

Institution: Imperial College London

Unit of Assessment: Chemistry (B8)

1. Unit context and structure, research and impact strategy**Overview**

The aim of the Chemistry Department at Imperial College (Imperial) is to inspire world-class chemical science, empowering staff and students to fulfil their potential within our inclusive scientific community. Our vision for chemistry builds upon our culture of collaboration transcending traditional disciplinary boundaries; we organize ourselves according to the potential impact of our research on society and industry addressing challenges in health, energy, sustainability and materials. Our research covers the full gamut of theoretical and experimental chemistry, allowing us to respond to opportunities such as Digital Chemistry and Synthetic Cells. From the discovery of a drug target for the common cold drug through to the synthesis of a hexagonal planar transition-metal complex that solved a 100-year old challenge set by the Nobel Prize Winner Werner, the Department has continued to pioneer frontiers in Chemistry during REF21. These breakthroughs have supported an impact pipeline that is unlocking applications from novel hydrogen fuel cells through to life-saving cancer drugs.

During REF21 Imperial invested £170M in a major new building for Chemistry research, the Molecular Sciences Research Hub (MSRH), on our White City Campus (see REF5a Institutional Environment Statement, IES). This 24,000m² cutting-edge research facility fulfills our strategic aim of obtaining state-of-the-art infrastructure for Chemistry. Reflecting Chemistry as a priority for Imperial, this investment is the first major science building at White City and represents a once-in-a-generation opportunity to change the way we work across disciplines, industry and local community. The White City Campus is an innovation ecosystem, including space and support for companies and entrepreneurs. The Department has grown from REF14, providing a home to 66 group leaders, including 13 staff holding independent research fellowships (63.3 FTE REF21). Additionally, our research community encompasses 100 postdoctoral research associates, 49 technical/operational staff, 7 teaching fellows, ~230 PhD and ~125 MRes students. This community is underpinned by our inclusive culture rewarded by renewal of our **Athena SWAN Gold Award** in 2019. A summary of our position relative to REF14 is provided below.

Chemistry Department	REF14		REF21	
Staff Returned (FTE)	54.9		63.3	
	Total	Per FTE	Total	Per FTE
Research Income	£60M	£1.0M	£86M	£1.4M
Publications	1,750	32	3,223	51
Citations	27,416	499	74,404	1,175

To take advantage of new opportunities, we restructured our research around 7 cross-disciplinary themes: i) Chemical Biology and Healthcare; ii) Energy; iii) Environmental and Green Chemistry; iv) Imaging, Sensing and Analytical Chemistry; v) Materials and Molecular Design; vi) Synthesis and Catalysis; vii) Theoretical, Computational and Data-driven Chemistry. Research is not siloed into formal groups and staff are encouraged to collaborate and interact via these themes. Our success in building our community around this strategic reorientation is evidenced by the substantial uplift in key performance indicators per FTE including: **~85% increase in publications, ~170% increase in citations and 43% increase in research income**. Reflecting our focus on impact, we leveraged our new infrastructure for knowledge transfer and exchange: we collaborate with >40 industrial partners directly investing in the translational impact of our research and have spun out >10 start-ups attracting >£ in funding.

Research Vision

During REF14, the Department pursued a growth strategy, with increased focus on multi-disciplinarity; this continued through REF21, accelerated by the 2018 MRSH opening. The

following aims underpin our vision:

- **Foster an inspiring and positive environment** enabling our community to thrive in the pursuit of blue skies research whilst attracting and nurturing new talent (11 lecturers were appointed during REF21).
- **Provide leadership** for inter-disciplinary collaboration within and beyond IC (e.g. London Centre for Nanotechnology (LCN)).
- **Recruit, train and retain leaders of tomorrow** providing a collaborative professional ecosystem (e.g. new academic appointments include 5 Royal Society URFs).
- **Support multidisciplinary training** for research and industry future leaders (e.g. 3 Centres for Doctoral Training-CDTs).
- **Deliver impact and support UK research capability** providing specialist infrastructure and facilities and partnering with external stakeholders to realise translation (e.g. £4M Agilent Measurement Suite (AMS)).
- **Promote early-stage commercialization** (e.g. leadership of an accelerator supporting >60 start-ups securing >\$300M).
- **Play leadership roles in national and international consortia** (e.g. multi-million InnoHub research cluster with Hong Kong).

Progress in delivering our research vision and aims is evidenced by:

1a. Support for multi-disciplinary research through the provision of world-class research facilities and co-location. Our research was already cross-disciplinary and cross-departmental in 2014; recognising the opportunity to unlock our potential further, Imperial committed to a major investment of £170M in the 24,000m² MSRH, allowing us to bring our Chemistry vision to life. MSRH is one of the most advanced chemical facilities in the world with a capacity for 80 groups and >800 researchers including collaborating groups from other departments stimulating connections between the chemical sciences and other disciplines. The carefully designed modular open-plan framework (section 3b) has created a dynamic research environment where static laboratories have been replaced by reconfigurable spaces able to adapt to changing research directions. MSRH allowed us to increase our research capacity and bandwidth (according to our strategic needs) by making 11 new academic appointments, attracting new industrial collaborations and transforming our research infrastructure: we implemented new Cat II biological facilities and anti-vibration laboratories that were previously unavailable. It fostered greater collaboration by bringing the community under one roof, rather than our three previous research buildings. We now have the infrastructure required to co-locate academic and external collaborators. This integration of themes and people is central to our vision for the future of Chemistry.

1b. Enabling Research Themes to excel in key areas identified by staff. In 2015, pre-empting the opportunities envisioned for our MSRH move, we developed our new framework of seven Research Themes. Each is challenge-led, outward-facing, multidisciplinary and designed to promote engagement with other Imperial departments. The Department pooled resources, intellectual and financial, and oriented recruitment around them, committing us to a collaborative outlook and strengthening implementation of our vision. Below we describe theme aims and exemplar achievements (sections 3 and 4 provide further funding and collaboration details).

Chemical Biology and Healthcare (CBHC) 4 strategic appointments created new capability in drug delivery (*Kamaly*), carbohydrate chemistry (*Schumann*), biological EPR (*Roessler*) and high-throughput chemical biology (*Walport*). Our research, cutting across chemistry applied to biology, drug discovery, nanomedicine, synthetic cells and diagnostics, was transformed through the provision of 2130m² of new chemical biology infrastructure (section 3c). These activities were complemented by the £5M EPSRC Chemical Biology CDT renewal and MRes programmes in Chemical Biology and Drug Discovery. Members engage in blue skies research through to translation e.g. small molecule/immuno-oncology drug discovery progressing from hit to clinical development. Activities have been transformed by proximity to the Hammersmith Medical Campus

following the White City move. An exemplar activity (Nature Chemistry, 10.1038/s41557-018-0039-2) on picornavirus inhibitors (Altmetric score=1251) was featured by >130 news outlets. The theme was key to a series of therapeutic breakthroughs underpinning two impact case studies (C1/C4, section 1e). These included the launch of the start-ups Myricx Pharma (*Tate*), NK:IO (*Fuchter*) and OneFour Discovery (*Armstrong*) raising >£5M and research on a CDK7 inhibitor (*Barrett/Fuchter*) that entered Phase II cancer clinical trials. Theme members play leadership roles in large-scale initiatives including the Imperial-Institute of Cancer Research (ICR), £13M CRUK Convergence Science Centre and £4.5M CRUK Imperial Centre. The theme established strong links with the Francis Crick Institute through joint appointments (*Schumann/Walport*) and satellite groups (*Tate/Di Antonio*). Members are directors of the Institute of Chemical Biology (ICB) (*Vilar*), Centre for Drug Discovery Science (CDDS) (*Tate/Fuchter*) and fabriCELL (Network of Excellence in Synthetic Cell Science) (*Ces/Di Michele*) bringing together >100 research groups and >15 industrial partners. *Tate*, *Fuchter*, *Long*, and *Vilar* secured £2.6M as part a £50M InnoHub Cluster in Biomedical Research with Hong Kong. Collaborations with industry include GSK and Pfizer.

Energy (ENE). The appointment of *Bakulin*, and provision of new energy research facilities further strengthened capabilities in optoelectronic research. We pioneered breakthroughs in the synthesis, characterisation, theory and simulation of energy materials, energy generation (fuel cells, solar cells) and energy storage (batteries, supercapacitors, chemical fuels). Research quality is manifest in members (*Heeney/Durrant*) featuring amongst the top 1% most highly cited scientists (ISI Highly Cited Material Scientists). A highlight combined spectroscopic and quantum-chemistry approaches to identify rules for transforming organic solar cell performance (*Bakulin*, Nature Materials, 10.1038/s41563-018-0128-z). Members are leaders in photovoltaics research leading to collaborative grants (e.g. EPSRC Programme grant on Targeted and Integrated Photovoltaics, £5.99M, (*Durrant/Heeney*)). Strategy documents such as the Royal Society policy document “Options for producing low-carbon hydrogen at scale” (*Durrant/Kucernak*) provide community direction. Pioneering research into battery technologies plays a central role in case studies C2/C3 (section 1e) with the *Kucernak* led launch of start-ups Bramble Energy, RFC Power, and Sweetgen Ltd raising >£5M. With the Physics Department, members run a Plastic Electronic Materials MRes. Members play leadership roles in College Institutes such as the Energy Futures Lab (*Kucernak*) and national initiatives (Faraday Institute, *Kucernak*). Industry links include Johnson Matthey, ITM Power and Tronox-Cristal.

