellows and 3 EPSRC Fellows (§3.1). All fellows benefit from support tailored to their level, with duties adjusted according to the scheme (§2.6).

2.5 Staff Profile

Success of our staffing and recruitment strategy is evidenced from the number of submitted "teaching and research" staff increased since 2014 from 34 to 43 (26% increase) and the number of females has doubled (3 to 6) (**Figure 2**). An overall shift toward higher grades (**Figure 2**) demonstrates success in senior staff appointment and career progression and is in line with the much-improved research output and income indicators (the average age has modestly increased from 41.9 to 44.7). Our reputation attracts international overseas research staff and academics (50% non-UK new starters since 2014) with 33% of returned staff from outside the UK.

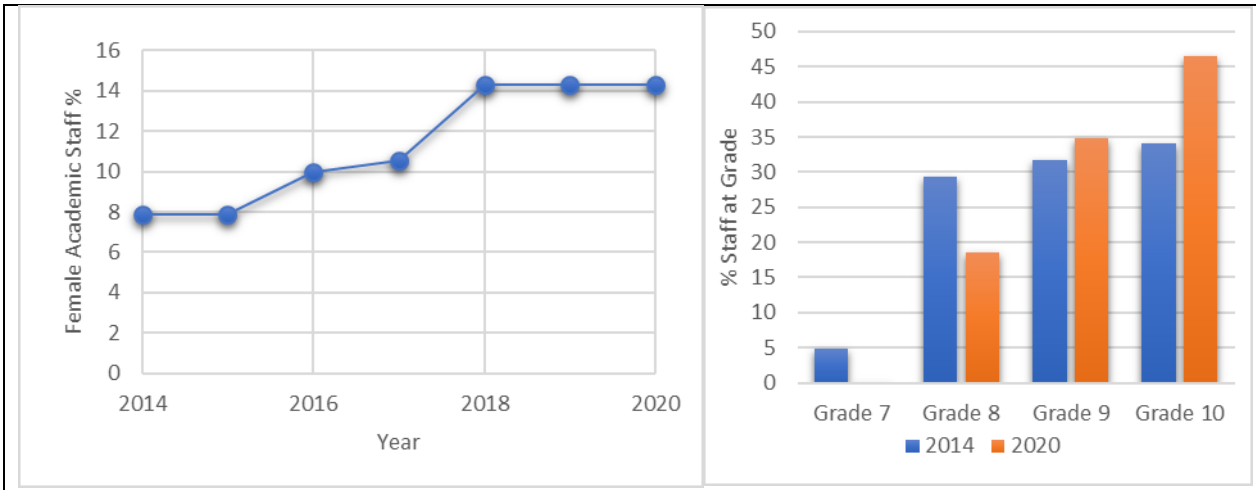

Figure 2 Gender Split and Faculty Grade Profile 2014 to 2020

2.6 Staff Support and Development Strategy

To provide support and development opportunities for all stages of the academic career equally, producing an inclusive, vibrant and productive department in line with our vision.

Induction

All new staff receive induction and training, including on EDI and Unconscious Bias, and are introduced to the University's Occupational Health service, which provides free counselling. The School of Physical Sciences hosts welcome events for all new staff.

Support and Development

Our provision is aligned with the Concordat to Support the Career Development of Researchers. Every member of staff has an annual Personal Development Review (PDR) discussion with an experienced, trained colleague. PDR enables reflection on overall contribution, plans, training needs, workload, career progression and recognition. Support required to achieve targets is provided including the institution's training programmes in management and leadership. PDRs enable effective succession planning, with more experienced colleagues mentoring staff taking on new roles, spreading best practice. PDR is underpinned by the workload model, which aims to ensure academic staff have time dedicated to research (minimum 1 day a week free from teaching during term) while balancing teaching, administration and leadership activities.

Recognition

We encourage and support staff via PDRs to apply for additional increments, exceptional performance awards and promotion. Promotions are awarded through a University process that recognises research, impact, teaching, administration and leadership contributions, accounting for individual staff circumstances such as parental, carers or sick leave. Since REF2014, 7 staff members have progressed from lecturer to senior lecturer, 5 staff promoted to Reader and 7 awarded Personal Chairs.

Sabbatical

Research or impact leave for all academic staff, of 1 semester following a five-year period of qualifying service, is operated at the discretion of the line management. Sabbatical leave is awarded to pursue novel research directions, including **Carnell** who was later promoted to reader through his work on biocatalysis, or impact activities, where **Greeves** developed a novel chemistry Open Educational resource (one of our impact case studies).

2.6.1 Support for Early Career Academics (ECA)

Further support is available to ECA:

Induction and Monitoring

Induction includes time with the HoD and introductions to key staff. HoD is the PDR reviewer for probationary staff so that necessary support can be implemented.

Mentoring and Training

A dedicated *research mentor* helps new staff settle into our Department providing advice and feedback on grants and papers. A dedicated *teaching mentor* advises new academics on preparation, delivery, assessment and quality monitoring of teaching. Peer mentoring is provided through the School's ECA forum. New academics complete teaching training, leading to Fellow of the Higher Education Academy status. A programme of researcher development events is delivered by the School including "Applying for a Fellowship", "Finding Funding Opportunities", "Making an Impact" and "Research Leadership".

