Institution: University of Southampton

Unit of Assessment: 08 Chemistry

1. Unit context and structure, research and impact strategy

1.1 Overview

The School of Chemistry contributes to the University of Southampton (UoS) mission to "*Change the World for the Better*" (**REF5a§1.2**) through excellence in chemical research, education and enterprise activities. Notable achievements since REF2014 that advance this mission are:

- Continued development of a diverse, international researcher community (53% of our Teaching & Research and Research-only staff are international), including: the recruitment of 7 new permanent staff; confirmation of 3 research fellows and transfer of 1 technical staff to permanent academic roles; 6 associate professor and 10 full professorial promotions and the graduation of 272 PhD students (33% female) (see **§2**).
- Embedding of a collegial and inclusive culture in the development of the School, underpinned by the values articulated in our *Chemistry Code of Conduct* (**§2**) and as indicated by the award of an Athena SWAN Silver award in 2015, renewed in 2018.
- Strong growth in research income, with a 32% increase in mean annual research income over the period (£7.9 M/yr *c.f* £6.0M/yr in REF2014), supporting the delivery of a diverse research portfolio (**§3.2**).
- The publication of influential work with a global reach, including 1403 ISI papers, 25 patents granted; 60 patents filed. International collaboration has increased steadily over the period with 52% papers involving international collaborators in 2019.
- Establishment of Chemical Engineering (**§1.2**) as a strategic University priority that will sit within the School of Chemistry, supported by a capital investment of £5.5M.
- A major (>£16M, 2016-20) refurbishment of the original Chemistry building (**§3**).

As one of 5 Schools in the Faculty of Engineering and Physical Sciences (FEPS), Chemistry is led by Head of School, **Reid** (to 8/2020)**,** with Deputy Heads of School, **Linclau** (Research and Enterprise) and **Hector** (Education), and Director of Infrastructure **R Brown**. Together with the School Finance Officer, Executive Officer, HR and H&S Advisers, they form the School Operational Board. The new Director of Chemical Engineering (Zhang) joined the School Operational Board in early 2019. The Heads of Research Groups (**§1.2**) form the *Research & Enterprise Committee* chaired by the DHoS-R&E, reporting to the School Board.

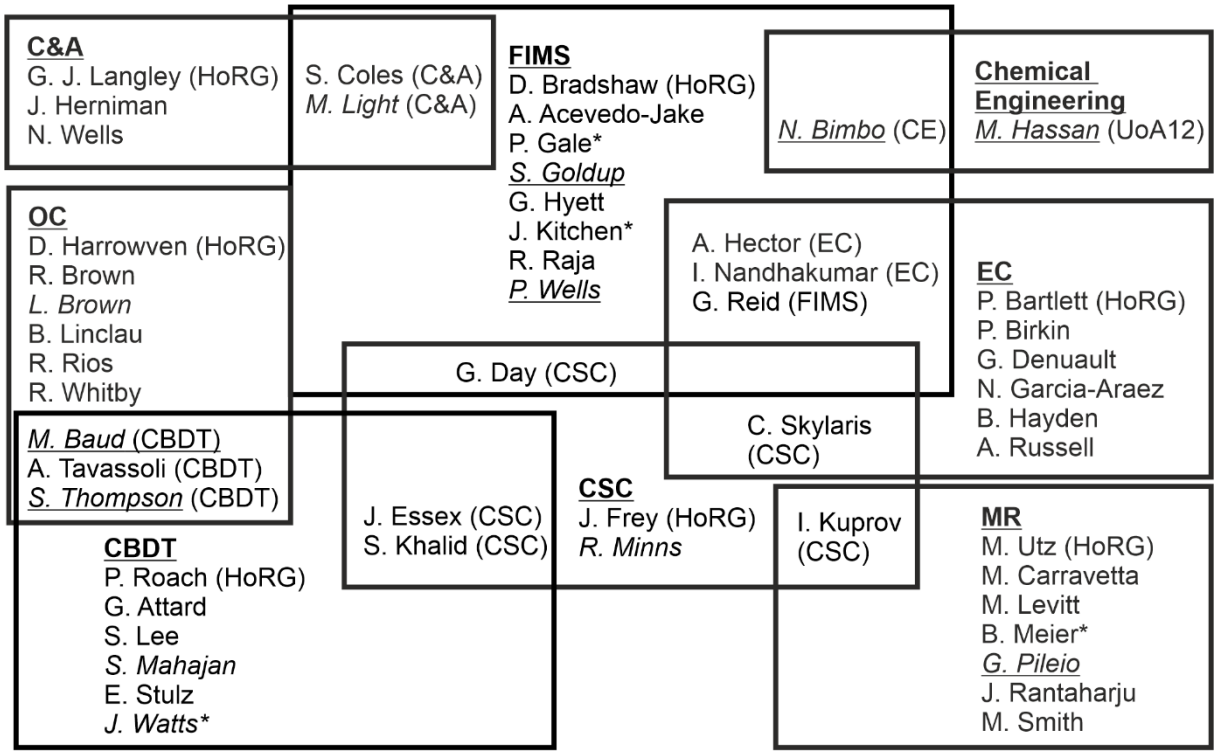
We are deeply committed to the values of EDI, reflecting our belief in the importance of ensuring an inclusive culture that welcomes and values equality and diversity for the continued success of the School and the well-being of all of our community. The School Operational Board, like the other committees, ensures EDI in all business and decision-making.

1.2 Research strategy

The School's ambition is for sustained internationally-leading research across the breadth of chemistry defined by our research groups and is built on:

- Recruitment and development of diverse staff and students, fully supported in their research activities and wellbeing;
- Establishment and maintenance of state-of-the-art facilities with sustainable research income;
- To deliver a stimulating and supportive environment promoting intellectual development and timely world-class innovation, capitalising on cross- and inter-disciplinary synergies across the School, Faculty and more widely.

Our five Research Groups in **Electrochemistry** (EC); **Magnetic Resonance** (MR); **Computational Systems Chemistry** (CSC); **Chemical Biology, Diagnostics and Therapeutics** (CBDT) and **Characterisation and Analytics** (C&A) reflect our strengths in these areas, particularly in the context of emerging societal challenges and government initiatives, and recognise the critical role of advanced analytical methods in C&A for delivering our research mission. The continuation of these groups was reaffirmed through an internal strategic review in 2017/18, which also created two new research groups: **Functional Inorganic, Materials and Supramolecular Chemistry** (FIMS) and **Organic Chemistry: Synthesis, Catalysis and Flow** (OC). This revised structure represents a refocusing of our previous REF2014 structure, with an increased focus on innovative chemistry to create a more *sustainable* and *healthier* world.



HoRG = Head of Research Group
Italics = Research fellows and technical staff appointed to academic permanent positions in this period.
Underlined italics = permanent staff appointed in this period.
For staff associated with multiple research groups, their principal group is given in parentheses.
* have moved from UoS in this period

Figure 1. Overview of Research Groups.

All staff are affiliated with primary groups, and some with multiple groups reflecting strong cross-disciplinary research in Chemistry (Figure 1). Additionally, our **Education** Group in Chemistry provides cross-cutting support to our academic staff, through translating innovative educational approaches across the School, supporting the preparation of UGs for chemical research and developing outreach to inspire the next generation.

Chemistry's strategy has been backed by significant support from the University through new staff appointments and cash contributions to support large and strategic equipment bids (**§2** and **§3**). Our new Category A staff have been recruited to align with our strategy, to strengthen and complement our research and to bring new research opportunities and synergies.

The expansion of Chemistry to include research and education in **Chemical Engineering** (CE) was identified as a strategic priority, taking advantage of the new Faculty structure that encompasses Chemistry and Engineering, building on the strengths in both Schools and the range of existing collaborations (**§1.3**). Significant investment has been committed to afford dedicated CE facilities (**§3**), with PGT and UG programmes launched in 2020 and 2021, respectively. We have appointed the first two specialist CE staff, providing educational contributions in CE, but research contributions more widely across the School's research spectrum. Their focus in sustainable, low energy CE aligns with both key societal challenges and the UN Sustainable Development Goals, bringing research in continuous flow chemical processing, porous inorganic solids, heterogeneous catalysis and battery technologies, complementing existing strengths in Chemistry. A detailed Business Case for both the capital investment and further staff appointments over the next 5 years has been approved by the University Executive Board.