Environmental and Green Chemistry (EGC). Research focusses on molecular technologies to impact agri-sciences, green synthesis and the environment. This includes catalytic systems for bio-based polymers and novel reagents to recycle hydrofluorocarbons. A joint appointment (*Kafizas*) and investment in new plant growth facilities opened new directions in light-activated materials for renewable fuel. Breakthroughs included a low-cost arsenic sensor (*Cass*) to test drinking water (sold by Aquafirm) and polymer membranes to separate mixtures (e.g. crude oil) without energy costly refinery distillation (*Jefferies*, Science, 10.1126/science.aba9806). Activities have been supported through a £1M Leverhulme CDT in Cellular Bionics (*Ces*) and Green Chemistry MRes. Our leadership in establishing the Centre for Climate Change Innovation (CCCI) (*Templer*) draws upon our Grantham Institute for Climate Change partnership. This allowed us to engage with the Mayor of London in defining London climate change policy and seed a new generation of clean-tech start-ups as outlined in Case Study C2 (section 1e). Further initiatives include a \$1M Human Frontiers of Science Program (*Ces*). The theme was involved in further impact activities including start-ups such as ECONIC (*Williams*) (C5, section 1e) which is addressing CO₂ global emissions with novel technologies that use this gas as a feedstock for polymers and Lixea (Brandt-Talbot) that is developing a biomass fractionation process using low-cost ionic liquids (C2, section 1e). Members play leading roles in the AgriFutures Lab (*Barter/Woscholski*), Ocean Plastic Solutions network (*Romain/Britovsek/Welton*) and the Centre for Translational Nutrition and Food Research (*Barter/Woscholski*). The theme has strong industry links including Syngenta.

Imaging, Sensing and Analytical Chemistry (ISAC). The appointment of *Ivanov* has strengthened the area of nanoscale sensors and the AMS has transformed analytical

capabilities. The theme has developed cutting-edge detection strategies to improve molecular specificity and sensitivity for early-stage diagnostics, medical imaging and pollutant sensing. An exemplar was the development of nanoscale tweezers for single molecule/organelle biopsies on individual cells (*Edel/Ivanov*, Nature Nanotechnology, 10.1038/s41565-018-0315-8). Further examples include tools for personalized therapies, rapid clinical diagnostics, label-free detection, electrotunable plasmonics, portable diagnostics and super-resolution time-resolved live-cell imaging. Biomedical imaging led to large grants including a £6.4M EPSRC Programme grant and £6M Medical Imaging CDT with Kings College London (*Long/Miller*) and an £1.7M ERC Consolidator Award (*Edel*). ISAC runs a Bioimaging Sciences MRes and members are involved in the LCN and Rutherford Lab (section 4a). The theme launched start-ups including Vidya Health (*Klug*) (C4, Section 1e) developing microfluidic disease diagnostics and Droptech Ltd (*Edel*) and Nanoprofiling Ltd (*Edel*) raising >£10M. The theme underpins industry collaborations including Oxford Nanopore.

Materials and Molecular Design (MMD). The appointments of *Di Michele* and *Torrissi* opened-up new areas in DNA nanotechnology, biowearable bioelectronics and 2-D materials. MMD activities were enhanced through new materials and characterization facilities (section 3c) including a £2.3M-Pulse Electron Paramagnetic Resonance spectroscopy (PEPR) national facility. Research focusses on development and optimization of molecules, nanostructured architectures and materials for applications including pharmaceuticals, self-healing materials and materials for energy. Research is highly regarded e.g. *McCulloch* (elected FRS 2020) features amongst the top 1% most highly cited scientists (ISI Highly Cited Material Scientists). An example breakthrough was a photocatalyst based on organic semiconductor heterojunction nanoparticles exhibiting unprecedented hydrogen evolution rates (Nature Materials, 10.1038/s41563-019-0591-1). High profile projects include a £7.7M EPSRC programme grant on fibre reinforced composites (*Shaffer*). The theme runs a Nanomaterials MRes and members are involved in industry collaborations e.g. a £3.2M EPSRC BP Prosperity Partnership.

Synthesis and Catalysis (SC). The appointment of *Bull* underpins theme focus on novel synthetic and catalytic methods for molecular discovery. Research in SC addresses challenges in synthetic chemistry and catalysis with the aim of developing fast, selective and clean chemical processes. Activity has been enhanced by access to >360 new fumehood spaces. The theme placed strategic focus on sustainable chemical manufacturing, recycling and digital chemistry complementing breakthroughs in late-stage functionalisation, biological probes and drug delivery polymers. Highlights include the first well-defined hexagonal planar transition-metal complex that was nominated for the 2019 Molecule of the Year (C&EN) (*Crimmin*, Nature, 10.1038/s41586-019-1616-2). Members spearheaded breakthroughs in Digital Chemistry developing high-throughput automation for the synthesis of molecular organic materials and supramolecular assemblies. This area is supported by the Institute for Digital Molecular Design and Fabrication (DigiFAB) (*Yaliraki(director)/Hii/Jelfs/Greenaway*). Activities supported a £6M CDT in Synthesis and Reaction Technology (*Hii/Yaliraki*) and a £2.8M EPSRC facility on Rapid Online Analysis of Reactions (ROAR) (*Hii*). SC activity stimulated a £1.7M ERC consolidator grant (*Crimmin*). Members deliver MRes courses in Advanced Molecular Synthesis and Chemistry and Engineering. The theme has partnerships with Johnson Matthey, Ineos, BASF and Polymateria.

Theoretical, Computational and Data-driven Chemistry (TCDC). Recognising the importance of computational materials discovery, the recruitment of *Jelfs* extended our capability in a theme encompassing computational chemistry and modelling, theoretical chemistry and data-driven approaches to chemistry. Growth includes data-driven approaches to chemistry, the application of unsupervised learning to biomolecular systems and AI to predict material properties. These topics complement the design and study of catalysts, modelling of electrochemical materials and studies of biomolecule function. Highlights include modelling of the first reversible electrotunable liquid mirror based on voltage-controlled self-assembly/disassembly (*Kornyshev*, Nature Materials, 10.1038/nmat4969). Large funding includes a €1.5M ERC grant (*Jelfs*) to accelerate materials discovery and a £1.3M EPSRC fellowship on electrochemical phenomena theory (*Cucinotta*). Members have developed (or contributed to) >10 software packages including

open source (e.g. *Jelfs*, SupramolecularToolKit; *Gould*, AMBAT), open access (e.g. *Yaliraki*, ProteinLens; *Cucinotta*, cp2k) and commercial (*Robb*, Bearpark Gaussian16; *Gould*, AMBER; *Harrison*, CRYSTAL) software. Early career training is a priority, e.g. €4.1M Marie Curie ITN (NanoHeal) partnership to study mineral interface healing (*Bresme/Harrison*). Members are involved in leadership of the Institute of Molecular Sciences and Engineering (IMSE) (*Harrison*) and its MRes and the Thomas Young Centre (TYC). Members work closely with industry including AstraZeneca (AZ).

1c. Increase the quality and volume of research activity with a balanced portfolio: We have strengthened our ability to deliver research through an investment of >£200M towards infrastructure, equipment and strategic staff appointments (section 2). We aimed to increase research bandwidth and unlock new areas of science including growth areas such as synthetic cell science and digital chemistry. This strategy, enhanced by collaborations supported by a network of multi-disciplinary institutes (section 1b, section 4a) and new ways of working with industry proved extremely successful, leading to >3,200 peer reviewed publications (~85% higher than REF14). The associated >74,000 citations are ~170% higher than REF14 (>27,400). Our community has been supported at all career stages: publication submissions are equally spread among our Fellows, Lecturers, Senior Lecturers, Readers and Professorial staff, mapping onto cohort size and male:female staff ratio. Additional performance indicators showed strong growth including a 43% increase in research income, 16% increase in PhD students, 98% increase in MRes students, 16% increase in academic staff numbers and 24% increase in patents filed. With active management this portfolio is well distributed (>93% of staff named as investigator). Post-graduate (PG; MRes+PhD) numbers have grown from 260 (2013/14) to 354 (2019/20) through investments in new CDTs that secured £1.2M industry funding, alongside a wider £2.4M PhD industry investment into the Department. Our community launched 4 new MRes courses in Advanced Molecular Synthesis, Molecular Engineering, Catalysis and Drug Discovery. The increase in MRes courses reflects a desire to enhance training in areas of specific research providing collaboration opportunities with other Departments (MRes projects combine two complementary supervisors). During REF21 we graduated 628 MRes and 384 PhD students.