Research Support

ECAs benefit from start-up funds for equipment/consumables, a PGR studentship (whilst attending supervision training) and a reduced teaching and administration load (30% initially built up gradually over the first 4 years of appointment). For example, the flow reaction system provided to **Slater** has underpinned her research so far.

The success of our approach is testified by a number of notable achievements by our newly-recruited staff: International Union of Crystallography Young Scientist Award (**Chong**, 2016), European Young Chemist of the Year (**Hasell**, 2014), RSC Macro Group Young Researcher Award (**Hasell**, 2020), BTM Willis Prize (**Clark**, 2019). Conference chairing (**Slater**, **Chong**, **Dyer**), editorial board memberships (**Slater**), panellist in funding bodies (**Chong**, **Slater**), honorary academic position in international institutions (**Hasell**, **Hong**). ECA staff have been encouraged to take leadership roles within our Department (**Hasell**, PGR Deputy Coordinator, **Slater** and **Giardiello** EDI lead and deputy).

2.6.2 Support for PDRAs

PDRAs are integrated into research clusters and our research strategy (§1.2). Additional support is available to PDRAs (beyond that in §2.6) including the School PDRA forum. This was instrumental in establishing the annual Postdoctoral Development Awards (£2500) (§2.1.2): an awardee (**Cauldbeck**) is now a Unilever Research Fellow. A programme of career development events is regularly run including "Becoming an Entrepreneur" and "Academia into Industry", complementing the University's Prosper initiative.

2.7 Postgraduate Research Students

We aim to attract the very best and brightest students, increasing their number and improve the quality of their training and employability.

2.7.1 Profile and Funding Sources

Figure 3 summarises the PGR student body. The strong increase of student numbers (66% since REF2014) is in line with our strategy and is due to an increase in industrially funded studentships (>30 in REF period) and by an "International PGR fee waiver" scheme. The fraction of female PGR is 38%, in line with the national benchmark (RSC Diversity Report, 2018).

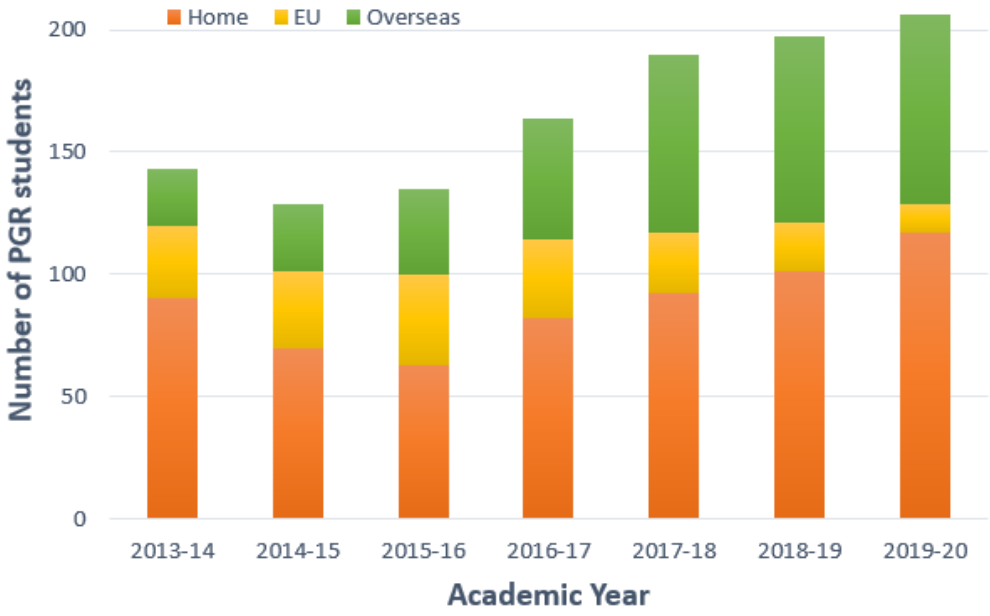

Figure 3 Number of PGR Students by Year

We secure a range of funding routes for studentships: EPSRC DTP, EPSRC CDT, ERC, China Scholarship Council, School, industry and self-funded students. We have a wide variety of partners which include other academic institutions such as Xi'an Jiaotong-Liverpool University, external research institutes such as Cambridge Crystallographic Data Centre and industry such as Unilever and IBM. The Leverhulme Centre for Functional Materials Design (£10M) supports 50 PGR students (2019-2024). MIF hosts an Advanced Training Centre, training PGR graduates to operate at the interface of physical science, data science, and robotics.

2.7.2 Research Degree Management

In the REF period 183.73 PGR degrees have been successfully awarded. All our PGR procedures are aligned with the principles of the Quality Assurance Agency.

Induction, Supervision and Monitoring

Students receive comprehensive induction including research integrity, EDI and support available outside of the supervisory team, covering health, disability, and international support. PGR students have at least 2 supervisors. Monthly meetings with supervisors are recorded and the timeliness and the records are monitored by the School PGR team.

Development

Professional skills development is organised by the Liverpool Doctoral College with training events including Communication & Writing, Research Methods, Impact, Ethics, Public Engagement, Careers and Entrepreneurship. In consultation with supervisors, PGRs prepare an annual 'Development Needs Analysis', which is discussed as part of their progression.