1.2.1 Research Groups

Electrochemistry (EC) (Head of Research Group (HoRG)=**Bartlett)** has a focus in *Energy Conversion & Storage*, where the section brings distinctive, internationally-leading expertise in the application of synchrotron methods to *in operando* studies of fuel cell catalysts (**Russell** with Johnson-Matthey and Diamond Light Source (DLS)). In this period, the group has made major contributions to the development of high throughput methodologies for materials discovery (**Hayden** with Ilika, Electronics and Computer Science (ECS) and the Zepler Institute (ZI) at UoS), particularly for proton exchange membrane fuel cells, solid-state Li-ion batteries and functional ceramics for energy harvesting. A major theme on energy storage and battery development (**Hector, Garcia-Araez, Hayden, Skylaris**), receives funding through the Faraday Institution (**REF5a§2.5**), in addition to industrial and InnovateUK projects and **Garcia-Araez**'s EPSRC Early Career Fellowship. The deposition of functional nanostructures, one of our priorities in REF2014, has been advanced significantly through two EPSRC Programme Grants (**§3, Bartlett**, **Hector, Reid**, with ECS and Physics), which is complemented by the electrodeposition of bulk thermoelectric materials for energy harvesting (**Nandhakumar**).

Distinctive interdisciplinary work in *sonoelectrochemistry,* (**Birkin,** with Engineering) has led to innovations in cavitation detection, surface cleaning and studies of bubble dynamics. **Denuault**'s work focuses on theory and application of microelectrodes, scanning electrochemical microscopy and nanostructured microelectrodes for electroanalytical applications. Collaboration with the National Oceanography Centre (NOCS) in Southampton focusses on determination of dissolved oxygen and other analytes in sea water. **Bartlett** also works with the Optoelectronics Research Centre (ORC), Dstl and Southampton General Hospital on biodetection and waveguide Raman-based diagnostics.

Magnetic Resonance (MR) (HoRG=**Utz**) employs quantum theory, numerical simulations and MR experiments to design and apply new techniques to problems ranging from physical science to medicine. Distinctive and unique strengths are the integration of high-resolution NMR spectroscopy with microfluidic lab-on-a-chip devices (**Utz**), the use of advanced MR methods to study endofullerenes (**Levitt, Carravetta, Pileio**), the exploitation of long-lived nuclear spin states - a phenomenon first discovered in the **Levitt** group - to develop new magnetic resonance imaging (MRI) methods, NMR of superconductors and biomolecular structure determination by NMR (**Carravetta**). In line with our objectives from REF2014 to build upon the world-leading work of **Levitt**, the appointment of ECR **Pileio** brings expertise in theoretical spin dynamics and NMR methodology. EPSRC Early Career Fellow (**Meier**) was appointed in this REF period, developing 'bullet dynamic nuclear polarisation' for the generation and utilisation of hyperpolarization in NMR and MRI, before moving to a permanent position at Karlsruhe Institute of Technology. Work in MR enjoys strong links with OC (synthesis: **L Brown**, **R Brown**, **Whitby**), CSC (simulations: **Kuprov**), FIMS and EC (inorganic materials: **Hector** and heterogeneous catalysis: **Raja**), as well as Biology, Medicine, Physics and Engineering across UoS.

Chemical Biology, Diagnostics and Therapeutics (CBDT) (HoRG=**Roach**) delivers internationally-leading work in chemical biology and at the life science interface, collaborating closely with clinicians in Medicine. **Tavassoli**'s design and development of protein-protein interaction inhibitors has led to extensive collaborations with industry, revealing important insights into several proteins in cancer biology, and leading to significant CRUK funding (£1M). Early career academic staff appointed in 2016 (**Baud**, **Thompson**) focus on synthetic probes for cancer targets and protein-protein interactions. Mechanistic enzymology and crystallography using the DLS and ESRF synchrotrons (**Roach**) feature strongly, particularly radical SAM enzymes and novel antibacterial targets. In diagnostics, the group has strengths in novel *in vitro* and *in vivo* molecular imaging techniques, DNA bionanotechnology and nano-sensors for medical diagnostics (**Roach, Stulz,** with Engineering), an area further strengthened by **Mahajan**, who is coupling advanced optical imaging with Raman spectroscopy. CBDT is also active in the emerging field of synthetic biology, with **Tavassoli**'s bacterial high-throughput screening platform being exploited through spin-out *Curve Therapeutics* (est. 2019), developing novel inhibitors of therapeutic targets previously regarded as 'undruggable'. **Roach**, **Lee** and **Tavassoli** target different aspects of antibacterial development, often with industrial engagement (e.g. Dstl, Merck). Projects with structural aspects benefit from significant crossover with CSC (**Essex**, **Khalid**).

Functional Inorganic, Materials and Supramolecular Chemistry (FIMS) (HoRG=**Bradshaw**) was established as a focus for research across molecular inorganic, supramolecular, materials and structural chemistry. A key aspect of the FIMS strategy has been to deepen its partnership with DLS to allow the School to leverage the national synchrotron facilities. Hence, **P Wells** was appointed jointly with DLS and has established a leading position in the application of synchrotron techniques, coupled with spectroscopic methods, for *in operando* catalytic studies, collaborating closely with industry and the Catalysis Hub (Harwell). A developing theme is in new inorganic late-stage ^{18}F radiolabelling strategies for medical imaging (PET) (**Reid** with GE Healthcare). The appointment of **Goldup**, together with the work of **Bradshaw** and **Raja,** has broadened and deepened efforts in supramolecular chemistry, bridging the development of organic, metal-organic and inorganic framework materials and their composites in separation,

sensing, and multifunctional catalysis. **Hyett** is developing porous hybrid solids, and CVD of thin film visible light photocatalysts.

The group's objective to be an internationally-leading centre for research in solid state materials and in the rapidly developing fields of nanomaterials and new materials chemistry, has stimulated strong links to both Electronics and Physics, benefiting from Southampton's nationally leading nanofabrication and clean-room facilities. **Raja** (with Sazio, ZI) is integrating photonic fibres with inorganic catalysts for CO_2 photo-conversion, and **Reid** leads research on electrodeposition and CVD of non- and few-layer transition metal dichalcogenides for next generation devices with ECS and Deregallera Ltd.

Organic Chemistry: Synthesis, Catalysis and Flow (OC) (HoRG=**Harrowven**) consolidates specialisms including: target synthesis, synthetic photo- and electrochemistry; endofullerene, organofluorine, carbohydrate and flow chemistry; reactor and experiment design and organocatalysis. The development of new continuous flow methodologies and reactors for the sustainable synthesis of fine chemicals, agrochemicals and pharmaceuticals by electro-, photo- and thermal chemistry (**R Brown**, **Harrowven**, **Whitby**) is aligned to key themes of the EPSRC *Dial-a-Molecule* Grand Challenge network (lead=**Whitby**) which brings together a large body of industrial and academic collaborators. **Linclau** heads the IBCatalyst-UK research consortium investigating the enzymatic glycosylation of modified carbohydrates to generate biologically relevant glycans. **Rios** adds expertise in organocatalysis focussed on the enantioselective synthesis of complex scaffolds, and extends to multi-hybrid green catalysis in collaboration with **Raja** (FIMS).

The OC group collaborate widely on interdisciplinary projects at various TRL levels, *e.g.* on orphan nuclear receptors (**Whitby**); engineers on power transmission (**R. Brown**); eTextiles (**Harrowven**); MR on imaging (**Whitby**, **L Brown**, **Bloodworth**); reactor designers (**R Brown**); materials chemists (**Harrowven**) and astrophysicists (**Whitby**).

Computational Systems Chemistry (CSC) (HoRG=**Frey**) is broadly based, with research covering multiple length-scales and time-scales, unified by the common theme of exploring interacting systems, where larger scale behaviour arises from a series of complex interactions of individual smaller components. Particular strengths, incorporating *multi-scale* approaches, are in modelling biologically relevant systems (**Essex**, **Khalid**, **Skylaris**) at increasing levels of organisation, from nucleic acids and proteins, to membranes and the whole cell and in predictive modelling of materials (**Skylaris**, **Day**), from nanoparticles for catalysis to the *ab initio* prediction of functional crystalline materials. **Kuprov** develops theoretical methods for modelling spin dynamics.

As proposed in REF2014, the group has moved in the direction of 'big data' and data-driven modelling, hosting the EPSRC Physical Sciences Data-science Service (PSDS) (**Frey, Coles,** with C&A) and the EPSRC AI Network+ (**Frey**) (**§**4). CSC collaborates widely with all research groups Chemistry, the wider University (e.g. **Khalid** with the National Biofilms Innovation Centre and Network for Anti-Microbial Resistance and Infection Prevention) and externally, providing the computational expertise that informs other research projects. The group collaborates extensively with industry through consultancy, funded PGRs and RAs.