1d. Working with industry and end users to deliver impact: Impact is deeply embedded in our 21st Century Chemistry vision. From co-location at scale through to multi-disciplinary networks and institutes with no barrier to entry (section 4a) we have pioneered collaborative models where researchers from different backgrounds work together and with external stakeholders on discovery and translation. As demonstrated through our impact case studies (C1-C5) these fused problem-led pulls from end users in healthcare and industry with bottom-up chemical sciences innovation. This enabled impact on challenges in health (C1/C4), energy (C2/C3), sustainability (C2/C5) and materials (C3/C5).

- C1** The Invention of Samuraciclib, a Highly Selective CDK-7 Inhibitor, the Formation of Carrick Therapeutics and Clinical Trials on Treating Patients with Resistant Cancers.
- C2** Green chemistry research and innovation policy driving a world-class cleantech Cluster in London.
- C3** Bramble Energy – Exploiting Materials Chemistry to Manufacture Practical Hydrogen Fuel Cells.
- C4** Interdisciplinary Chemistry-led research leading to new ventures in drug discovery, diagnostics and personal care.
- C5** ECONIC – Catalysis to Deliver Polymers from Carbon Dioxide.

Each case builds on fundamental breakthroughs including small molecules to treat cancer (C1), the design of near net zero industrial economies and regenerative fuel cells for use in renewable energy grids (C2), hydrogen fuel cells (C3), single-cell microfluidic platforms (C4), protein-protein interactions as cancer drug targets (C4) and catalysts which incorporate CO₂ into polymers (C5). These developments benefitted from researchers having access to world-class facilities which we invested in throughout REF14 and REF21. These have been key to unlocking new science alongside our multi-disciplinary approach to research. C1 emerged from a collaboration between

Chemistry and Medicine, C2 between Chemistry and the Grantham Institute, C3 between Chemistry, Electrical Engineering (UCL) and the Energy Futures Lab and C4 a series of collaborations between Chemistry and Physics at Imperial with the ICR, NHS and Francis Crick Institute. Our strategy aligns with that of Imperial, emphasizing cross-disciplinary quantitative research, impact and collaboration with external stakeholders.

Our impact agenda has continued to evolve in scale and ambition. In addition to commercialisation of in-house research we work with >40 companies who invest in our innovation pipelines (section 4c) with a view to addressing industry challenges. In parallel, a rapidly growing impact strategy has been to directly support research pipelines within industry by providing access to facilities and expertise they do not have access to. Key to this has been engagement with the industry and SME ecosystem that has grown at White City. This has acted as a catalyst for fostering collaborations, with dedicated MSRH co-location spaces driving pre-competitive research with companies such as Puraffinity and DNAe. MSRH is within 800m of the Imperial Hammersmith Medical Campus and NHS Trust bolstering biomedical engagement.

Hammersmith and Fulham Council (H&F) developed an industrial strategy to support Imperial-industry collaborations including the “Upstream Initiative” (a joint enterprise unit). Upstream and the Department co-established the Deep Tech Network interfacing >50 SMEs/industry partners in White City including MiNA Therapeutics and Novartis with Imperial researchers including those in Chemistry.

Further collaboration opportunities have arisen between Chemists based at the MSRH and I-Hub (22,000m² incubator). These buildings are physically conjoined stimulating collaborations with companies such as Polymateria and Sixfold Bioscience. This adjacency led to partnerships with the co-working ventures Central Working (>60 SMEs) and I-Hub Incubator (>15 SMEs) who meet regularly with our Director of Development and organise show and tell events with Chemistry staff. An example of the serendipity engineered through co-location with industry is our partnership with Clustermarket based in the I-Hub. Clustermarket pioneered a scientific equipment marketplace through which local SMEs can book and access MSRH equipment and expertise. This has been transformational for local SMEs who now access expensive equipment (e.g. confocal microscopes/NMRs) that would otherwise limit growth.

The Department played a leading role in co-founding the Imperial College Advanced Hackspace (ICAH) (section 4a) a prototyping warehouse where members rapidly convert ideas into prototypes. Working with ICAH the Department delivered a Hackers-in-Residence Programme for >50 start-ups giving them access to ICAH and MSRH equipment and expertise. This was pivotal to ventures such as Pregenerate.

Industry engagement has been strengthened locally and nationally through staff-led consortia and research centres (section 4a) including Agri-net which brings together >1000 members of the agri-science research and industry communities (e.g. Sainsbury's). These networks are complemented by CDT-SME Business Clubs supporting >35 companies (e.g. Calix, Deepmatter). The Department hosted visits from >90 other universities and national/international governmental agencies keen to learn best practice with regards to multi-disciplinary collaboration and new ways of working. Section 4c provides full details of the success of our impact strategy in driving industry engagement.

1e. Future strategic aims and goals for research and impact: We have identified research areas that build on emerging strengths and will foster cross-Departmental collaboration which we will support through MSRH satellite groups and Imperial's networks and Institutes. We will be appointing 6 new lecturers/senior lecturers and 2 readers/professors aligned to these areas over the coming 12-24 months. These include the interface between industry 4.0 and the Chemical Sciences which will revolutionize chemical synthesis, materials development, drug discovery and is an industry priority area. We will build a chemical hackspace, DigiFAB will foster cross-Department collaborations and a Digital Chemistry MSc will be launched (2022). The White City ecosystem, Francis Crick Institute, Hammersmith Medical Campus, Uren Biomedical Engineering

Hub and forthcoming School of Public Health represent an exceptional framework for growth in healthcare technologies and drug discovery. Strategic appointments in translational therapeutics are planned. Our CCCI and Agri-Futures Lab involvement reflects our long-term focus on climate change technologies, agri-tech and the circular economy. We plan appointments in sustainable carbon technologies, food security and will launch a Climate Change Innovation MSc (2022). The Department will expand activities in energy technologies and electronic structured materials including energy storage and fuel production by CO₂ reduction. To support impact, we will build on collaborations in health with the Rosalind Franklin Institute (RFI) and in energy and materials with the Faraday and Royce Institutes. Income diversification through pre-competitive research with local SMEs will be an increasing focus activity.

1f. Research integrity: This is an essential Departmental pillar. Imperial is signatory to the Concordat to Support Research Integrity and adopted the Council for Science and Technology's Universal Ethical Code for Scientists upholding its three principles. Imperial provides training in topics related to research integrity aimed at PG students, PDRAs, Fellows and Academic staff. It has transparent and fair processes to deal with allegations of research misconduct. To aid researchers in considering Responsible Research and Innovation (RRI), the Department set up training courses covering how project design can impact RRI, research ethics and bioethics, professional integrity and plagiarism. The Department is committed to encouraging research to be accessible through open access routes (e.g. Spiral, the institutional open access repository, IES) and for publications to incorporate FAIR data. The Department is a leader in FAIR developments through the IUPAC working party on FAIR Spectroscopic Data, Open Reaction Database initiative and new FAIR Chemistry tools e.g. the FAIRSharing record and automated workflows for FAIR NMR data publication.

2. People

Our submission of 63.3 FTE represents all permanent academic staff as well as ECRs with independent fellowships. Contract categories are 31.3 Professors, 6 Readers, 7 Senior Lecturers, 6 Lecturers, 13 Research Fellows (including 4 Imperial College Research Fellows, ICRFs). The ECRs with fixed-term contracts receive Department and College support for career progression at the end of their long-term fellowships. For the REF21 submission all staff submitted up to 10 outputs with the final selection made by a panel (HoD, Deputy HoDs, cross-Departmental representatives). Attention was paid to achieve representative outputs in terms of staff career stage (47% by Professors who make up 49% of submitted staff) and gender (19% by women making up 20% of submitted staff). 40% of impact case studies include companies led by women.

2a. Staffing strategy

Academic staff: Our focus has been on recruiting scientists according to excellence and strategic fit (see table below). We recruited 11 lecturers (L)/senior lecturers (SL) – four of them female. Recruitment advertising is framed around open research themes recognising that open adverts attract more women and BAME candidates. We formed search committees to encourage applications from across cultures and circumstances and offered mentoring to unsuccessful female candidates with exceptional potential (one of them, *Cucinotta*, securing an EPSRC Fellowship, joining us in 2018). This process has been recognised as best practice (Athena SWAN Gold and highlighted as a “beacon activity” by the Institute of Physics) and the percentage of female academic staff has increased (12.3% to 19.7%). ~10% staff turnover across REF21 ensured vitality and we supported staff to achieve their personal ambitions e.g. moving to other Universities (Oxford, Birmingham, Wellington) or enabling impact industry secondments (Vidya Health).

Research Theme	New Permanent Recruit	Expertise
CHBC	<i>Kamaly (L)</i>	Imaging/drug delivery
	<i>Roessler (SL)</i>	Bioinorganic chemistry/EPR
	<i>*Schumann (L)</i>	Carbohydrate chemistry/glycobiology
	<i>*Walport (L)</i>	High-throughput platforms/chemical biology
MMD	<i>Torrise (L)</i>	2D materials/wearable bioelectronics
	<i>Di Michele (L/URF)</i>	DNA nanotechnology
SC	<i>Bull (L/URF)</i>	Synthetic methods for molecular discovery
ISAC	<i>Ivanov (L)</i>	Nanoscale sensors
ENE	<i>Bakulin (L/URF)</i>	Organic optoelectronic discovery
TCDC	<i>Jelfs (SL/URF)</i>	Computational materials discovery
EGC	<i>*Kafizas (L)</i>	Light-activated materials for renewable fuels

* Crick Institute / * Grantham Institute Joint Appointment

Personal research fellowships won in open competition: Potential fellows apply via a dedicated website to a selection committee which identifies candidates. Subsequently we support them throughout the application process (mentoring, administration, mock interviews). We are proud to have had >45 externally funded fellows since 2014 including 30 Marie Curie Fellows and 9 newly hired independent research fellows, four of whom are female (see Table below).