Progression

2 members of academic staff with relevant research profiles, act as members of the annual Independent Progress Assessment Panel, providing feedback and pastoral support to each PGR. A written report from the PGR is reviewed and discussed in person with the panel. PGRs deliver a formal presentation in their third year at the annual PGR conference, with our Department funding prizes for the best talks and posters. If annual progress is unsatisfactory or the students raise concerns, there are support mechanisms and robust processes in place managed by the Faculty.

2.7.3 Additional PGR Support

Our PGR staff student liaison committee meets tri-annually to address issues: from these meetings a dedicated space in the Department for PGRs has been established recently. The PGR and PDRA communities are included in decision making, including the detailed plans for resuming research during the COVID-19 pandemic and the development in 2019 of the PGR-led "Careers Day".

The Department funds travel bursaries to support the dissemination of PGR's research work. A number of PGRs have been awarded student prizes including Wallace (subsequently UKRI FLF, University of East Anglia).

2.7.4 PGR Evaluation and Employability

From the 2019 PRES, Chemistry PGR students are in the top quartile of the Russell group concerning PGR resources and development of student's confidence to be creative or innovative.

The employability data (latest Chemistry data from Destination of Leavers from Higher Education survey) indicate that 95% of our PGR graduates are in work or study 6 months after completing with job destinations in areas closely related to their research.

3. Income, Infrastructure and Facilities

3.1 Research Funding

The quality of our staff, research strategy, cluster structure (§1.2) and recruitment strategy (§2.3) enables us to be agile and collaborative whilst fully exploiting our infrastructure and facilities.

Research income totals £73M during the REF period, a 121% increase from REF2014, comprising 301 externally funded research projects placing us in the 90th percentile in the Russell group for Chemistry. **Figure 4** shows the cumulative grant income of awards by source demonstrating strong performance with the dominance of UKRI funded research in-line with our strategy (§1.2).

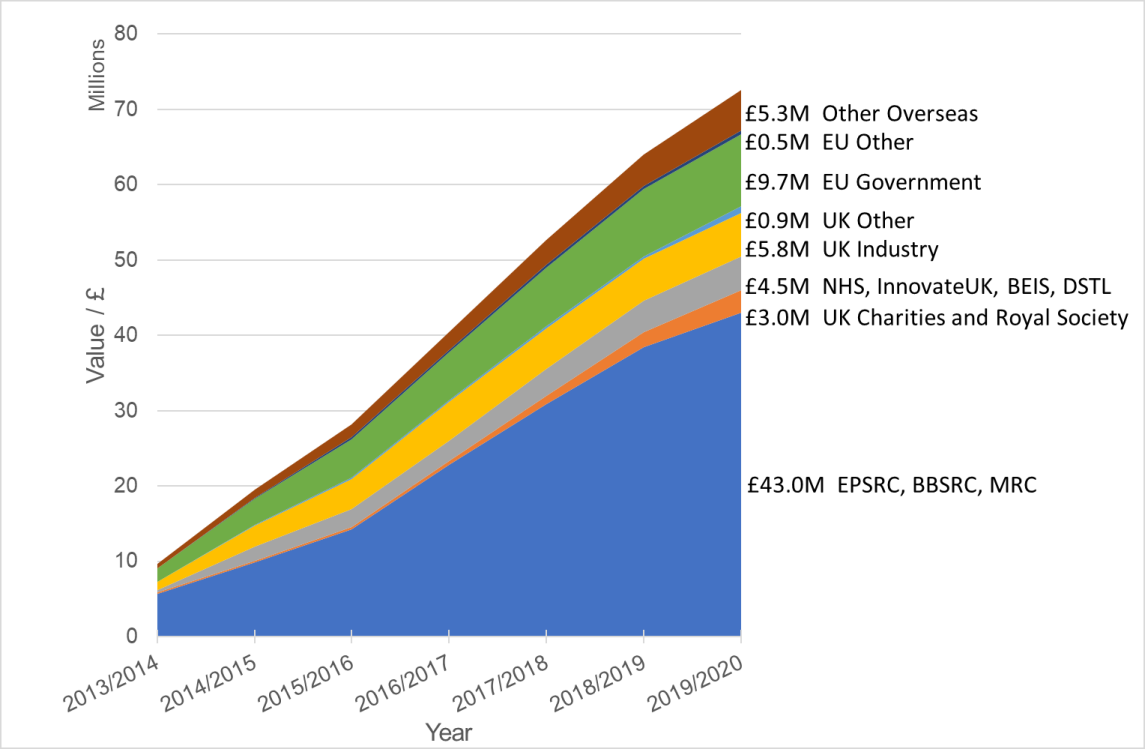

Figure 4 Cumulative Value of Research Income for Liverpool

We attract funding from a diverse range of funding sources (**Figure 4**), embedding resilience in our income model. Notable is the 119% increase from UK industries (£6M, £2M of which from Unilever) and the >£150M new research grants have commenced in the period (>250% increase from REF2014). The Department also attracted £572k through the University-managed EPSRC "Impact Acceleration Awards". Departmental endowment funds have contributed to the enhancement of our analytical facilities (~£400k, not in **Figure 4**).

Our research strategy (§1.2) aimed to target Materials, Medicinal Chemistry, Nanomedicine, Energy, Functional Interfaces and Catalysis and we have achieved substantial grant award success in all these areas.