Characterisation and Analytics (C&A) (HoRG=Langley) focuses on the development and use of advanced analytical methods, leading to significant industrial and UKRI-funded activity. C&A combines expertise in modern analytical instrumentation, the EPSRC UK National Crystallography Service (NCS, **Coles**), thin film and powder diffraction, including pair distribution

function analysis of amorphous materials (**Light**), state-of-the-art mass spectrometry (Langley, Herniman) and solution NMR spectroscopy (N Wells). Specific interests include the application of hyphenated approaches, GC-MS, UHPLC-MS, UHPSFC-MS and GCxGC-HRMS, to analyse small molecules: pharma and agro chemicals (with Environmental and Life Sciences); petrochemicals (with Engineering, Innospec, BP); lipids, oligonucleotides and polymers (AZ, Huntsman) and fundamental MS/MS fragmentation processes (AZ, Syngenta). **Coles**' group specialises in charge density distributions, structure-property relationships (with **Day**) and crystal growth. Distinctive structural science projects in macromolecular crystallography (with Biological Sciences), X-ray laser spectroscopy and imaging (with ORC) and CT Imaging (with Engineering) are complemented by well-funded research in informatics and AI, with **Frey**. Specialist projects include, biological screening and target discovery (**Baud**), ^{19}F logP measurements (**Linclau**), and characterisation and binding of novel catenanes and rotaxanes (**Goldup**).

1.2.2 Strategic priorities for the next REF period

Building on existing and emerging strengths, synergistic expertise between Research Groups, and maximising interdisciplinary opportunities, our strategic priorities include:

1) In the area of molecular and materials discovery and applications, particularly aligning with our priority of creating a more *sustainable* world:

- Establishing an interdisciplinary Centre of Excellence in Continuous Digital Chemical Engineering Science (CDCES), bringing together science and engineering expertise from across the University, with industrial partners, for the discovery and production of new compounds and materials using smart, sustainable processes and methods (**FIMS**/**OC**/**CSC**/**CE**).
- Exploiting expertise in molecular, supramolecular and materials chemistry with a sharpened focus on sustainable chemistry (porous materials, energy harvesting, flow catalysis, photocatalysis) and medical diagnostics (**FIMS**/**CSC**/**CE**).
- Building upon our excellence across fundamental and applied electrochemistry for energy storage and batteries, fuel cells, energy harvesting and chemical sensing (**EC**/**FIMS**/**CSC**/**CE**).
- Developing Artificial Intelligence and machine learning, applied to drug development, synthesis planning, modelling methods and materials discovery (**CSC**/**CBDT**/**OC**/**FIMS**/**CE**).

2) On the interface with biological and medicinal science, creating a *healthier* world:

- Applying chemical understanding to biological systems: understanding protein ligand interactions for enzymes and other drug targets; developing cyclic peptide clinical candidates with trials underway against several cancer targets (**CBDT/CSC**).
- Strengthening ties with medicine through target synthesis and an understanding of molecular interactions; working with engineers to solve topical problems through molecular synthesis and/or degradation under stress (**OC**/**CSC**).

3) In advancing methods for characterisation, which underpin the other priority areas:

- Driving innovations in combined diffraction and simulation methods for structure analysis of crystalline and amorphous materials, including hybrid catalytic materials and crystal sponges (**C&A**/**CSC**/**FIMS**).

- Exploiting recent breakthroughs in NMR studies on living tissue slices; development of new hyperpolarisation strategies (**MR**/**CBDT**).
- Establishing a regional Centre of Excellence for multi-inlet 2D GC-MS to advance the research of UK synthetic and catalysis chemistry communities working with volatile compounds, environmental scientists detecting low level and air-borne pollutants, and engineers researching the evolution of small organic gases and low-level contaminants (**C&A**).
- Establishing a new facility using a unique combination of correlative SEM, confocal RAMAN and windowless EDX imaging for in situ studies of battery electrodes and structures (**EC**).

1.3 Interdisciplinarity

UoS has a strong culture of multi- and interdisciplinary research and encouraging collaboration including strategic allocation of PGR and research funding to interdisciplinary projects. Interdisciplinarity is a strength in the School, and staff collaborate and influence across disciplines to address major societal challenges, e.g. through our strategies for Chemical Engineering and the Institute for Life Sciences (IfLS), a UoS priority integrating bio- and life-sciences, bringing together expertise across science, medicine and engineering. Chemistry engages with most cross-faculty University Strategic Interdisciplinary Research Institutes and University Strategic Research Groups (**REF5a§2.6**) and co-leads (**Whitby**) CDCES (**§1.2.2**), one of 4 newly established (2020) Faculty-based Centres of Excellence, with strong alignment to our Chemical Engineering, flow processing and AI priorities. In his leadership role as Associate VP, **Attard** oversees interdisciplinary research across UoS

Within Chemistry, interdisciplinary research is supported by fostering our staff's ambitions to allow them to be successful and removing barriers to collaboration within UoS and more widely. Interdisciplinary success is valued, celebrated and recognised in our promotion process (e.g. **Mahajan**, **Minns**, **Tavassoli**). Examples of interdisciplinary work in Southampton (Chemistry/Physics/Electronics/ORC; Chemistry/Medicine/Biology) are illustrated in the Research Sections above. Further examples include: significant multidisciplinary activity in AI, with Computer Science and Mathematics (e.g. **Frey** and **Whitby**'s Dial-a-Molecule and AI3SD networks), and through **Day**'s ERC Synergy grant with Liverpool (materials discovery) and Rostock (robotics); **Mahajan**'s Transformative Healthcare Programme Grant with the ORC, Medicine at UoS and Edinburgh; **Bradshaw** and Langley's work with NOCS on porous hybrid solids for bioremediation of nuclear waste from legacy sites and dissolved organic matter composition, respectively; **Utz** with Medicine on microfluidic NMR metabolomics of cancer cell lines.

Chemistry is very strongly engaged with the IfLS (Deputy Director: **Mahajan**). Nineteen Chemistry staff representing all seven research groups are members of the IfLS and are strongly engaged with medicine, bioengineering and biological sciences. Two themes of the University's Life Sciences Strategy are led by School staff: Biophotonics & Imaging (**Mahajan**) and Chemistry of Life (**Roach** then **Baud**).

Facilitation of interdisciplinary research also sits behind our philosophy of embedding research groups from other disciplines within the Chemistry building complex, as set out in REF2014 and extended during this period. Chemistry hosts the groups of Ponce de Leon and Wills (Electrochemical Engineering), Kanaras (Physics), Cruden (Energy Storage) and the nCATS

group (Tribology) led by Wood. This has deepened collaborations with groups in **EC**, **CSC** and **FIMS**, in particular. Similarly, **Frey** collaborates with Physics, Biology and the ORC developing soft X-ray laser imaging for biological samples. The imaging experiments, together with **Minns**' fast laser spectroscopy experiments are hosted in a dedicated lab in Physics, and with strong links to the hardware development at the Central Laser Facility. Staff (including **Frey**, **Khalid**, **Lee**) are engaged with the Rosalind Franklin Institute and we have agreement to locate the next generation of soft X-ray imaging hardware at the RFI.

Over 30% of staff in Chemistry have funded collaborations with other Schools in FEPS, exploiting distinctive UoS facilities (e.g. ZI cleanrooms), the complementary expertise in molecular-level control that enables bottom-up atom-by-atom materials growth (Chemistry), through to fabrication, testing and evaluation of high-tech devices (Electronics Engineering) and large-scale equipment (Electrical, Mechanical and Materials Engineering).

1.4 Facilitation of Impact

UoS has a strong track record in realising impact from its research with support delivered through Research and Innovation Services (RIS, **REF5a§1.5**) including contracts and partnerships, consultancy, IP protection, fund-raising, legal services, spin-outs, etc., with incubation facilities at the Southampton Science Park.

Chemistry surpasses this university-level support to achieve impact from our research. Under Chemistry's leadership, Southampton became a partner (2016) of the Knowledge Centre for Materials Chemistry (KCMC), which brings materials chemistry-using industries together with academic research expertise and facilities to drive UK industrial growth. **Reid** sits on the KCMC Governing Board, while **Hector** and **Bradshaw** are UoS leads on the Management Board. The KCMC has led to collaborations with a range of SMEs and large organisations including, Victrex, Carrington Textiles, Urgo, Deregallera, Merck, Pilkington NSG, City Technology. Furthermore, Chemistry was instrumental in UoS being a founding partner in the Faraday Institution (**REF5a§2.5**), which strategically aligns with priorities in **EC**, **CSC** and **FIMS,** fostering research collaboration between universities and businesses as part of the UK's industrial strategy.