Research Theme	New Hires on Fixed Term contracts	Expertise
CHBC	<i>Di Antonio</i> (BBSRC David Philips)	Nucleic acid chemical biology/epigenetics
	<i>Aprile</i> (UKRI Future Leader)	Antibody engineering/protein aggregation
	<i>Barnard</i> (Wellcome Trust Henry Dale)	Protein chemical biology
SC	<i>Chadwick</i> (ICRF)	Organometallic catalysis
	<i>Lewis</i> (ICRF)	Supramolecular chemistry
MMD	<i>Greenaway</i> (URF)	High throughput automation/porous materials
ENE	<i>Gasparini</i> (ICRF)	Photovoltaics, bioelectronics
TCDC	<i>Cucinotta</i> (EPSRC Fellow)	Computational electrochemistry
EGC	<i>Brandt-Talbot</i> (ICRF)	Renewable materials

The internally funded ICRF scheme (11 fellows to Chemistry in REF21) attracts talented ECRs, providing four years funding to establish independent careers. Six of these ICRF fellows secured permanent positions at Imperial or elsewhere. Fellows benefit from a tailored training programme provided by Imperial's Postdoc and Fellows Development Centre (PFDC) and fellowships are formally reviewed at their mid-point to ensure the fellow maximises opportunities for career advancement and can exploit opportunities for permanent positions in

the Department and elsewhere.

2b. Staff development, support mechanisms and career progression

Academic staff: The HoD (*Armstrong* 2015-19, *Ces* 2019-present) is responsible for line management, supported by seven senior academics who undertake line management of staff sub-cohorts (6-10). A 6-month induction programme introducing new staff to the department and vice versa is provided, guided by a mentor. We introduce new academic staff to relevant companies with the mentor providing guidance on impact philosophy. New appointees are provided with start-up packages including equipped labs/office/funding (£60k-£180k) and allocation of at least one PhD. Staff are encouraged to take advantage of training via the Imperial Learning and Development Centre (LDC) and Educational Development Unit (staff attended 37 different courses filling 74 spaces during REF21).

All staff have an annual personal review and development plan (PRDP) meeting with their line manager identifying support to achieve career goals, recognising achievements and discussing research impact. Coaching is offered to staff with management responsibilities and the Department contributes to mid-career leadership courses. With input from Chemistry, the Faculty runs a programme on “Strategic Training in External Partnerships” providing new academic staff with know-how on routes to delivering impact.

As part of the annual promotion process, the HoD and line managers invite applications and identify candidates to be encouraged to apply. They identify potential candidates for future years (providing application support) and look for candidates to nominate for prizes (particularly historically underrepresented groups). ~95% of promotions during REF21 were successful (total 36) and of those 22% (8) were for female staff (19% of all staff are female). We attribute this parity to rigorous and fair Departmental promotion procedures. During the annual pay relativity exercise the HoD recommends those with major achievements (e.g. impact, community) receive financial bonuses.

Our workload model ensures equitable distribution of work and enables those who need it to be released from some duties. The model is based upon parity of core teaching ensuring all staff can engage in research and impact. Fellows are restricted to minimal teaching and new staff members ramp up from 0.2 to 1FTE over 2 years. The model captures activities associated with research and impact allocating the remaining time to management and administration. This transparency led to 81% of Chemistry staff indicating they “knew what is expected of me in my role” (Imperial Staff Survey 2019). The model allows for a smooth transition back from long-term leave and promotes rotation of responsibilities and succession/handover planning.

The Elsie Widdowson Fellowship releases academic staff returning from maternity/adoption/surrogacy leave from all teaching and administrative duties for one year enabling them to maintain research momentum. Five Elsie Widdowson Fellowships were awarded during REF21. During parental leave, academic staff may request Department funding for a PDRA to support research during leave (5x6 months awarded) and flexible working is supported upon return. Since its introduction (2015), two women and six men took shared parental leave.

Research Staff: We are dedicated to supporting fixed-term research staff through implementing the Concordat principles. During REF 21 >326 RAs completed their post. We offer research staff career advice and support through direct mentoring, including the PRDP, PFDC and Chemistry Post-Doc and Fellow Committee (CPFC) (6 Departmental Reps and 2 Champions) who ensure the PFDC stays well-informed about researcher needs. The CPFC Chair meets monthly with the HoD and sits on the Department EDI committee. The Department supports the CPFC with a £5k budget for networking events. During Women@Imperial weeks, the PFDC runs “Paths for Postdoc” events involving women speakers from Chemistry.

Research staff have ten annual development days written into contracts. During REF21 they registered for 56 different LDC courses, filling 127 spaces. PDRAs enjoy outstanding support from the PFDC which offers >50 bespoke courses (132 Chemistry PDRAs [40%] registered during REF 21) including ones specifically designed for women and BAME staff, funder showcases, one-to-one support (128 PDRAs) and mock interviews (49 PDRAs, double REF14). PDRAs involved in student supervision can apply for the title of Assistant Supervisor and attend Graduate School training recognising the valuable contribution they make towards student supervision (currently 18 PDRAs hold this status).

The Department supported the Irene Joliot-Curie conferences (co-founded by *Welton*) designed to promote womens' careers in science providing speakers and mentors, and bursaries for PDRA attendance. Programme success led to it being transferred to the RSC and other learned societies.

2c. General Professional support

Effective, transparent management for a sustainable Department: Our Departmental vision was developed bottom-up and the result of a large-scale consultation involving all staff, Departmental Champions across Imperial and >80 external stakeholders from industry, academia and government. To support the new vision, we recently refreshed our External Advisory Board (EAB), bringing together internationally leading academics (*Yellowlees*, *Edinburgh/de Mello*, *ETH/Blackmond*, *Scripps/Bassereau*, *Institute Curie Paris*), industrial leaders (*Skingle*, *GSK/Haywood*, *MedCity*) and engagement leaders (*Caddick*/former Director of Innovation Wellcome Trust). The EAB will provide strategic insight into our next 10-year strategy.

More broadly, Departmental staff are supported by a management structure which includes the Executive (HoD/Associate HoDs/Director of Research (DoR)/Recruitment and Safety), responsible for coordinating large initiatives, Imperial Strategy integration and EAB engagement. The Research Strategy Group (RSG) led by the DoR (*Vilar*) promotes industry engagement and is responsible for developing and maintaining facilities to enable staff to achieve their research ambitions. It includes Research Theme Leads, the Research Development Manager (new post, section 3a) and rotating ECRs who gain planning insight. The Management Committee coordinates operational mechanisms and monitors performance. H&S is overseen by the Director of Safety, Safety Committee and Faculty H&S staff who are sector-leading e.g. their RSC book ('Challenges for Health and Safety in Higher Education and Research Organisations', 2020) is regarded best practice. In the Imperial Staff Survey (2019) 96% of staff said "they were aware of their personal H&S responsibilities".

Professional and Technical staff: We are committed to supporting and celebrating the contribution and career progression of Professional and Technical staff. E.g. five technicians gained "chartered scientist" status during REF21 with the Department contributing financial support, study leave support and career planning sessions.

Community, well-being, mental health: We actively seek out and create opportunities to nominate staff for Honours and Awards. Bottom-up recognition is captured through the Chemistry Community Honours: community members nominate colleagues in recognition of positive contributions with citations published (~300 nominations per edition). We award annual Chemistry Prizes and publish a monthly Newsletter. All staff attend monthly Departmental meetings; in addition, meetings are organised between the HoD and different communities (Fellows/PDRAs/PhD students/Professional/Technical/Administrative/Teaching staff). These promote transparency and feed into the Staff Action Plan ensuring everyone has a say in the running of the Department. We introduced trained Mental Health (MH) First Aiders, a Support Services and Life Adviser and established a MH Safe Place. We run regular community events (e.g. guided meditations).

A key element of well-being is flexible working and all Academic, Learning & Teaching and Research staff benefit from home working, job-sharing, staggered hours, and condensed hours. Staff may also apply to reduce working hours on a short-term or permanent basis or request

special leave for reasons including study leave. In the 2019 Imperial staff survey 94% of Chemistry staff responded positively to 'As long as I get the work done, I am trusted to organise my workload in a way that suits me'.

Throughout COVID-19 we implemented a 'do what you can when you can' policy and asked staff to highlight changes in circumstances so that support could be provided. MSRH opening hours were extended and resourced to enable staff and students who needed to travel to do so at non-peak times and at times that worked around their circumstances.