The exceptionally strong funding generated by the **Materials** cluster emphasises the nationally and internationally leading nature of this activity. Materials is backed by a Leverhulme Centre award (£10M), Henry Royce Institute (£11M), ERC Synergy Grant (€10M, €4.1M to Liverpool), EPRSC Programme Grant (£7.3M), MRC (£3.3M), an ERC Advanced Grant (€2.5M), Faraday Battery Challenge (£2.2M), EPSRC (£953k, £928k, £916k, £902k), Royal Society (£916k), King Abdullah University of Science and Technology (£790k, £669k) and ExxonMobil (£650k).

Major programmes in **Nanomedicines** were funded by Unitaid ($32M, $20M to Liverpool), WITS Reproductive Health & HIV institute (£4.5M), EPSRC (£1.1M, £1.1M, £646k), CRUK (£856k), NIH (£460k) and industry (£826k, ViiV healthcare; £616k Nufarm).

International collaborations in **Medicinal Chemistry** have led to funding from the Bill and Melinda Gates Foundation ($5M, $1.2M to Liverpool), MRC (£1.5M) and Global Health Innovative Technology (£1.1M) for treatment of river blindness and elephantiasis. We received support from MRC for the development of drugs to treat fungal infections (£531k) and from industry for new anti-infective agents (Romark, £940k).

In the **Energy and Functional Interfaces** theme staff won significant funding from EPSRC for CO_2 to fuels project (£987k), electrochemical energy storage and batteries (£836k, £520k, £470k), carbon dioxide reduction (£904k), from Unilever (£2.2M, to access the MicroBioRefinery §3.4), from EU-FP7 (€615k) and an ERC Consolidator award (€2M). Funding has been secured to establish the National Biofilms Centre (BBSRC, £1.8M).

Sizable funding has been won in **Catalysis** including an ERC Consolidator Grant (€1.9M) together with awards from EPSRC (£437k) and the Royal Society (£405k) and, in molecular electronics, there have been awards from EPSRC (£451k, £497k, £599k) and the Leverhulme Trust (£413k).

Funding secured in **Chemical Models** is associated with many of the large initiatives above (*e.g.* Leverhulme Centre, Faraday Challenges) and theory-focused grants (ERC Consolidator Grant, €1.5M).

Cowan's EPSRC fellowship was renewed, **Boulatov** won an EPSRC early career fellowship and **Adams** (now Glasgow) won an EPSRC fellowship. **Hasell**, **Slater, Vezzoli** and **Greenaway** (now Imperial) won Royal Society University Research Fellowships, **Slater** was awarded a Dorothy Hodgkin fellowship and **Giardiello** won a UKRI Future Leaders Fellowship.

3.2 Future Funding Strategy

To expand existing research areas, develop new ones, fully exploit enhancements in our infrastructure and facilities and further diversify income streams through supporting interdisciplinary research.

We will target increased industrial funding, working closely with strategic partners including Unilever, Johnson Matthey, NSG Pilkington, BP, AstraZeneca, Pfizer, ExxonMobil, ViiV, NuFarm and Liverpool ChiroChem and others, enabled via our Impact Strategy (§1.3). We will further diversify our funding sources, such as NHS, MRC, BBSRC, NERC and NIH. Examples in place already include the Strength in Places grant 'Delivering Integrated Solutions for Human Infection' (**Raval**) and the £3.5M EPSRC Prosperity Partnership with Unilever.

3.3 Estate Infrastructure

The Department occupies >20,000 m^2 in 4 neighbouring buildings (Robert Robinson and Donan Laboratories, Materials Innovation Factory, Surface Science Research Centre and Stephenson Institute for Renewable Energy). We have lecture theatres and meeting rooms (one with virtual reality capabilities) available to all staff and students for seminars and networking meetings. All buildings have social areas for informal interactions to spark serendipitous collaborative ideas.

There has been substantial University and external investment expanding our research laboratories and equipment base since 2014, including £81M for Materials Innovation Factory (MIF), £5.2M synthetic organic lab refurbishment (Regius Chair), £2.2M refurbishment of Surface Science Research Centre, £1.8M EPSRC supported programme to upgrade NMR (**Blanc**) and £320k internally funded upgrade to mass spectrometry.

Our strategy is to focus on core strengths (§1.2), with the largest single investment in infrastructure in the period being the establishment of the MIF (11,600 m^2), one of 8 projects supported in the first round of the UK Research Partnerships Infrastructure Fund. The scale of the industry interaction is unprecedented in the UK in the area of Materials Chemistry, with >100 industry users co-located. Our expertise in Materials Chemistry, combined with unparalleled open-access facilities (>£20M, §3.4) and dynamic support infrastructure, enables revolutionary research and development in the MIF. Research activity includes Organic Materials (**A. Cooper**), Inorganic Materials (**Rosseinsky**), Nanomedicines (**Rannard**), Sustainability (**Lopez-Sanchez**), and High Throughput Formulation and Automation. The MIF houses the Leverhulme Research Centre for Functional Materials Design, created to drive a design revolution for functional materials at the atomic scale. This centre bridges the current design gap by fusing leading-edge synthesis concepts from the physical sciences with ideas from the forefront of computer science, alongside experts in robotics, engineering, management and social science. MIF hosts the Materials Chemistry spoke of the Henry Royce Institute, the UK's national institute for materials science

research and innovation. A distinctive innovation ecosystem of lab-robotics and digital companies has developed involving Croda, CSols, Labman, and Chemspeed all co-located in MIF. Research outputs include >25 papers in Science and Nature Journals.