Three spin-outs are currently resident in Chemistry space: *ATDBio* (created by former staff member T Brown); *Ilika Technologies* (**Hayden**) and *Curve Therapeutics* (established in 2019 by **Tavassoli,** attracting £4.5M of venture capital funding). These are at different stages of maturity, and all bring significant advantages to the wider School community through research synergies and access to specialist equipment, in addition to financial benefits through formal facilities and collaboration agreements that support their continued growth and contribute to the sustainability of specialist facilities, e.g. the Advanced Composite Materials Facility (ACMF, **§3.4**) through our partnership with Ilika.

Recent successes in translational activities include: IAA funding (**Linclau**, **Frey**, **Skylaris**, **Kuprov**, **Mahajan**, **Raja**, **Reid**), InnovateUK funding (**Garcia-Araez, Hayden, Hector)**, KTPs (**Frey, Russell**) and STFC IPS funding (**Reid, Hector**). Staff secondments are supported to enable the successful translation of technology (e.g. **Hayden**: 50% secondment as CSO, *Ilika*; **Tavassoli** 75% FTE as CSO, *Curve Therapeutics*).

Our REF2021 Impact Case Studies include two successful and mature spin-out companies (*Ilika* and *ATDBio*) that reflect areas of technology where we have focussed effort over a sustained period and where there has been demonstrable progress since 2013, one based on the development and commercialisation of a powerful computational software package (*ONETEP*)

that enables calculations on large scale assemblies at a level of accuracy that surpasses conventional software, and a strategic public engagement programme (*Water Transistor and Electrochemical Circus*) focussed on engaging audiences with research in electrochemistry for the production of smaller, faster and smarter high tech devices, and demystifying electrochemistry in the school curriculum for teachers and pupils.

Further impacts at an earlier stage of development include: the development of a diagnostic electrode in gas sensors (**Russell**), which is predicted to provide a financial benefit of $9M to sensor manufacturer City Technology over the first five years of sales, in addition to improved safety for end-users; based on Birkin's sonochemistry research, purchase of intellectual property by a US manufacturer and a new company, Sloan Water Technology Ltd., established on the Southampton Science Park; the creation of spin-out *HyperSpin Scientific*, based on **Meier**'s development of dynamic nuclear polarization at UoS. In addition, the development of the ViridiCO2 catalyst platform results from our nurturing of impact and business potential in our PGR students; the technology was developed by Stewart (PhD 2020, followed by IAA) under the supervision of **Raja**, winning the Energy and Environment category of the 2020 RSC Emerging Technology Competition. Stewart has been accepted into Innovate UK's entrepreneurial *ICURe* programme (**REF5a§2.3**).

1.5 Open Research Environment

The University has adopted a robust, progressive open access and open data position which, with support provided through the UoS Library and School ensures near 100% compliance. For UKRI-funded work, Green OA is the minimum position. The UoS institutional repository ePrints (**REF5a§2.4**) is used to make all outputs available, linked to authors, funding sources and data-sets, which are assigned a DOI.

Leadership in open data is provided by **Coles** and **Frey** through their vision for the PSDS. Funded by a £3M EPSRC grant (began 2019); the PSDS succeeds the National Chemical Database Service as an EPSRC National Research Facility, providing a hub for aggregating and integrating data resources for the Physical Sciences, opening avenues for application of machine learning and artificial intelligence techniques across the data.

1.6 Research Integrity

Chemistry adheres to UoS policies (**REF5a§2.8**) for ensuring the highest standards of research integrity amongst all activities. All students and researchers receive training and guidance on ethics, plagiarism and research integrity through the Doctoral College; the Faculty Ethics Committee provides guidance and promotes best practice. We are guided in identifying possible conflicts of interest by the "Nolan" seven principles of public life. Clear policies have been developed around expectations for those involved in consultancies. A Register of Interests is maintained centrally and updated by individual staff on an annual basis.

2. People

2.1 Delivering Excellence

UoS is committed to delivering excellence in research, education, ECR and PGR training and development. We have an excellent record of sustaining and improving performance by attracting, developing and retaining high-achieving staff, and by nurturing and developing younger staff in the early stages of their careers. Where possible, we prioritise permanent appointments for staff over fixed-term contracts; of 46 submitted staff, 43 have permanent contracts and 3 are independent researchers. We strive to accommodate part-time and flexible working requests from staff at all levels (academic, technical clerical, RAs, PhDs) to meet their individual circumstances or in support of impact (*e.g.* secondments, **§1.6**). Reflecting the School's commitment to provide flexible working opportunities, five of our Category A staff (3M,2F) are on fractional contracts.

In accord with our ethos for EDI, all staff and PGRs undertake mandatory EDI training, with a refresher after 4 years (100% completion). The introduction of the *Chemistry Code of Conduct* in 2019 further encourages positive, respectful relationships for staff and students at all levels. Our Common Room is used by staff and students across all areas, providing a central networking point within the School, helping to ensure a supportive community and strongly engaged staff. In the 2019 Staff Engagement Survey, Chemistry had a 77% response-rate, with 94% of staff agreeing/strongly agreeing that "My direct line manager treats me with respect", and 89% that "My direct line manager and I have a positive working relationship."

2.2 Staffing Strategy

Our research strategy informs the recruitment of internationally excellent researchers. Since the last REF census, we have appointed 7 new Category A staff to permanent contracts (**Baud**, **Goldup**, **Pileio**, **Thompson**, **P. Wells,** Hassan (UOA 12)**, Bimbo**), as strategic hires aligned to Chemistry's strategic priorities (**§1.2**), taking advantage of natural turnover to reinvest in younger talent and forward planning against upcoming retirements to provide continuity of internationally excellent research. Additionally, RS Dorothy Hodgkin Fellow **L. Brown**, RS URF **Minns** and IfLS Fellow **Mahajan** were confirmed to permanent positions.

Staff appointments are made where we are confident that the individuals can be supported appropriately and complement and enhance our existing activities, including alignment to development of research infrastructure. **Goldup** was appointed (2014, promoted to full Professor 2017) to enhance our portfolio in Supramolecular Chemistry. **P. Wells** was a strategic joint-appointment with DLS (promoted to Associate Prof., 2019), to build on the foundation of our strong links to the Catalysis Consortium and EPSRC Catalysis Hub via **Russell**, **Raja**, **Carravetta**, **Skylaris**. X-ray manager, **Light** transferred (2016) from the Technical pathway to the full academic pathway, aligning with investment in diffraction infrastructure, partly through renewal of the NCS (**§3.1**). As part of our strategic priorities for multidisciplinary research at the interface with biology and medicine (**§1.2.2**), **Baud** and **Thompson** were appointed to strengthen the **CBDT** group.

Beyond Category A staff, staffing strategy includes:

- supporting impact - KCMC Knowledge Transfer Manager, Swart, is embedded in Chemistry, bringing >30 years' experience in industrial R&D to the role. He facilitates

industry collaborations, highlighting funding mechanisms to support impact and assisting with applications (**§1.4**)

- maintaining and developing, through our commitment to the *Technician Commitment*, a community of technical staff to ensure strong support for research facilities throughout the School. For example, new research technician, **Zhelev**, supports research and infrastructure in **EC**, new research engineer, **Gong**, supports specialist NMR instrument development and new laboratory manager **Villa-Garcia** supports equipment in the ACMF.

The development of Chemical Engineering has already allowed the recruitment of 2 **CE** staff (Hassan**:** simulation and modelling of capture, discharge and utilisation of gases; **Bimbo**: research focus in chemical processing using porous inorganic pillared clays).

As well as strengthening our research groupings and developing cross-disciplinary synergies, we have sought to achieve a balanced age profile (35% staff <45, 41% 46-55, 24%>56). Academic posts are advertised widely with explicit consideration of EDI to seek applications from the widest possible talent pool. Currently, our M:F ratio among Category A staff remains almost unchanged from REF2014 (17% female cf. 18% in REF2014) and it is a priority to increase the proportion of female staff, partly through EDI considerations in our support and mentoring of younger researchers. Interview panels are gender balanced and receive guidance on unconscious bias. The three new non-UK appointments increased the proportion of international Category A staff to 39%.