We are constantly working to improve our physical environments. MSRH (section 3b) was designed with inclusivity in mind: wheelchair access, variable height benches and fume cupboards in every laboratory, a multi-faith prayer room and a mothers' room. The Department retains a 3000m² footprint at South Kensington supporting cross-campus collaborations and providing informal environments for staff to work and relax in (e.g. new staff common room). This supports sociability encouraging collaboration at all levels. In the College Staff Survey (2019), 91% of Chemists said they had a good working relationship with colleagues.

Building on measures aimed at increasing the visibility of our diverse community six members of the Department were included in the RSC project "175 Faces of Chemistry – Celebrating Diversity in Chemistry", and *Wilton* was awarded an OBE (2017) for "Services to diversity in education".

2d. Training and supervision of PGR students

We attract outstanding students from the UK and internationally. The Department has a vibrant community of ~230 PhD students (50% EU/overseas) and ~125 MRes students. We have a proud history of PG training and research with practical benefits to society with >50 external partners involved in co-funding/co-supervision/training of PhD students during REF21. All PhD students are part of the Graduate School, which provides development courses and Global Retreats. During REF21 Chemistry PG students took 1786 places across 166 different courses. Students attend a minimum of four professional skills workshops and a plagiarism awareness course during their PhD. Our CDTs have pioneered transferable skills courses that have been translated to the Graduate School and franchised to other institutions (e.g. BBC Science Communication). All students are aligned with Research Themes allowing them to benefit from cohort frameworks. A growth area has been MRes students (63 in 2014 to 125 in 2020). We run eight MRes courses reflecting our core capabilities and work at interfaces: Chemical Biology, Bioimaging, Drug Discovery, Biological and Physical Chemistry, Nanomaterials, Catalysis, Advanced Molecular Synthesis and Green Chemistry. Currently, the PG student-staff ratio is 4.2:1 for PhDs and 2:1 for MRes.

PhD Recruitment: Open days include Department tours where potential applicants meet students and group leaders and hear talks on MRes/PhD options. Department (DTP/CDT) and Imperial (President's PhD Scholarships/CSC) schemes are supplemented by studentships from various sources (industry/charities). The Department receives >200 formal applications p.a., resulting in ~65-70 new PhD students. These are typically funded: 25% CDTs, 20% Institutional, 10% overseas funders, 10% DTPs, 10% industry and 25% other sources. The conversion of applications-to-offers and offers-to-acceptances over REF21 reveals decisions are free of gender bias (40% female applicants and 42% female students). Recruitment is based on Imperial-EDI recommendations aimed at welcoming students across the neurodiversity spectrum and from diverse backgrounds (>40 different countries). A £2M donation supports two scholarships p.a. for students from Nigeria.

PhD Support mechanisms: Inductions include facilities, safety, professional development and talks by the Provost, Head of Graduate School and HoD. The Departmental PG Social Committee organizes events supported by £12k from the Department. Committees led by the Directors of PG (*Wilton-Ely*) and MRes (*Woscholski*) Studies (DPS/DPMS) provide support to PG/MRes students including PG and MRes Senior Tutors, Research Student Manager, MRes and PG Administrators, SSLA and MH First Aiders, CDT Directors, MRes

Course Directors, CDT Project Managers and an EDI Fellow. New supervisors are assigned experienced co-supervisors and take courses through the Faculty Educational Development Unit. The HoD meets the PhD community monthly to drive student experience improvement e.g. informed the decision to award PhD students who moved to MSRH a 1-3 month funded extension according to need.

Teaching and Progress monitoring: Assessments occur after 9 months (ESR), including an oral examination, and 24 months (LSR) as well as a PG symposium presentation. The ESR ensures the student can pursue independent research and checks they are being supported. Monitoring continues with 6-monthly progress questionnaires. In the LSR, progress is assessed in terms of results and project direction and includes a thesis plan. LSR assessors follow up at 30 months. These mechanisms provide warnings of conflict or student under-performance. 85% of PhD students submit on time (>4 years) (above national average of 80%).

PhD Career development: The Graduate School provides professional development for PG students (won 2017 Times Higher Education Award for Student Experience), through transferrable skills courses including a residential course and events in collaboration with the Careers Service. Complementing courses offered by the Graduate School, we deliver PG transferrable skills courses that drive cohort formation, promote student empowerment, facilitate early-stage commercialization, encourage networking and support multidisciplinary research. These include Science Communication with the BBC, HACKEDU offering industry 4.0 training with ICAH, Industry Innovation workshops and RRI and EDI courses. The Department organizes career seminars to ensure students are informed about career opportunities and benefit from help on job applications, CVs and interview practice from potential employers. >50 external partners work with the Department in training delivery including the chemical (BASF), pharmaceutical (GSK), personal-care (P&G), agri-science (Syngenta) and med-tech sectors (Oxford Nanopore) and additional organizations such as the National Physical Laboratory. The Department has several programs (EVOLVE, Wilkinson's fund) facilitating PhD student placements (from 2 weeks to 1 year) in other universities, industry or government organizations. Students benefit from a wide range of outreach opportunities (section 4).

The Department with the RSC, piloted a Membership and Accredited Recognition Scheme (MARS) supporting PG student progression through professional body membership categories. The pilot scheme proved popular with female postgraduates (54% of students were female). Of PhD graduates reporting a destination (2014-2018 data), 57% continued to a research post and notably 72% ended up in full-time employment within 6 months of completing their studies.

Pioneering Early Career Entrepreneurship: We have pioneered student entrepreneurship so ECRs can spin-out. PhDs students own 100% of IP they create independently; through a new Imperial initiative (Founders Choice) PDRA's own 95%. This approach stimulated PG/PDRA spinouts including FreshCheck. Students benefit from the Invention Works pipeline: entrepreneurship education (delivered via the Enterprise lab), ICAH access to build prototypes and space at the I-Hub incubator to scale-up. The Department supports seed funding programmes (Project Boosters) alongside the Imperial VC Challenge. There has been an emerging stream of achievement-we have supported a pipeline of female entrepreneurs including those pursuing agricultural productivity (Fungi-alert, *Weaver/de Manzanos*) and clean tech innovation (Lixea, *Brandt-Talbot*).

Awards: Our PG students have won numerous awards for conference contributions (e.g. Gold Medal, STEM for Britain) demonstrating the high level of research achieved and the effectiveness of our presentation skills training. Thirteen students won EPSRC Doctoral Prize Fellowships.

2e. Equality, Diversity and Inclusion

The Department established a new EDI Committee in 2015. It shares best practice, discusses concerns, invites speakers to update on EDI topics and ensures we embed EDI in all activities.

Chaired by two EDI Co-Directors (*Jelfs/Barnard*) it expanded to include sub-committees focused on e.g. Recruitment, Flexible Working, Inductions and EDI Training. **Our sector leading EDI environment was recognised through renewal of our Athena SWAN Gold award (2019) making the Department one of 16 UK Departments to hold an Athena SWAN Gold award and one of only two in Chemistry.** The award represented an opportunity to drive further positive change and we have since included: (i) 'Action on EDI' courses and annual unconscious bias staff training; (ii) introduced Bronze, Silver, Gold EDI training requirements; (iii) altered assessment processes for PhD scholarships to consider the diverse pathways of applicants. The Department has fostered an extremely supportive environment benefitting from a diverse international concentration of scientists and multi-disciplinary centres where collaboration is encouraged. Joint seminars and social events abound with a culture of interaction extending to other local institutions.

3. Income, infrastructure and facilities

3a. Research income: Our ambitious strategy to increase income, diversify funding and raise £170M towards construction and fit-out of the MSRH has been underpinned by the Research Strategy Group (RSG). We succeeded in achieving these objectives in parallel, capitalized on collaborative opportunities stemming from our multidisciplinary challenge-led themes and leveraged the MSRH development to unlock new funding streams including industrial philanthropic support. The RSG is supported by the Research Development Manager (RDM), a new post (2017) that monitors 12-month funding plans submitted following PRDPs, organises peer-to-peer grant reviews, mock interviews, compiles funding opportunities for staff, liaises with Imperial's Industry Partnerships and Commercialisation team and with Faculty Research Committee to promote inter-Departmental and inter-Faculty collaborations.

Grants Awarded: This strategy led to Chemistry being awarded £86M in REF21 (vs. £60M in REF14), made up of 329 new grants from ~90 funders. Funding sources were: £38.6M (45%) from UKRI/Royal Society, £22.1M (26%) from the EC, £10.5 (12%) from industry, £6.9M (8%) from charities and £8M (9%) from other sources.

To diversify our portfolio we engaged with EU partners and as a result increased EU funding by 50%. Most UKRI funding was from EPSRC (£30.4M) followed by RS (£4.7M) and BBSRC (£2.3M). Multiple examples have already been highlighted throughout section 1b. Additional prestigious exemplars include an EPSRC Programme grant in materials for energy, £1.83M (*Durrant/Haque/Kucernak*), senior fellowships from EPSRC, £1.58M (*Fuchter*) and 4 EPSRC-Horizons grants, £800K (*Bakulin/Heeney/Di Michele/Brooks*). BBSRC and MRC grants have supported research at the chemistry/life sciences interface, £1.5M (*Tate*). Notable EU funding includes a further three ERC starter grants, €6M (*Di Michele/Bakulin/Crimmin*). Industrial funding was £10.5M reflecting the translational impact of our research. Examples include a BASF Corrosion Cluster £500K (*Harrison*), a £1M AstraZeneca-BBSRC – Surface interactions with antibodies grant (*Bresme*) and an Ineos – Polymerisation catalysis initiative £900K (*Britovsek*).