Our Radio Materials Laboratory, created with Unilever, is a unique facility within the UK for generating traceable soft materials and drug compounds and was crucial for the human trials of the world's first orally dosed nanomedicine for HIV therapy.

Our Central Teaching Laboratory won a Higher Education Academy 2016 Collaborative Award for Teaching Excellence and embeds 'research-led teaching' in our degree programmes.

A £1B Estate Strategy has been approved by University Council (2017) and identified Chemistry as of long-term strategic importance, recognising the significant strengths of our research, enabling us to grow research activity in line with our ambitions (§1.2).

3.4 Operational and Scholarly Infrastructure

Any researcher or collaborator (academic or industrial SME or large corporation) can access our state-of-the-art facilities for research or impact projects or to trial ideas to support grant applications. Facilities usage is monitored and action taken if necessary with regard to EDI.

3.4.1 Technical and Business Development Staff

Communal facilities enable the efficient use of funds and encourage interdisciplinary research (§1.4). The MIF and Analytical Services equipment base (§3.4.2) are centrally shared and maintained with >20 dedicated staff (technical and business development) supporting our research activities. A user forum enables technical expertise to be shared and informs future strategic equipment needs. Technical staff engage with our research activities and frequently appear as co-authors of research outputs, including **Robertson**, 18 publications and **Clowes**, 43 publications since REF2014. The Department has a dedicated Safety Officer (**Jones** -2020, **Bergqvist Lane** 2020-) to coordinate safety policy, training, induction and implementation. The Department is 100% compliant in HASMAP at the "substantial" level and is working towards "high".

An overview of the University professional services including research support and library service is provided in the University environment statement (§4).

3.4.2 Core instrumentation and cutting-edge capabilities

We discuss below the most distinctive aspects or our vast range of equipment.

Chemical analysis

Advanced NMR spectroscopy provision include 6 solution state instruments ranging from 200 to 500MHz (with a cryoprobe), shared access to 600 and 800MHz (with cryoprobes), high pressure NMR capability and 3 solid-state NMR instruments (400MHz and 800MHz – 3rd highest field in the UK for solid-state). These facilities are managed by a dedicated specialist (**Luzyanin**) or by the research groups (**Blanc**, **Iggo**) and provide structural determination of samples across all our experimental clusters (§1.2). More than 200 users per month (PGRs, PDRAs) and all undergraduate students access the NMR facilities, analysing >60,000 samples each year.

Laser spectroscopy apparatus for femtosecond to nanoseconds transient UV/Vis spectroscopy enables detailed *in situ* analysis of charge carrier dynamics of photoactive materials and molecules. We have leading capabilities in broad-band Sum-Frequency Generation (**Arnolds**, **Cowan**), one of only 3 systems in the UK, and apparatus for femtosecond to milliseconds transient spectroscopy (**Volk**, **Cowan**). High resolution XPS instruments (**Raval**) are operated for the

determination of both elemental and chemical states in anti-microbial surfaces and *in situ* electrochemistry, complementing a number of *in situ* Raman and IR apparatus.

Diffraction facilities are a suite of 5 powder and 3 single crystal X-ray diffractometers with small angle capabilities, a wide range of sources (Co, Cu, Mo) and temperature stages for range of experiments from 12 to 1500 K currently solving >150 crystal structures per year. As part of pulsed laser deposition units, we have a KrF laser and a RHEED instrument for *in situ* monitoring of thin film growth.

Microscopy facilities include a comprehensive array of techniques to probe surface and interfaces of materials and include a suite of state-of-the-art UHV scanning probe microscopes with STM (**Hodgson**, **Nichols**, **Raval**), SEM with enhanced spatial resolution FIB and cryostage, EDS and WDS spectroscopies apparatus, SVET (**Shchukin**) coupled with high performance IR camera, as well as AFM and Raman.

Chromatography and mass spectrometry capabilities have been greatly expanded and now include a flow system (**Slater**), supercritical fluid chromatography, imaging MS, preparative HPLC (**Myers**) and GC, many of these are coupled with mass spectrometry instruments. Over 2400 samples are analysed by mass spectrometry each year.

Dedicated instrumentation gives access to a range of materials properties including magnetic (PPMS, MPMS), electrical (*e.g.* AC Impedance), thermal (*e.g.* TGA, DSC, Gas sorption), rheological and optical (*e.g.* time resolved fluorescence).

Automation and Robotics

The MIF is at the forefront of developing cutting-edge technologies in automated robotic equipment for the creation of new materials, including the bespoke £2.5M *Formulation Engine*. Robotics facilities include automated formulation platforms with 4 mixing stations preparing up to 800 formulations in 24 hours, dispensers for viscous material and powders, units to measure ionic transport and 2 high throughput rheometers. We have developed a revolutionary new technology of autonomous mobile robotic chemists plus an integrated suite of reaction and measurement stations in NMR, XRD, HPLC-MS to be used by these robots that have been highlighted in Nature (**A. Cooper**, **Figure 5**). The MicroBioRefinery (**Lopez-Sanchez**) enables high-throughput conversion of biomass, via bio- and chemo-catalytic routes, to high value chemicals.