2.3 Career development

2.3.1 Research Associates (RAs) and ECRs

Since 2014, on average 73 RAs (31% female), distributed across the research groups, have been in post. Induction of all new RAs is provided upon arrival and, following completion of probation (RAs: 12-months; academics: 24-months), all staff (including RAs, ECRs and technical staff) are appraised annually, with specific focus on career aspirations and development needs to reach those goals, with Line Managers actively encouraging promotion applications when appropriate. Reviews with RAs prior to departure explore potential career opportunities. As well as academic mentors, we have a network of area-specific mentors signposted for RAs and ECRs who want support on a particular aspect of their work or life, covering work-life balance, maternity/paternity/caring, and LGBTQI issues.

Since REF2014, we have consulted with researchers across the Faculty to develop an action plan that has prompted significant changes in our provision for our RA community. The Faculty policy complements UoS policies, focussing on disseminating the *Concordat to Support the Career Development of Researchers*, institutional review of practice, and establishing professional development support for researchers. Chemistry has a research and teaching fellow network to provide a cohesive identity for researchers and to ensure that the seven principles of the *Concordat* are implemented. RAs are represented on several committees, providing insight into decision-making processes in the School.

A package of events for RAs and ECRs has been developed in the Faculty and School, specifically intended to support their career and professional development. Training sessions tailored to RAs and ECRs are provided via the Centre for Higher Education Practice (CHEP, **REF5a§3.5**). All ECRs complete the PGCAP programme run through CHEP. This programme has a strong mentoring network to support staff towards achieving Fellowship/Senior Fellowship

of the HEA (Chemistry has 17 Fellows and 6 Senior Fellows of the HEA). RAs can take all or parts of the PGCAP course as part of their training, supported by teaching opportunities within Chemistry, potentially leading to FHEA status. Professional Development supports skills development in a range of other areas, including EDI, enterprise training, leadership and management skills. Examples of further bespoke training offered by Chemistry include external facilitator-led *Lumina Spark* reflective development training and group coaching (now being rolled out to other Schools in the Faculty), *Pitching Persuasively* (external facilitator) and grant-writing workshops. The School actively encourages participation in the annual UoS *SpringBoard* programme, supporting the development of early career female staff.

We raise awareness of activities through a monthly newsletter and focussed advertising of funding opportunities specifically aimed at RAs and ECRs.

To support the transition to independent academic positions for both internal and external candidates we have introduced a competitive selection process for encouraging and supporting fellowship applications. Independent research fellowships in Chemistry during this period include:

- RS URF: **Carravetta** (2007-15), **Minns** (2011-19), **Goldup** (2009-17)
- RS Dorothy Hodgkin Fellowship: **L Brown** (2009-15)
- EPSRC Early Career Fellowships: **Kuprov** (2009-14); **Garcia-Araez** (2016-21); **Meier** (2018-19)

Fellowship holders are supported at Faculty and School levels through the Fellowship Champions network, with assigned senior mentors and a supportive senior team to provide clear career guidance, coaching and advice on progression targets. Chemistry has a strong track-record of independent fellows securing permanent academic positions at the end of their fellowships. While most have transitioned to permanent academic positions at UoS, we take pride in the success of ECRs who have found success elsewhere. As an example, **Meier** won an ERC Synergy grant (2020) in Karlsruhe to build on his work in Southampton.

New academics are supported by significant start-up funds, PhD studentship funding, as well as reduced teaching/administrative work-load allocations during their first 3 years. The effectiveness of support, including mentoring by senior staff through their probationary period and beyond, is evidenced by a 100% success rate for those new Chemistry staff eligible to apply for EPSRC First Grants or New Investigator Awards during this REF period, all of which were supported by PhD studentships.

Career development and recognition for our technical staff (e.g. through staff achievement awards) is a focus at institutional level and ensured through the *Technician Commitment*. As examples, **Zhelev** was admitted to MInstP and achieved CPhys status, while an annual budget (£2.5k) is allocated to our workshop technicians to participate in specialist conferences or training.

The annual Dean's Prize rewards excellence in research, education, enterprise, public engagement and citizenship, recognising all areas in which our RA, ERC and technical staff community support the work of the School.

2.3.2 Established academic staff

The development of all staff is discussed at annual appraisals, reflecting on the previous year, reviewing objectives and discussing career development (including opportunities for promotion), workload balance, research and funding strategy, publishing, outreach, education and work-life balance. An outcome of staff appraisals is to jointly set objectives for the coming period and to define development and training needs. Successful impact activities are recognised in our appraisal and promotion processes (**REF5a§3.3**, re-banding and additional increments and staff awards).

We operate a Workload Tariff Model for all teaching, management and administrative roles in the School. This provides the basis for allocating duties in an equitable way and helps with managing facilities use and external visits or secondments to pursue research and/or impact. For short external visits/secondments (1-2 weeks), we adopt a flexible approach, through careful scheduling of teaching and having deputies for other duties; all UG modules are taught by two members of staff to maximise flexibility. Many staff have had leave to facilitate experimental beam-time at major UK (e.g. DLS: **Russell**, **Hector**, **Stulz**, **Wells**; ISIS: **Raja**; CLF: **Minns**, **Frey**) and international research facilities (e.g. **Minns**, **Russell**, **Wells**). Requests for longer visits are considered more formally by the School Operational Board, with input from the relevant Head(s) of Teaching to manage individual staff workloads. Recent examples include **Levitt** (TIFR Hyderabad; IISC Bangalore), **Kuprov** (University of Lille), **Birkin** (University of Utah), **Carravetta** (National Institute of Chemical Physics and Biophysics, Talinn).

Our mentoring and support has proven successful in enabling career progression. Since 2014, 10 staff (1F,9M) have been promoted to full professor and 6 (3F,3M) to associate professor. The success of our academic staff is also reflected in fellowships of prestigious learned societies; **Bartlett** and **Levitt** are Fellows of the Royal Society; **Bartlett** is a Fellow of the International Society of Electrochemistry; **Levitt** is a Fellow of the National Academy of Sciences, India and a Fellow of the International Society of Magnetic Resonance; 22 staff are Fellows of the Royal Society of Chemistry (RSC).

2.4 Equality, Diversity & Inclusion

The University recognises the importance of improving gender and diversity equality in STEM disciplines, which can otherwise both severely reduce the quality of our research and negatively affect female and minority group career progression. In Chemistry, EDI training has been compulsory since 2014 and has been completed by 100% of our staff and PGRs. University policies (**REF5a§3.8**) are promoted within Chemistry, which has played an important pioneering role including as the first School at UoS to renew its Silver Athena SWAN Award in 2018, following a first Silver award in 2015. Receiving this for the second time highlights Chemistry's continuing efforts to support the career aspirations of female chemists, whilst eliminating gender bias and promoting opportunities for all.

As a founding signatory of the Athena SWAN Charter, we aim to maximise the potential of all our available talents. Several initiatives have been implemented, including: career guidance and development; peer mentoring; a Diversity charter; well-being surveys; changes to recruitment and selection policies to fully reflect our EDI ethos; all job adverts are screened by our Chemistry HR lead to ensure they conform to the School's policies and to avoid unconscious bias. Three female professorial staff (**Khalid**, **Reid**, **Russell**) with School leadership responsibilities provide highly visible role models.

Chemistry prioritises family support and many policies implemented from our Athena SWAN awards have been adopted University-wide. We operate a core-hours policy - all meetings are held during 'family-friendly' hours, enabling all staff to engage. Email policies have been introduced to promote good work-life balance and manage staff and student expectations. Flexible working is at the heart of our ethos in Chemistry, reflected at all levels. Part-time and flexible working is considered on a case-to-case basis with line-managers and the HoS – we always aim to support these. Variations to working hours have occurred at all levels irrespective of gender, both shorter and longer term, to accommodate caring responsibilities, individual health and well-being needs.

The Chemistry EDI Committee (chair: **L Brown**), meets regularly with the HoS to reflect on Chemistry's Action Plan and to identify good practice. It includes PGR, UG, ECR, technical and administrative staff representatives, our LGBTQI and Concordat champions and an outreach/admissions lead. The EDI report is a standing agenda item for the School Operational Board. An annual budget (£2k) is allocated for promotion of EDI in Chemistry.

Full regard to EDI issues has been paid in the preparation of our submission, following the institution Code of Practice (**REF5a§3.9**). All staff have had the opportunity to input to this **REF5b.** Of the final selection of outputs, 17% are attributed to female colleagues, matching our staff ratio, and the main authorship of Chemistry's four impact case studies also closely matches the gender split of our staff ratio (1F,3M). We have encouraged all Category A staff to declare (confidentially) any individual circumstances that may have influenced their productivity over the REF period.