Philanthropic income was £3.9M (96 individual gifts) enabling us to strengthen equipment provision (Agilent), widen participation for home students and improve socializing spaces (Dr Cross) and attract exceptional ECRs from Nigeria (Jack Hirst Scholarship).

3b. Infrastructure: Our strategic expansion with respect to bandwidth, co-location, collaboration models and facilitating research in new areas (e.g. plant chemical biology, label free imaging) has been supported by MSRH linked investments.

MSRH was built to high energy efficient standards, certified BREEAM excellent and awarded a 2019 global laboratory design S-Lab prize. It spans 9 floors, each benefitting from dedicated technical support and offers access to high-quality research space and flexible infrastructure fostering collaboration. This includes large-scale open-plan laboratories (10x500m²) and writing-up areas and >360 fume-cupboard workspaces. MSRH has a 200m² social common room and exhibition atrium. Specialist areas include 23 laser/microscopy bays (330m²), low-electrical noise laboratories (220m²), a

cleanroom-suite, glove box and solvent drying tower areas, furnace room, fuel-cell laboratory, workshops, cold rooms/laboratories, plant growth, autoclave rooms, protein production and cell culture areas, radioisotope and nanoparticle laboratories (211m²). Further facilities include a 242-seater lecture theatre, seminar rooms, common room, MH suite, exhibition atrium and instrument rooms.

3c. Research facilities and equipment: The RSG oversees Departmental equipment planning including identifying strategic opportunities to invest in new facilities. We have been extremely successful, opening a series of national instrumentation facilities with each supporting multiple themes whilst promoting a broader cultural change with a move towards shared equipment clusters pooling equipment and staff resources. These have driven efficiency savings and promoted knowledge transfer. A measure of success is that 15% of all instruments on the Imperial shared equipment register are registered to Chemistry, the largest contribution by any Department. The following examples highlight new capabilities that support our Research Themes and enhance partner collaborations.

The AMS (£4M) is the largest university investment by Agilent in the world and provides unrivalled walk-in capabilities for researchers to apply the latest measurement technologies. Up to 50% of AMS user time is dedicated to supporting external users which now number >30 from other Imperial Departments and >15 users from other universities and industry, e.g. Syngenta. The AMS offers: (i) High-end analytical and preparative chromatography (LC, GPC, SEC) and capillary electrophoresis; (ii) Single and triple quadrupole-LCMS; (iii) ICPMS; (iv) FTIR-Chemical Imaging; (v) Seahorse analyzer. Smaller items worth £1M (HPLC, spectrometers) are distributed throughout MSRH. It supports >100 projects helping researchers evaluate methods for e.g. delivering therapeutics to the brain and understanding interstitial fluid composition.

The Department identified Digital Chemistry as a growth area requiring infrastructure investment. We raised funding from EPSRC (2018) and industry to establish ROAR (£2.8M). ROAR is the first EPSRC Dial-a-Molecule Grand Challenge institute providing Imperial researchers (>15 research groups from Chemistry and Chemical Engineering) and >10 external partners (e.g. BASF) with access to instrumentation for data-centric synthetic research. It incorporates: (i) High-throughput robotic reactor platforms (e.g. three UnChained Labs Junior platforms, Opentrons OT-2 platforms) (ii) *In situ* real-time reaction monitoring; (iii) Continuous flow reactors; (iv) Automated parallel synthesis reactors; (v) uPLC-SFC-MS systems for high-throughput reaction analysis. ROAR supports our CDT in Synthesis and Reaction Technology and the DigiFAB community providing an integrated suite to synthesise and characterise molecules in high-throughput and analyse reaction progress online.

The Department sought to support instrumentation to study unpaired electron systems securing EPSRC funding (£2.3M) (2020) and partnering with Bruker to establish PEPR at MSRH. PEPR combines EPR spectroscopy with film electrochemistry: (i) X/Q-band pulse Spectrometer; (ii) continuous-wave X-band Spectrometer; (iii) cryogen-free cryostats. PEPR enables pulse measurements at multiple frequencies of a range of systems from membrane proteins to hydrogen production catalysts.

Chemical Biology has been a strategic growth area (section 1b). We invested in dedicated infrastructure and equipment including 4 fully equipped category-2 tissue culture rooms and protein production facilities. MSRH offers equipment for automated peptide and oligonucleotide synthesis, and instrumentation to analyse biomolecules and cells (e.g. IncuCyte live-cell imaging system, flow cytometer, SPR, MS proteomic facilities, Zetasizer). Our new capabilities allowed us to integrate biophysical characterisation and synthesis of biomolecules with detailed cellular studies and expand plant chemical biology activities.

An additional strategic area is molecular materials (with emphasis on energy, section 1b). We enhanced materials fabrication and characterization capabilities. This encompasses a 160m² class 7/8 clean room housing suites for soft electronic and microfluidic materials including glove boxes, evaporators, spin coating and doctor blading equipment, solar simulators and external

quantum efficiency spectrometers. We offer microscale polymer processing, atomic layer deposition, sputter coating, high-temperature furnace rooms and core characterisation (PXRD/TGA-MS/DSC). Printing, coating techniques, additive manufacturing processes, AC/DC temperature-dependent electrical and Vis-NIR optical material characterisation setups are available. Imperial is a Henry Royce Institute partner with equipment from the £10M node housed in the MSRH (confocal optical microscopy, advanced electrochemical facilities) and UREN Engineering Hub (SEM/FIB/high-power XRD/RIE/MOCVD). The Department offers transient laser spectroscopies for soft electronic materials, including eleven ultrafast (fs) and eight slower timescale laser systems.

To complement chemical biology and materials research the Department offers a microscopy suite. MSRH allowed us to co-locate these in a dedicated area making this facility safer and more efficient to operate. It includes super-resolution fluorescence microscopes (STED/dSTORM), fluorescence imaging including confocal microscopes (single/double photon excitation), high-resolution Raman imaging (visible/infrared), fluorescence lifetime imaging (femtosecond time resolution), 2D-IR microscopes and dark-field imaging microscopes (visible/NIR/IR). The Department has >15 optical microscopes for bright field microscopy with detectors capable of low-light detection, single photon counting, and ultrafast high-speed imaging (100,000 fps). Optical polarization microscopes and holographic optical trapping platforms are available. We house AFMs, SEMs and a Scanning Ion Conductance Microscope.

The Department has a long track record of innovation in organic/inorganic synthesis and homogeneous catalysis. Further to ROAR investments we have a core instrumentation suite supporting this area including an NMR Spectroscopy facility (290m²) measuring ~90,000 samples pa. We have one 500MHz and five 400MHz Bruker spectrometers (-80 to +130 °C) with multinuclear probes. For solid samples, two Bruker spectrometers are available (200MHz/600MHz) with VT capability. The Department benefits from access to the Cross-Faculty NMR facility including three Bruker spectrometers (800MHz/two 600MHz). In addition to AMS capabilities we have a cutting-edge Mass Spectrometry facility supporting >70 research groups (>400 users) and >20 companies, analysing >12K samples p.a. Techniques include (low/high resolution): EI-MS (Direct Insertion and coupled to GC)/APCI MS/CI MS/MALDI-ToF/UPLC (ES) Electrospray ToF/UPLC-ES/QQQ-MS/UPLC-ES/SQ-MS/DART analysis/NanoFlow LCES Orbitrap-MS/TGA-EGMS. For solid state characterisation we have an X-ray facility including two 4-circle (kappa geometry) single crystal X-ray diffractometers and powder/thin film XRD. MSRH enabled us to further expand capabilities in synthesis providing air-sensitive characterisation suites, centralised solvent drying columns and a high-pressure reactor suite to study catalytic systems.

Soft condensed matter studies are supported by six SAXS/WAXS X-ray beamlines. These have been enhanced through strong engagement with large scale facilities such as Diamond, ISIS and the ESRF where we secured >170 beamtime shifts.

The Department has access to state-of-the-art computing facilities including an in-house computational suite housing 82 workstations (450m²) and a bespoke MSRH NVIDIA GPU cluster (48 GPU's). Imperial invested £25M during REF21 in Research Computing Service (RCS) providing an extensive range of central computing technologies (fast networking, large scale data storage, high performance computing) and support services (clinics, training). >250 Chemistry researchers are registered to use RCS with usage during REF21 exceeding 55 million CPU hours. High Performance Computing (HPC) coupled with a Research Data Store (RDS) is hosted in an external data centre (one of the largest UK facilities with 72,000x86 CPU cores with 500 terabytes of main memory, together with >5 petabytes disk storage). Chemistry has access to the national EPSRC Materials and Molecular Modelling Hub HPC system. Access to these is central to computational and theoretical chemists, allowing them to perform cutting-edge simulations (e.g. molecular dynamics simulations of membrane proteins). These facilities enable storage and processing of large imaging and digital chemistry data sets.