Figure 5 Smart Autonomous Mobile Robot Performing Photocatalyst Discovery Without Human Guidance (Figure adapted from https://doi.org/10.1038/s41586-020-2442-2)

Formulation Facilities

Our Ultra Mixing and Processing Facility (UMPF, **Shchukin**) is a bespoke facility, home to the Controlled Deformation Dynamic Mixer which works from the bench (mg) to the pilot-plant (tonnes) scale and is designed to access extreme processing space at pressures of up to 5000 bar, flow rates of 1/2 tonne per hour, and rotor speeds of up to 20,000 rpm. Our MIF formulation measurement facilities provide tools for characterisation and stability assessment of materials with complex microstructures from the nanometre up to the millimetre.

3.4.3 Computing Facilities

Free access to high-performance computing facilities is provided centrally by the University to promote shared use of high-value facilities and include an HPC system with 4200 CPU cores plus dedicated GPU nodes. The Chemical Models cluster has secured access to further national (ARCHER) and international (PRACE) computer resources enabling large scale parallel computations that contributed to some of the unit's most significant research outputs, including 19 papers in Science or Nature family journals.

3.4.4 Technical tools

Examples of novel tools developed in Liverpool include:

- *Novel instrumentation*: IR-Vis Sum-Frequency spectroscopy (**Cowan**), UMPF upgrade (**Shchukin**), Central archive of NMR data (**Iggo**).
- *New Software/Database*: Crystal Structure Prediction Software FUSE, MC-EMMA, ChemDASH (**Dyer**, **Darling**, **Rosseinsky**), Charge mobility calculation code TransLoc (**Troisi**), Contributors to electronic structure calculation software MOLPRO (**D. Cooper**) and ONETEP (**Teobaldi**).

3.5 Instrumentation Outside the University

We access national and international research facilities, notably at the Institut Laue-Langevin (France), STFC including ISIS, DIAMOND and the Central Laser Facility, EPSRC including NMR and EPR, and the American Light Source and Mag Lab (USA). Competitive access to these facilities has been awarded worth >£6M which led to outputs including in Nature Physics.

3.6 Consultancies and Professional Services

Consultancy is encouraged (via PDR, §2.6) to foster professional development, generate impact and develop contacts with industry. Since 2014, the University CONSULT framework has brokered 27 commercial consulting projects (£785k) between researchers in the Department and clients include spin-outs, high-growth start-ups, and large multinationals (*e.g.* Boots, M&I Materials, Solvay, ExxonMobil). These relationships help inform our research and impact strategies (§1.2, §1.3).

4. Collaboration and Contribution to the Research Base, Economy and Society

4.1 Research Collaborations, Networks and Partnerships

In line with our strategy (§1.2), we are dedicated to enhancing collaboration at the *individual*, *institutional* and *extra institutional* level.

We support *individual* researchers to grow their networks and develop collaborations through 22 Impact Acceleration Account awards, strategically allocating PGR studentships, our strong base of facilities and analytical equipment and providing physical space for hosting workshops and conferences (§4.5). We strongly advocate for our academic staff to take up *visiting or honorary academic positions*: 18 honorary appointments within international academic institutions have been taken up by 11 staff members in this REF period. We enthusiastically support incoming visits of scientists at all career stages – hosting long-term visits of 43 post-graduate students, 34 postdoctoral researchers or permanent academics and 9 competitively funded postdoctoral fellowships including Marie-Curie and Newton fellowships.

We enhance cross-disciplinary activities through our role as founding members of several multidisciplinary research centres (§1.1, §1.4) reflecting our belief that major chemistry developments are increasingly rooted in interdisciplinary science. We enhance cross-disciplinary activities through strategic decision making on new academic appointments (§2.3), facility upgrades (§3.3-3.4) and support for fellowship applications (§2.4, §2.6). We have *joint projects* with >10 departments in the institution, 70% of all our grants by value are collaborative and, of these, 27% are interdepartmental (>10% of our PGRs have co-supervisors outside Chemistry).

We believe that *external networks and partnerships* are essential to maximise the societal and economic impact of our research (§4.3). Our Impact Strategy group (§1.3) is dedicated to establishing and supporting major, long-term, collaborations with partners across the public, private and third sectors. Our current and developing strategic partnerships include: *Materials Innovation*: Unilever (also supported through capital investment), Henry Royce Institute, Centre for Process Innovation, National Biofilm Innovation Centre; *Medicinal Chemistry*: GlaxoSmithKline, AstraZeneca, Anacor, Romark Pharmaceutical and establishing the Liverpool-Guangdong University of Technology Joint Laboratory for Drug Discovery; *Energy*: NSG Pilkington, Ceres, Faraday Institute.

We proactively engage with national and international funders to promote a sustained exchange of scientists hosting visits from the China Scholarship Council and King Abdullah University of Science and Technology. This has enabled us to diversify *joint-research projects* in response to global challenges from the: Royal Society - Newton Advanced Fellowships; European Commission – University of Liverpool led consortia on rechargeable batteries; NIH (USA) – Reverse Transcriptase Inhibitors therapies for HIV; Unitaid (UN) – anti-malarial drugs; Global Heath Innovation Technology Fund (Japan) – anti-Wolbachia drugs; Bill and Melinda Gates Foundation – anti-infective agents.

Aggregated indicators show that the Department of Chemistry is highly successful in turning its networks and partnerships into world-class research. Of >900 Chemistry papers published since 2014, >74% have a non-Liverpool author, and >54% have a non-UK based co-investigator (SciVal report).