2.5 Well-Being

The well-being of our staff and students is a priority and our approach aligns closely with that of the University. We commissioned an external provider to deliver bespoke training for staff around well-being and resilience. Our School well-being champion promotes opportunities for support and training across our community. In addition to pastoral support from Personal Tutors, PG Supervisors and the Graduate School leads, the University's Enabling Services and First Support teams are available 24/7 to provide professional support for research students. All staff and their families can receive advice and support via a confidential Employee Assistance Programme provided by Legal & General. Referrals to Occupational Health (OH) are also encouraged where appropriate, initiated either via the individual or their line manager. 'Return to Work' meetings are held for staff returning from long-term absence or leave, and OH guide on adjustments or phased return to smooth the transition back into the School.

The School well-being champion has played a crucial role in supporting staff and students during the COVID pandemic. Our response to the pandemic has also included regular meetings with staff and students, social activities, the circulation of on-line resources related to mental health, financial support for home working and actively encouraging line managers and supervisors to be mindful of student and staff well-being.

2.6 Research Students

Chemistry works closely with the UoS Doctoral College and FEPS Graduate School to coordinate training and monitor the progress of our talented and vibrant cohort of PhD and MSc research students. They form a large, diverse, international and truly multidisciplinary research community. Over the REF period 272 FPE (Full Person Equivalent) students (89F,183M) have been awarded Chemistry PhDs. The research training and skills development in the Graduate

School is valued by the companies and SMEs that employ our graduates, e.g. BP, AWE, GSK, AZ, Merck, Novartis.

Year	2013/14	2014/15	2015/16	2016/17	2017/18	2018/19	2019/20
PhDs awarded (FPE)	41.15	36.10	43.80	35.95	51.30	30.60	33.50

Since 2015, 14 EPSRC Doctoral Prizes have been awarded to exceptional PhD graduates in Chemistry *via* the University panel, helping to develop these talented ECR staff in research careers, supporting their leadership development and maximising the impact from their research.

Recruitment: PGR recruitment has continued to be strong since 2014, averaging 45 students per year. The cohorts have a large international contingent, with 39% entering from the EU or overseas. PhD students are supported variously by EPSRC DTP, CDTs, iCASE awards, industrial sponsorships, competitively awarded UoS President's Scholarships, IfLS studentships, School funds, and a range of EU, Interreg and international scholarships (including Conacyt, Chinese Scholarship Council, *etc.*). An increasing number (12 UK, 19 international) of research MSc/MRes students have enrolled in Chemistry since 2014.

All PhD projects are advertised widely using national and international recruitment websites, with adverts checked to ensure they meet our EDI expectations; candidates are interviewed by at least 2 independent staff, with gender balance where possible. The PG Admissions Officer, HoS and DHoS (Research) are gatekeepers to ensure the best candidates receive DTP or internal funding, in line with Chemistry's strategy. PGR funding is prioritised for ECR staff, excellent research that leverages external industry funding, impact development and interdisciplinary research.

Training and support: All PG students receive stipends at or above UKRI levels and are treated equally with regards to supervision and training opportunities. They engage in subject-specific training and safety following a quarterly 'training needs analysis' performed jointly with their supervisory team, as well as generic, transferable skills training. There is a wide range of advanced skills and knowledge courses and PG students are required to attend a subset of these relevant to their research and to broaden their scientific knowledge. Students are expected to attend relevant seminars and symposia selected from a vibrant programme including internal, UK and international speakers, as well as symposia delivered by final year PhD students. They are also strongly encouraged to contribute to national/international conferences, and we are proud of their successes while representing Southampton. Many of our PGs have received awards (e.g. PhD student Stephanie Chapman was selected to present her work at the 67th Lindau Nobel Laureate meeting in 2017; Sylwia Ostrowska received the 2019 Magnetic Resonance in Chemistry Young Scientist Award at Euroismar 2019; Hannah Macdonald won 1st prizes for her talks at the German Conference on Cheminformatics (2017) and the Young Modellers' Forum (2017); Lee Steinburg won a MGMS/UK QSAR student prize (2018)).

PGR reps from each section (75% F) meet regularly with the Graduate School leads. The School allocates an annual budget (£1k) for organisation of additional career development, networking and training opportunities and 'PGR coffee and cake', helping to build the

community. Team-building training has been introduced to develop soft skills and to build the cohort.

Recruitment and training of high quality PGRs has benefitted from our leading or involvement in 5 EPSRC Centres for Doctoral Training in:

- Complex Systems Simulation (2009–18, PI=**Essex**);
- Theory and Modelling in Chemical Sciences (2014–22, co-directors=**Essex, Day**, with Oxford, Bristol);
- Integrated Magnetic Resonance (2011–18, **Levitt**, with Warwick, St Andrews/Dundee, Nottingham, Aberdeen);
- Next-Generation Computational Modelling (2014–22, Engineering, Physics, Chemistry);
- Energy Storage and its Applications (2014–22, Engineering and Chemistry with Sheffield)

and the LabFact EU Interreg programme (PI=**Harrowven**, with Caen, Rouen, Le Havre, East Anglia).

Monitoring: PGR progress is monitored formally via the Faculty Graduate School, with the Chemistry lead and deputy providing oversight and pastoral support to Chemistry PGRs. Each PGR is assigned primary and secondary supervisors who provide guidance on direction and progress throughout the PhD through regular informal discussions, group meetings, quarterly reports, *etc*. Formal progression hurdles occur at 9 and 18 months, involving written reports, inspection of experimental records, and a *viva voce*. Independent academics perform the role as one of the Examiners in the progression reviews, and as Internal Examiner for the PhD *viva voce*. Less experienced ECRs supervising students co-supervise with more senior staff to ensure appropriate guidance and support is available, and an experienced academic provides oversight of the examination processes.

3. Income, infrastructure and facilities

3.1 Infrastructure and facilities

Chemistry is housed in facilities that are either purpose-built and/or have undergone major refurbishment since 2000, providing excellent containment via ~170 fume cupboards, facilities for high pressure chemistry and a Cat 2 laboratory for biological samples. In addition to the capital investment in Chemical Engineering (£5.5M), since 2014 UoS has demonstrated its strong commitment to Chemistry by investing significantly (>£16M, 2016-20) in a major refurbishment of the original Chemistry building that houses the Electrochemistry research group. The works included complete replacement of the extraction system (plant and fume-cupboards) to create a much more energy-efficient wind-responsive system, provision of chilled recirculating systems to reduce water usage, improved fire safety (including fire trace systems in all fume-cupboards and external gases), as well as refurbishing the teaching laboratories. Other improvements include complete re-enveloping of the building and replacement of all windows, to increase the sustainability of the infrastructure and ensure the integrity of the building for at least 25 years. The building upgrades also include improving Disability Discrimination Act access for staff and students, part of our commitment to EDI. Our target is to secure ~£20m funding to refurbish the Synthetic Chemistry Building (opened in 1999) in the coming REF period.

Research is supported by the C&A group with expert staff, including specialists in NMR, mass spectrometry and diffraction (7 FTE), while computational support for CSC is provided centrally via the University's iSolutions team. Two FTE mechanical workshop staff interface with a specialist NMR engineer. We also have 2 FTE Chemistry stores staff and an exceptional scientific glass-blowing workshop (3 FTE). A dedicated H&S Adviser leads training in risk management, COSHH and chemical safety, while our Facilities Manager is responsible for infrastructure maintenance across Chemistry.