Staff have access to a range of Imperial facilities. Examples include: Electron Microscopy (Cs-corrected/monochromated S(TEM)/dual beam slice and view) to support materials' characterization; cryo equipment for imaging biological, soft, and hybrid materials; radioisotope production ($^{11}\text{C}/^{18}\text{F}$) for PET imaging. Inter-institutional sharing is established, e.g. via LCN, giving access to lithography cleanrooms, STMs and neon-ion microscopy.

3d. Professional Services Support: Research benefits from four Departmentally funded teams. Three analytical scientists run our core instrumentation (NMR, MS, XRD), two run ROAR, one the AMS (supported by Agilent personnel), and two PEPR. Seven research technicians provide general chemistry support including a mechanical workshop technician, electronics expert and instrument tester (working together as an instrument design team capitalising on ICAH), a chemical waste and inventory coordinator, and a tissue culture technician. This team has oversight from the Technical Operations and Technical Services Managers. The team frequently appears as output co-authors. The Department employs LabCup management software to improve safety and avoid chemicals duplication. Through a Clustermarket partnership supported by Stratocore PPMS, equipment is accessible to internal and external stakeholders.

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

4a. Contributions to the research base

Support and mechanisms for interdisciplinary collaborations: We recognise that working collaboratively with colleagues across Imperial and other institutions provides unique opportunities for multi-disciplinary research. Collaboration is the lifeblood of our research ethos with joint projects and grants with almost every department at Imperial. 63% of grants are inter-departmental and 35% are with external institutions. >80% of papers submitted to REF21 involve collaborations with other Departments at Imperial, other universities or both. 18% of Chemistry-registered PhDs are co-supervised by non-chemists, with a similar number registered elsewhere co-supervised by chemists.

We are strong advocates of joint appointments as a mechanism for supporting collaborations. In addition to those highlighted in section 1b examples include joint appointments with other Departments/Institutes within Imperial (*Shaffer/Materials*; *Templer/Grantham Institute*) and other universities (*Durrant/Swansea*; *McCulloch/KAUST*; *Torrisi/Catania*), growing activity in materials and climate change technologies. To further promote collaborations we held >300 seminars with international (30%) and industrial (12%) speakers at the Department and >160 other events including distinguished prize lectures e.g. Sir Derek Barton Centenary Celebration, 2018 and Nobel Prize Winners Szostak and Moerner. We benefit from seminars organised by interdisciplinary centres that Chemistry staff lead e.g. IMSE (41) and LCN (200).

Chemistry Leadership in Multi-disciplinary Institutes/Centres: As highlighted in section 1b a key mechanism to foster collaboration is via the 56 Imperial Global Challenge Institutes and Centres & Networks of Excellence that enhance our co-location strategies. All our staff are associated to at least one of these Institutes/Centres with the following 7 Chemistry-led:

- Our research in sustainability benefits from collaborations with: (i) the Grantham Institute (*Templer*-Director of Innovation) driving collaborative climate and environment-related research with real-world impact; and (ii) the Energy Futures Lab (*Kucernak*-Director) which promotes energy innovation across >300 active projects and advances systemic solutions for a sustainable energy future.
- Novel approaches to synthesis and catalysis and their scale-up benefit from collaborations with IMSE (*Harrison*-Director) which brings together Imperial researchers to fuse molecular-based innovation with engineering solutions (>140 affiliates across all Faculties)
- DigiFAB (*Yaliraki*-Director) brings together cross-faculty expertise in molecular synthesis, artificial intelligence, robotics, automation, materials science, sensor technologies and big data to drive advances in Digital Chemistry (>45 affiliates across all Faculties).

- Our research in chemical biology and healthcare benefits from: (i) the ICB (*Vilar/Director*) focusing on the development and application of novel molecular technologies for solving challenges in the life and biomedical sciences (>130 affiliates across all Faculties), and (ii) the CDDS (*Centre/Tate, Fuchter-Directors*) developing therapeutics against cancer, antibiotic resistant infections and neurodegenerative diseases (>60 affiliates across all Faculties).
- Our ability to turn ideas into prototypes is enabled by ICAH (*Ces-Director*), a prototyping Centre where researchers work alongside external partners (>3500 members (students and staff) across all Faculties).

National Collaborations: The Department also plays a leading role in stimulating collaborative research across the UK. Examples include:

- LCN (*Shaffer* was 2010-2020 Director) bringing together >200 academics from IC, UCL and KCL, with dedicated nanofabrication and nanometrology facilities. The LCN was pivotal to securing the £10M Henry Royce Institute Hub “Atoms to Devices” at the MSRH and UREN Hub.
- The Francis Crick Institute dedicated to understanding biology underlying health and disease (*Tate/Di Antonio/Schumann/Walport-see section 1b*).
- The £13M CRUK Convergence Science Centre (*Tate/Vilar*), a partnership between Imperial and ICR addressing cancer challenges, building on our capabilities in Chemical Biology.
- RFI bringing together UK strengths in physical sciences, engineering and life sciences. A partner in our Chemical Biology CDT and co-developing 2DIR technologies with the Department (*Klug*).
- TYC (*Cucinotta/Jelfs/Bresme/Yaliraki/Harrison*), an alliance of >120 groups from IC/KCL/Queen Mary/UCL focused on materials modelling.
- Faraday Institute (*Kucernak*) for electrochemical energy storage research, including the Lithium-Sulfur Technology Accelerator (Co-I, *Kucernak* with UCL, £7.5M).

International Collaborations: We are a globally minded Department and value international partnerships as a core part of our research and learning communities. Within Europe, our research collaborations have been developed through FP7 and H2020 Networks which extend across 17 EU countries and partners from outside the EU and involves 49 research institutions and 32 industrial partners. We are also engaged in over 55 international collaborations worldwide, including Harvard, MIT, EPFL, Technical University Munich, Peking University and Tokyo Tech. To facilitate these collaborations we drive associated policy development for instance with the UK government, Japanese Society for the Promotion of Science and Japanese government on UK-Japan academic collaborations (*Willison*) and a BEIS-commissioned report on international collaborations in manufacturing research (*Hii*). Examples of large strategic international initiatives established by Chemistry staff include:

- InnoHub Cluster in Biomedical Research. Funded by Hong Kong Innovation and Technology Commission (£50M; £2.6M to Chemistry) bringing together Hong Kong University, Peking University and Imperial on a large-scale pan Asia-Europe Chemical Biology Laboratory (*Long/Fuchter/Tate/Vilar*).
- Membranes in Photosynthetic Organisms. \$1M Human Frontiers of Science Programme studying photosynthetic organisms (with European Spallation Source (Sweden) and University of Auckland) (*Ces*)
- South Korean NRF-Global Research Lab. \$2.5M collaboration with Gwangju Institute of Science and Technology developing organic/perovskite photovoltaics (*Durrant/Heeney*)
- Network to Revolutionise Indian Solar Energy (SUNRISE). £7M EPSRC-GCRF project developing solar cells in Indian communities, involving UK universities including Imperial (*Durrant/Haque*) and Institutes in India
- Delivering essential medicines to Africa. A £332k GCRF-funded project (with University of Pretoria and CSIR-South Africa) to support drug manufacturing in South Africa (*Hii/Miller*).

4b. Leadership in the Academic Community

Awards and honours: The quality of our research has been externally recognised by a range of prestigious awards and honours awarded to staff for their scholarship and outstanding contributions to the national and international science community. Highlights during REF2021 from learned and related societies include:

- **National awards:** OBE for services to diversity in education (*Welton*)
- **From the Royal Society:** Wolfson Research Merit Award (*Heeney, Long*); RS Hughes Medal (*Durrant*)
- **From the RSC:** Harrison Meldola (*Fuchter, Crimmin, Jelfs*); Corday Morgan (*Shaffer, Tate*); Medimmune Protein and Peptide Science (*Tate*); Norman Heatley (*Tate*); Sir George Stokes (*Cass*); Rita and John Cornforth (*Brooks/Law/Seddon/Ces*); Marlow (*Bakulin*); Frankland (*Long*); Exceptional Service (*Griffiths*); Chemistry of Transition Metals (*Crimmin*); Interdisciplinary (*McCulloch*); Peter Day (*Heeney*); RSC Macrogrouper medal (*Heeney*); Bob Hay Lectureship (*Jelfs*)

The breadth and significance of our work is evidenced in the receipt of awards from a wider range of bodies:

- **Awards from other organisations:** Asian Rising Star (*Hii*); IUPAP Young Scientist Prize (*Kuimova*); BASF Catalysis (*Ashley*); Eli-Lily OIDD-Outstanding Contribution to Compound Screening (*Bull*); Ben Sturgeon Lectureship-British Liquid Crystal Society (*Seddon*); Thieme Chemistry Journal Award (*Braddock, Fuchter*); German Association of Glycosciences-Excellence in Glycosciences (*Schumann*); Alzheimer's Society Early Career Award (*Aprile*); MPS Otto Hahn Medal (*Schumann*); Institute of Physics Liquids and Complex Fluids Early Career (*Di Michele*); Vice.com Humans of the Year (*Torrisi*); Lynden-Bell (*Kornyshev*); Newton Prize (*Haque*); Tetrahedron Prize Young Investigator (*Fuchter*); Philip Leverhulme Prize (*Bakulin, Jelfs*); Microscopy Today Innovation (*Ivanov, Edel*); Sir David Cooksey Prize in Translation (*Tate*); CAMS Lectureship (*Edel*); Society of Porphyrins and Phthalocyanines Young Investigator (*Kuimova*); World Economic Forum Young Scientist (*Gasparini*); Chemistry Finalist-Blavatnik Awards (*Fuchter*); European Climate Impact Battle (*Brandt-Talbot*).