4.2 Engagement with Key Research Users

The Department of Chemistry has developed a unique approach to translation science. Our unit is a founding partner of the Knowledge Centre for Materials Chemistry (KCMC), with a KCMC knowledge transfer manager based within Chemistry (**McBride,** 0.5 FTE). Both our Materials Innovation Factory (2017-) and previously our Centre for Materials Discovery (2007-2017) are founded on the Liverpool Model, encouraging external parties to provide guidance on industry drivers and needs, and to use our world-leading departmental facilities and leverage our academic expertise and knowledge leadership. The Liverpool Model has generated a high level of engagement, with industrial research users embedded on campus from 12 different companies within CMD (2014-2017) and 6 within the MIF over the REF period. To realise the full potential of academic-industrial partnerships, and the wider economy, one of Unilever's R&D leaders (**Reed**) began a long-term secondment to the MIF as a Strategic Director in 2019 to exploit the key

learnings from the success of the Unilever-Liverpool partnership and create a range of high-impact strategic partnerships with other R&D intensive UK manufacturers.

Our research strategy stems from consultation with end-users across the private sector, engagement with learned societies (§4.5) and specialist research domains (§4.6). We complement University level initiatives (led by our Research, Partnership and Innovation team) with our own bespoke activities, dedicated staff and promotional materials (§1.3), including advertising externally at major international industry events such as the Shanghai International Fair. We host an annual Liverpool Industry-Chemistry Engagement event (attracting over >100 companies across 2018 and 2019) providing an opportunity for our academics, existing and potential industrial partners and funders to collaborate.

4.3 Contributions to the Economy and Society

Our broad and flexible engagement pathways have led to significant and far reaching economic, societal and environmental impacts including: 6 spin-out companies, 20 licencing agreements, 27 consultancy projects, >30 industry/academia joint PGR students (including with Unilever, IBM, NSG Pilkington, Johnson Matthey, Croda, ExxonMobil, Arkema), 55 patent families filed and involvement on >25 advisory boards during this REF period.

Spin-out companies launched within the REF period include Liverpool ChiroChem (**Xiao**), Porous Liquid Technology (**A. Cooper**), Cage Capture (**A. Cooper**), Mobotics (**A. Cooper**) Polymer Mimetics (**Rannard**, jointly Scott Bader) and Tandem Nano (**Rannard**). These companies have received high levels of financial backing (>£6M) and are generating economic benefit through the creation of jobs, with Liverpool ChiroChem alone generating >60. Cage Capture won the RSC Emerging Technologies prize in 2016 and was a finalist in the Nature Spinoff Prize 2020.

The MIF and its predecessor CMD have engaged with >25 companies during the REF period, and their importance are recognised in the Liverpool City Region's science and innovation audit, which lists Materials Chemistry as one of three regional strengths. For Unilever, the lead partner in the CMD and MIF, new products launched in the REF period based on research carried out in these 2 specialist chemistry academic led centres are achieving sales of >€500M p.a. (details in our impact case study "High Throughput Polymer Discovery through the Centre for Materials Discovery"). Our strength in automated materials chemistry has led to Unilever re-focussing this research in the North West UK (Ellesmere Port). Furthermore, the specialist equipment developed and used by the MIF academics has led to new products being launched, such as by Micromeritics Instruments, and the relocation and expansion of Chemspeed UK to within the MIF.

Within the SIRE, coatings based upon nano-encapsulation (**Shchukin**) are being translated into products for thermal management of buildings and as antifouling coatings for shipping with large reductions in CO_2 emissions being achieved on test fleets.

Working with **Iggo**, Lucite funded PGR students and have filed 2 new patents for conditions and catalysts (2016, 2018) for the second stage of the ALPHA methyl methacrylate production method – a process which has led to the elimination of 130 ktonne p.a. waste and generated >$1.4 Bn in revenue.

Over this REF period, BP's (now INEOS) AVADA process for the synthesis of ethyl acetate (**Kozhevnikov** REF2014 impact case) has grown by 30% to >300 ktonne p.a. (2017).

Research from Medicinal Chemistry and Nanomedicine has contributed to 3 clinical trials within this REF period. Nanomedicine has contributed to 2 world-first human clinical trials (first orally dosed nanomedicine trials for HIV). The Abbvie compound ABBV-4083, developed in collaboration with the Liverpool School of Tropical Medicine, designed to treat the tropical diseases river blindness and elephantiasis which affect >120 million people, is entering Phase 2 trials.

4.4 Engagement with Communities and the Public

Outreach initiatives are now integral to our core departmental activity, included in an individuals' workload and considered within promotion and sabbatical leave cases. The diversity of activities is exemplified below:

- *Museum Exhibitions* including the creation of a Royal Society Summer Science exhibition called "The Hole Story" (2017, 14,000 attendees), and exhibiting at Tate Liverpool (2018), Royal Albert Hall "Illuminating Atoms" (2014), and Big Bang North West fair (2019).
- *Public Lectures* at science fairs such as Pint of Science, Wirral Arts Festival, Liverpool LightNight, SciBar, Science in the Snug, Science in the City, AAAS Science Webinar with a total of more than 35 lectures related to our research.
- *Workshops for Schools and Colleges* Our hands-on activities reach ~1000 students p.a. across the Northwest, targeting local underprivileged areas. Many are research-themed including practical nanotechnology workshops, and are delivered by a diverse set of academics, research staff, and PGR students. The menu of activities is refreshed yearly by UG project students.
- *Outreach for school teachers* through 4 specialised lectures at teachers' conferences, and the development of novel teaching materials for chemistry teachers, such as resources on molecular modelling for post-16 chemistry and biology students' as part of the National STEM Centre (**Berry**).
- *Development of Diversity and Equality* by participating in dedicated policy forums. Our academics give lectures and sit on panels within LivWiSE (Liverpool Women in Science & Engineering) events (**Nixon**) and have engaged with UKRSA to look at the needs of researchers taking periods of parental leave (**Slater**).
- We proactively engage with local, national and international print and broadcast media including opinion pieces in the New Statesman and our work on robotic chemistry (**A. Cooper**) was covered by the BBC (World, News, Radio 2 and 4 and all local radio stations).

4.5 Contribution to the Sustainability of the Discipline

Chemistry is a constantly evolving discipline that relies on learned societies and peer reviewed journals to promote its achievements and drive innovation. It also requires active participation in the operation of funding bodies and national facilities to maximise the benefit of public investment. We are involved:

- In *learned societies*, where 10 staff members have served as a committee member in this REF period, and *researcher associations*, where **Slater** chaired the UK Research Staff Association and the Royal Society Research Fellows Network.
- As *Editors* of peer reviewed journals, including Biocatalysis and Biotransformation (**Carnell**), Journal of Molecular Catalysis A (**Xiao**), Electrochimica Acta (**Hardwick**), Nanomedicine (**Rannard**), Chemical Science (**A. Cooper**); 12 staff members contribute to the editorial or advisory board of 16 scientific journals from RSC (5), ACS (4), Wiley (4) and others.
- As members of the *scientific committee of national facilities*, including Chair ISIS FAP1 and SIG3-ECA (**Claridge**), Facility Access Panel for STFC Lasers for Science (**Volk**) and Diamond (**Claridge**, **Chong**), ISIS (**Clark**) and allocation panel for UK solid-state NMR National Research Facility (**Blanc**).
- Contributing to national (EPRSC and RSC) and international (EU, South Korea, Saudi Arabia) funding bodies as *panellists* (16), *chairs of panels* (2) or as an *advisor* (EPSRC Council member, **Rosseinsky**).
- Redefining the disciplinary landscape by *organising conferences/workshops* with 50 events organised by Liverpool staff members including symposia in established conferences such as Materials Research Society and large international conferences including Materials Chemistry 13.

- Advancing the discipline by *publications* that consolidate knowledge and set possible roadmaps. Over 150 *reviews and perspective papers* (receiving >12,000 citations, Web of Science) have been published by our Department in addition to a scholarly book (**Zhang**).

4.6 Wider Influence and Contribution to the Research Base

Our staff members are encouraged to leverage their scientific knowledge leadership nationally and internationally to drive policy development:

- *Government advisory roles*. Our staff has membership in the Science Minister's Advanced Materials Leadership Council (**Rosseinsky**), and the Innovate UK Emerging Technologies & Industries Steering Committee (**Rannard**). We also contribute to the development of UK government briefing papers, with examples including "The opportunities and limitations of CO_2 utilisation" (**Rosseinsky**, **Cowan**, **Xiao**), "Green Hydrogen" (**Cowan**), and "Sustainable Synthetic Fuels for Transport" (**Rosseinsky**) as well as policies on national facilities, including the STFC Neutron Strategy Review 2017 (**Rosseinsky**).
- *Advisory or steering roles* are taken up in external national institutions including the Wellcome Trust (**Nixon**), Carnegie Trust (**Rannard**), NPL, Cardiff Catalysis Institute (**Rosseinsky**); international institutes and bodies like the Max Planck Institute for Solid State Research, Max Planck Institute for Microstructure Physics, US Department of Energy Materials Synthesis Review, CICECO-Aveiro (**Rosseinsky**), Chemistry Department at HK University of Science, Chemistry Department at Shanghai Jiao Tong University, International Center for Chemical and Biological Sciences at University of Karachi (**Xiao**), the Lawrence Berkeley National Laboratory (**A. Cooper**), Medicines for Malaria Venture (**O'Neill**), IMDEA Nanoscience Centre, Madrid, School of Chemical Technology, Aalto University (**Raval**), as well as private companies including RDGraphene (**Hardwick**), Gilead, Scott Bader (**Rannard**).
- Active *roles in National Networks* addressing specific challenges include UK Solar Fuels Network (**Cowan**, chair from 2020), Dial-a-Molecule (**Slater**, steering board), Directed Assembly Network (**Slater**, committee member), COVID-19 preclinical drug development and N8 Chemical Biology initiative (**O'Neill**, advisory boards), BIOCATANET, CoEBio3 (**Carnell**), Connect NMR UK (**Blanc**).
- Important recognitions received by our staff include: **Rosseinsky**, Royal Society Research Professor 2013-, re-awarded 2018; Royal Society Davy Medal 2017; **A. Cooper** Elected Fellow of the Royal Society 2015; Royal Society Hughes Medal 2019; **Bower** RSC Hickinbottom Prize 2015; Philip Leverhulme Prize 2016; **Nichols** RSC Geoffrey Barker Medal 2016; **Xiao** RSC Tilden Prize 2020.