3.1.1 Key facilities

- The NCS and Southampton Diffraction Centre, led by **Coles**, provide world-leading expertise for structure determination and is amongst the highest throughput and most powerful crystallography labs in the world. These provide state-of-the-art ultra-high flux X-ray sources for single crystal structure determination with 2 Rigaku Superbright FR-E+, Rigaku 007 and Rigaku R-axis Spider diffractometers (the latter optimised for PDF analysis), a macromolecular crystallisation pipeline with robots and imaging facilities, a Bruker D2 Phaser for PXRD and a Rigaku SmartLab optimised for thin film and microfocus diffraction; a new Hypix 2D detector has enhanced our capabilities for GISAX analysis. The latest renewal (§**3.2.4**) has allowed, for the first time, contract research with industry and SMEs.
- Materials deposition and analysis capabilities have been enhanced significantly by establishment of the ACMF in 2014 (§**3.2.4**), housing a multi-chamber UHV system for combinatorial thin film material synthesis, device fabrication and surface analysis, coupled with a manufacturing cluster tool based on PVD methods (donation from Ilika). The School also hosts CVD rigs for thin film and nanoparticle growth, environmental SEM with EDS/WDS detectors. Photo- and e-beam lithography, sputtering, fabrication, FEGSEM, AFM, Raman and electrical characterisation facilities are available *via* the ZI and TEM *via* the Southampton General Hospital.
- NMR facilities include open-access service instruments (3 x 400MHz, 500MHz, incl. multinuclear capabilities) and specialist instruments. Specialist equipment for cryogenic NMR (to 1K) includes a unique cryogenic high-resolution MAS NMR probe for solid-state NMR experiments down to 9K; a home-built dissolution-DNP polariser (94GHz) with a dissolution wand capable of generating NMR signal enhancements by factors of up to 10^5 at room temperature.
- The mass spectrometry facility includes a unique suite of instrumentation, affording the only open access GC-MS, HPLC-MS and Supercritical fluid chromatography (SFC)-MS facility worldwide, affording a comprehensive separation science suite to provide high-throughput solutions for a wider range of applications. This capability is complemented by higher performance, specialist instrumentation, including FTICR-MS, ion mobility MS, specialised capability in oligonucleotide analysis, high resolution MS, structural elucidation (MS/MS), petrochemical analysis and lipidomics (with Medicine). This facility has been enhanced further by an EPSRC capital equipment funds (§**3.2.4**). EPSRC Maximising Capability funds (£187K, 2018-20) fund a specialist analyst for our ion mobility mass spectrometer, to develop bespoke methods for advanced research projects, locally and regionally, and to engage other researchers by developing training activities.

- Electrochemical equipment, specialist multichannel potentiostats, high-pressure equipment, battery lifetime cycling equipment and glove boxes for experiments associated with nanomaterial electrodeposition and battery research. A dedicated technician oversees these facilities, increasing their efficiency for external and internal projects, as well as providing training for Chemistry PGRs and RAs.
- 10 dedicated glove boxes for synthesis, materials chemistry, electrodeposition and battery research.
- Integrated suite of flow reactors and in-line analytical tools for synthesis/electrosynthesis/ catalysis.
- Multiple IR, Raman and UV-visible and fluorescence spectrometers.
- DNA synthesisers for oligonucleotide work, ITC and cold rooms.

Maximum usage across UoS and externally and the sustainability of core facilities is achieved through their operation as Small Research Facilities.

As evidenced by the recent refurbishment, sustainability is embedded in the School's culture. Chemistry's Sustainability Officer works as part of the Chemistry Energy Group (CEG) towards reducing our carbon footprint, feeding into the building refurbishment project. Energy efficiency improvements and carbon reduction initiatives are supported through a dedicated UoS carbon management fund, to which the CEG has bid successfully for several projects. These included funding (£50k) to replace all glassware drying ovens and funding to investigate solvent recycling, yielding significant savings.

3.2 Research funding portfolio and plans:

3.2.1 Research income

Income in this period was £55.6M (**REF4b**), a 32% increase in funding rate since REF2014 (£7.9M/yr cf. £6.0M/yr). This increase is due, in large part, to healthy increases in mean annual funding from UKRI sources, the Royal Society and BEIS (35% increase to £5.2M/yr). EPSRC is a major funding agency, together with BBSRC. EU and ERC sources have contributed ~£12.9M. Industry sources total £1.7M (excluding industry funding associated with PhD studentships and project partnerships on UKRI grants), with a further £1.8M from charities. Chemistry has very strong industrial commitment to its postgraduate research with over £3.6M in industry studentships since 2014, e.g. through CASE, CDT and individual contracts.

In addition to the Fellowships detailed in **§2**, major strategic funding awarded in this REF period *include*:

- EPSRC Programme Grants:
  - *Advanced Devices by Electroplating*, £6.3M, PI=**Bartlett**, with **Hector**, **Reid**;
  - *Photo-Electro* (£6.5M; Nottingham-led, with **R. Brown**, **Harrowven**);
  - *Physics & Technology of Photonic Metadevices & Metasystems***,** £4.5M, PI=Zheludev (ORC) with **Hayden**;
  - *Next generation molecular imaging & therapy with radionuclides*, £6.4M, KCL-led with **Reid** and Imperial College.

- *Lighting the Way to a Healthy Nation*, Transformative Healthcare Programme Grant, £4.5M (£2M to UoS), **Mahajan** with ORC and Medicine, UoS, and Edinburgh

- EPSRC Platform Grant (*A Multidisciplinary Research Platform for Nuclear Spins far from Equilibrium*), £1.5M; PI=**Levitt**, with **R Brown**, **Carravetta**, **Pileio**, **Whitby**;
- BBSRC Industrial Biotechnology Catalyst (IBCAT), £3.5M; PI=**Linclau**, with **Lee**;
- CRUK Programme Grant, £1M, PI=**Tavassoli**;
- EPSRC Automating Science Discovery AI Network+, £1M, PI=**Frey**.

Staff in Chemistry have an excellent track record of securing prestigious ERC funding; grants held over this REF period include:

- Starting Grants: **Bradshaw** (2010-15), **Day** (2012-17), **Mahajan** (2016-20);
- Future and Emerging Technologies (FETOpen) grant: **Utz** (2016-2020);
- Consolidator Grant: **Goldup** (2017-22);
- Advanced Grants: **Levitt** (2012-16 and 2018-23);
- Synergy Grant: **Day** (2020-26).

These large research programmes sit alongside a broad portfolio of standard grants, held across all research groups; 93% of our Category A staff held EPSRC or BBSRC awards during the REF period. We are confident that our research strategy will facilitate continued success in securing funding from a range of sources, maintaining a diverse research income portfolio.

3.2.2 Professional services & facilities access

Our staff consult for biotechs, large pharma, fine chemicals industries and Government agencies. We operate a successful professional service, **Southampton Chemistry Analytical Solutions** (led by Langley), providing commercial access to specialist spectroscopic, diffraction and scientific glass-blowing facilities and the collective expertise of the C&A group. This activity supports the instrumentation base in Chemistry and resources for future investments.

3.2.3 Major Facility Use

Chemistry makes considerable use of large facilities (synchrotron, neutron, lasers, *etc*.). The value of access to UK facilities is £10.4M since 2014 (**REF4c**). Staff have also been awarded >130 days at European (e.g. ALS, APS, Spring-8, ESRF, SOLEIL, ILL, SLS, HASYLAB) national facilities since 2014.

3.2.4 Capital equipment

The NCS National Research Facility was renewed for 2016-21 with £4.7M EPSRC funding, with £350K strategic UoS funding, allowing state-of-the-art instrumentation upgrades, as well as new advanced technique services (high pressure crystallography, gas cells, charge density analysis).

The ACMF (**§3.1**) was established in Chemistry (2014) through EPSRC Capital Funding (£3.3M and £0.6M from Ilika; PI=**Hayden**), allowing the scale-up of materials on wafers using molecular-beam epitaxy based methodologies developed in Chemistry and their incorporation in advanced thin film devices in the energy, electronics, optoelectronics sectors, and compatibility with the

clean-room fabrication facilities in the ZI. The ACMF has been enhanced further in 2019 through high-throughput equipment upgrades donated by Ilika (valued at £350k).

The MR group has expanded its facilities with a £2M EPSRC equipment grant for advanced NMR instrumentation (**Utz** & **Levitt**, 2017), including a 700 MHz liquid state NMR system, two dedicated 400 MHz liquid state NMR spectrometers to support the group's research in dynamic nuclear polarisation, and replaced the 400 MHz solid state NMR console. The equipment supports extensive collaboration across UoS, nationally and internationally.

In 2019, an EPSRC Strategic Equipment grant (£856k, **Langley** (PI)**, Herniman, Attard and Raja** with Bath, Swansea, Portsmouth) funded a multi-inlet gas chromatography high-resolution mass spectrometry, a unique capability within the UK academic sector. This capability is used by researchers across the southern region and will be extended to other academic and industry researchers to form a new Centre of Excellence (**§1.2.2**).

3.2.5 High Performance Computing (HPC)

HPC is a strategic enabler to many of our research goals and UoS has made significant investments in this area (**REF5a**). Iridis, the University's HPC, remains one of the most powerful computational facilities in the UK. In 2017, Iridis5 joined the elite of the world's top 500 supercomputers and, running alongside Iridis4, provides over 32,000 processor-cores, as well as a new Data Intensive service, 20 of Nvidia's enterprise GPUs, and a dedicated data visualisation service. The machines are free to access for all research staff and students, supporting ambitious research in the **CSC** group and facilitating widespread use of computational approaches across Chemistry. The **CSC** group also secures regular access to national Tier 1 (ARCHER) and Tier 2 HPC facilities through competitive applications, membership of High-End Computing consortia and Tier 2 computing centres. Southampton is a founding member of Science and Engineering South, the Materials Modelling Hub (**Skylaris** as co-I) and JADE (**Khalid** as co-I), the Joint Academic Data Science Endeavour. **Essex**, **Skylaris**, **Day, Khalid** have received > 2,000,000 kAUs (kilo-allocation units) on ARCHER since 2014, with a value of *ca.* £1.6M.