Fellowship of Learned Societies: Staff support their areas through learned society fellowships, including 5 Fellows of the Royal Society (*Barrett/Robb/Durrant/McCulloch*), 23 Fellows of the RSC, 3 Fellows of Institute of Physics (*Harrison/Seddon/Kornyshev*), 2 Fellows of Royal Society of Biology (*Cass/Tate*) and 1 fellow of the Academy of Medical Sciences (*Barrett*).

Supporting Learned Societies: Commitment to the broader chemistry community is reflected in the leadership and advisory roles our staff play in learned societies. *Welton* was elected **President of the RSC** (2020-2022) with a further 20 academics from the Department serving as members of RSC division councils, groups and committees as well as in advisory boards for 6 other societies (e.g. Academy of Medical Sciences and the Royal Society)

Editorships: The scholarship of our staff is reflected in their contributions as editors of 10 journals including ACS Sustainable Chem. Eng. (2019-present, *Hii*), RS Open Science (2019-present, *Jelfs*), RSC Med. Chem. (2015-2020, *Fuchter*), as well as being members of >25 editorial boards.

Invited Lectures: staff delivered an extensive series of invited lectures with >140 talks in industry, >700 research talks at other HEIs and >600 invited conference lectures. Examples include plenary lectures at the International Conference on Photochemical Solar Energy Storage (*Durrant*, China, 2017/2019), GSK Emerging Academics Symposium (*Fuchter*, UK, 2016) and World Economic Forum – Intelligent Food Systems (*Barter*, Davos, 2018).

Organisation of conferences: We organised >80 national and international conferences with examples including the European Material Research Society (*Kamaly*, Poland, 2018), RSC Next Generation Materials for Solar Photovoltaics (*Haque*, UK, 2016) and International Union of Crystallography congress (*Brooks*, Montreal, 2014)

Visiting and Honorary positions: Chemistry staff have held visiting/honorary positions in >15 other universities reflecting the esteem in which they are held internationally. Examples include Hong Kong University (*Hii*, *Long*); Tokyo Institute of Technology (*Willison*, *Edel*); CSIRO, Australia (*Fuchter*); Institute for Chemical Engineering Science A*Star, Singapore (*Britovsek*).

Serving the Research Community: Our staff are recognised for their expertise and in demand to serve on national and international science and policy committees, and as reviewers for international agencies as outlined below:

- For EPSRC, staff served on Physical Sciences prioritization panels, as co-chairs in grant meetings (*Seddon*, *Welton*), in the CRUK-EPSRC Multidisciplinary Review Panel (*Fuchter*) and in the Scientific Advisory Committee for Energy (*Harrison*).
- For BBSRC staff have e.g. served on panels for New Technologies (*Tate*) and Transformative Technology SAP (*Edel*)
- For the Royal Society staff served on Royal Society URFs (*Crimmin/Shaffer*), International Exchange (*Armstrong*) and Newton Fellowships (*Barter/Durrant/Bull/Ashley*) committees
- A selection of other funding committees includes the Ramsay Memorial Trust (*Armstrong*), Leverhulme Trust (*Robb/Parsons*), STFC Lasers for Science Facility (*Kuimova*), Swiss National Science Foundation (*Hii*), Ireland Science Programme, (*Long*), Deutsche Forschungsgemeinschaft (*Kornyshev*), EC-H2020 FET (*Edel*).

Advisory national and international committees and boards: Our staff are internationally recognised for their expertise and in demand to serve on national and international committees. They served on >15 advisory boards for other universities and >10 advisory committees of other institutions including large facilities (e.g. Diamond, *Brooks*) and prizes (e.g. King Faisal International Prize, *Spivey*, *Yaliraki*).

4c. Collaboration and contribution to the economy

Supported by our impact strategy (section 1d), our major user group during REF21 has been industry, resulting in global economic impact. We have collaborated with >40 companies (e.g. AZ/Shell/BASF/GSK/P&G/Airbus/Polymateria) who directly funded our research (>£10.5M) recognising its translational impact. We have a thriving technology transfer pipeline. Staff had 144 Invention Disclosures submitted and assessed by Imperial Innovations. 63 separate patent families were published (24% increase on REF14), spanning 10 business sectors. Staff are involved in 19 commercial licenced deals (revenue of £730k). During REF21, the Department spun out >10 companies based on Chemistry research that raised >£10M in funding. These include Sweetgen, OneFour Discovery, Bramble, Myricx Pharma, Vidya Health and NK:IO. Led from within Chemistry, a cleantech accelerator supported the creation of over >60 SMEs securing >\$300M. These ventures are at the heart of Case Studies C1-C5.

Our success in EPSRC impact schemes includes two outgoing Knowledge Transfer Secondments (KTS) grants and four KTS grants for incoming staff and seven Pathways to Impact grants (£950k). We have been involved with 7 Confidence in Concept grants (Wellcome Trust/MRC-£430k). Each year the Department enters into CASE award agreements with external bodies (10 different organisations e.g. Merck). >57% of staff participated in >165 consultancy or advisory boards in energy, pharmaceuticals and the environment generating £1M consultancy income. Impact extends further with staff sitting on the research boards of 11 companies including Cyclofluidics.

4d. Collaboration and contribution to society

Promoting EDI around the world: The Department has engaged in >60 activities during REF21 that promote best practice. We have influenced policy makers and national bodies (MPs, NHS,

UKRI, Royal Society, RSC, IoP), launched the Women in Cleantech report at London City Hall (*Templer*), chaired the National Athena Swan Panel (*Welton*), become members of the UKRI EDI external advisory group and shared our Athena SWAN experience with colleagues in Universities across the UK, Ireland, Canada and Australia.

Government policy development: Chemistry academics served society in key policy committees including the London Sustainable Development Commission (*Templer*) leading to a report embedded within the London Mayor's and Secretary of State's policy measures to support a London Cleantech Innovation Cluster. *Templer* spearheaded initiatives to increase female participation in cleantech innovation (Women in Cleantech Initiative) and advised the West London Alliance with low-carbon recovery plans (C2, section 1e). *Kafizas* contributed to the Environmental Industries Commission on the effectiveness of photocatalytic materials in tackling local air pollution. *Klug* advised Government and NHS on innovation in healthcare and *Willison* contributed to the Government response to Covid-19 through a House of Lords Committee paper and Adam Smith Institute paper. *Yaliraki* and *Welton* supported science policy through membership of the All-Parliamentary Group for Social Science and Policy and the Science Minister Senior Stakeholder Group.

Society engagement and outreach: We seek to inspire public debate about our work through media including radio, television, internet, public events (WIREDLive, New Scientist Live) and museum exhibitions. Examples include a Science Museum showcase (part of 200th Anniversary of Frankenstein) addressing misconceptions around synthetic cells attended by >20,000 people. To mark the 150th anniversary of the Periodic Table we ran a series of events with the RSC, V&A and Science Museum to give insight into future chemical science developments and how they might impact society (Chemistry2040). This culminated in the MSRH opening by the London Mayor.

Inspiring and connecting with London students and the wider community is a core strength. A fulltime Departmental outreach officer has driven engagement with >8000 students (ages >10) through school lectures and visits, summer schools and in-house demonstrations. Female students account for >60% of participants. We supported an additional >5000 students via >240 school visits through the RSC Spectroscopy in a Suitcase Programme.

Wade organised a Women in Chemistry Wikithon. Eighty girls from local secondary schools researched the careers of female chemists leading to >1,300 women and BAME chemists being added to Wikipedia. Subsequent edit-a-thons attended by thousands around the world have taken place supported by the RSC, ACS and AAAS.

The Department takes part in the Imperial Festival, an annual celebration of discovery in South Kensington bringing together 20 cultural institutions. The Festival has grown to audiences >20,000 in 2018. Such was its success that in 2019 the College partnered with other institutions in the 'Albertopolis' to launch the Great Exhibition Road Festival which attracted >60,000 people. As always, the Department was heavily involved in this success, running numerous talks, stands and workshops on everything from the basic principles behind soap through to solar technologies and science-led escape rooms.

White City is a low educational attainment and high poverty area. With the Imperial outreach team the Chemistry Director of Development worked to stimulate social value culminating in a £2M donation (Marit-Mohn Foundation, 2017) to establish the Reachout Makerspace (adjacent to ICAH), a workshop where school students innovate alongside Imperial researchers. Chemistry staff and students support Makerspace courses that have been attended by 1000s of children. Local engagement is further strengthened through regular involvement in the W12 Festival.