3.2.6 University Library

The Library provides electronic access to >1200 chemistry journals, including Gold level RSC subscription and all ACS journals, as well as access to online databases, including Web of Science, Scopus, SciFinder Scholar, Reaxys and INSPEC.

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

4.1 Collaboration overview

Chemistry's strategic links with academic and industrial research around the world are supported through EU networks, programmes such as the EPSRC/NSF and EPSCR/SFI collaborations, Erasmus programmes, the World University Network and others. A key example is the ARAP scheme with A*STAR, Singapore (15 joint PhD students), supported at University level through bilateral 2+2 PhD programmes.

We host many distinguished international visitors, most with prestigious scholarships, including from the US, Canada, China, India, Singapore and Europe. As well as externally-funded visits, international collaboration is supported by the University's Global Fellowships scheme,

developing collaborative partnerships through support of a range of activities, including significant time spent at UoS.

4.2 International, national and industrial research collaborations

We have a wide range of collaborations where the team brings together the appropriate combination of expertise and skills to meet the scientific challenge. Important *examples* of international activities include:

- **Harrowven** is PI on an EU Interreg programme (€5.7M), LabFact, uniting world-class research centres located in the Channel area (Caen, Rouen, Le Havre, East Anglia, Southampton).
- **Raja** is a member of the EU-funded MULTI2CAT program with academic and industrial partners in in Spain, Germany, Italy, Belgium and France.
- **Levitt** is PI on a Marie Skłodowska-Curie Innovative Training Network, with partners in Germany, Poland, Italy, France, Spain and the UK.
- **Garcia-Araez** and **Bartlett** hold a Royal Society International Grant with the University of Buenos Aires and Research and Knowledge Transfer Centre of Jujuy.
- Extensive academic collaborations exist between Southampton and international research groups. 48% of 1403 papers published in the REF period have international collaborators.

Nationally, Chemistry has very strong links with academic and industrial partners. *Examples* include:

- **Frey** leads the EPSRC AI^{3}SD Network+ (Artificial Intelligence and Augmented Intelligence for Automated Investigations for Scientific Discovery).
- **Whitby** is PI on the EPSRC Dial-a-Molecule Grand Challenge network.
- Research Complex at Harwell through the EPSRC Catalysis Hub (**Wells, Russell**, **Raja).**
- **Roach** with Dstl on novel protein targets and their inhibitors for protection against bacterial biological warfare agents and antibiotic resistant pathogens.
- **Russell** with the Johnson Matthey Tech. Centre to advance development and understanding of the cathode & anode components in electrocatalysts and fuel cells.
- **Reid** with GE Healthcare, KCL and Imperial College, developing new metal fluoride complexes as scaffolds for rapid, late-stage F-18 radiolabelling; with Holmes (Cork), de Groot and **Hector** on chalcogenide semiconductors and applications; with Deregallera and Epivalence.
- **Langley** with Innospec on fuel quality and IDIDs, Waters on SFC-MS and Bath, Swansea and Portsmouth Universities on 2D GC-MS.

UoS encourages enterprise and innovation in science and, in keeping with this ethos, Chemistry has strong links with business and industry. Many examples were discussed in **§1.6**. 16 of our Category A staff have had active consultancies with industry since 2014, working with a variety of large, international companies and SMEs, e.g. Morgan Innovation and Technology (**L. Brown**), AstraZeneca (**Stulz**), Dassault Systèmes (**Skylaris**), Dextra Laboratories/New Zealand Pharmaceuticals (**Linclau**) and UCB (**Essex**).

4.3 Sustainability

Academics in the School contribute to the health and sustainability of the discipline through actively taking leadership roles, such as:

- Delivering Plenary and Keynote lectures: over half of our category A staff have delivered plenary or keynote lectures at international conferences, totalling > 110 in this REF period.
- Holding visiting professorships and visiting academic positions at international institutions, including: **Bartlett**: Visiting Professor, Memorial University, St John's, Newfoundland, Canada (2015); **Coles**: Visiting Professor, University of Cagliari, Italy (2015); Visiting Academic; **Denuault**: Visiting Professor, University of Sao Paulo (2015-16); **Khalid**: Distinguished visitor, Bangalore, India; **Kuprov**: Visiting Professor, University of Lille (2016); **Linclau**: Visiting Professor, Ghent University (2015-); **Nandhakumar**, Academic Visitor, Singapore ASTAR (2017); **Raja**: Eminent Visiting Scientist, Institute for Materials Research & Engineering, ASTAR Singapore (2016); Academic Visitor, IIT Madras (2018) and Jilin University, China (2018); **Rios**, Visiting Professor in SKKU, South Korea (2015-19); **Stulz**: Visiting Professor, University of Bordeaux (2016).
- Organising, chairing and co-chairing international conferences and meetings, *including*: Chairs of two Gordon Conferences (**Bartlett**, **Goldup**), two Faraday Discussion meetings (**Minns**, **Day**), co-organisers of ISACS16, Challenges in Chemical Biology conference (**Tavassoli**, ETH, Zurich, 2015) and co-organiser of CECAM workshop of Frontiers in Computational Biophysics (**Khalid**, Switzerland, 2018) and co-organiser, chair and co-chair respectively of Hyphenated Techniques in Chromatography (**Langley** Ghent 2016, Cardiff 2018, Ghent 2020).
- 23 staff are members of one or more journal editorial boards. Examples: **Associate editors**: **Bradshaw**: (*Coordination Chemistry Reviews*); **Goldup** (*Chemical Science*); **Kuprov** (*Science Advances*); **Editorial board members**: **Bartlett** (*ChemElectroChem*, *Current Opinion in Electrochemistry*); **Coles** (*Crystallography Reviews*, *Supramolecular Chemistry*); **Day** (*Faraday Discussions, CrystEngComm*); **Essex** (*Journal of Computer-Aided Molecular Design*); **Frey** (*Journal of Cheminformatics, Patterns (Cell Press)*); **Garcia-Araez** (*Journal of Materials Chemistry A*); **Khalid** (*Scientific Reports*); **Langley** (*Rapid Communication in Mass Spectrometry*); **Lee** (*Molecules (MDPI)*); **Levitt** (*Journal of Magnetic Resonance*, *Journal of Chemical Physics*); **Light** (*Transition Metal Chemistry*); **Nandhakumar** (*Scientific Reports*); **Raja** (*Catalysis*); **Read** (*Education in Chemistry*); **Rios** (*Frontiers in Chemistry*, *Scientific Reports*); **Russell** (*Chemical Society Reviews*); **Stulz** (*Cogent Chemistry*); **Tavassoli** (*RSC Chemical Biology*); **P.Wells** (*Catalysis, Structure and Reactivity*). **Advisory boards**: **Day** (*Molecular Systems Design & Engineering*); **Hector** (*Royal Society Open Science*).
- Standing on a range of national and international committees, steering groups and special interest groups, such as: **Reid** became President-elect of the RSC in 2020 (President 2022-24); President of the International Society of Electrochemistry (**Bartlett**, 2017-18); Chair of the Scientific Advisory Board for the ROAR centre at Imperial College, London (**Whitby**, 2018-), Expert Panel members of the Faraday Institution (**Russell** and **Owen**), EPSRC High Level Advisory Group for the National Research Facilities (**P.Wells**), IUPAC – GO FAIR Chemistry Implementation Network (**Coles**), **Khalid** leads the High End Computing Biosym consortium and **Day** led the organic and soft matter theme (2014-18)

and leads the materials discovery theme (2018-) on the steering committee of the Materials Chemistry Consortium; these consortia allocate national HPC time. **Langley** is President of the International Mass Spectrometry Foundation (2020-24), Vice Chair of IMSF (2016-20), Chair of the Separation Science Group of the RSC (2010-), chromatography-mass spectrometry lead for SCG4 of the Energy Institute (2009-), Member of RSC AD Council (2014-19).

- Advisory roles to the academic community, including: Member of International Advisory Board State Key Laboratory Physical Chemistry of Solid Surfaces, Xiamen, China (**Bartlett**); Chair of Royal Society Committee 3 (2019-20) (**Bartlett**); Royal Society URF Aii Panel Chair (**Bartlett**); International review of Chemistry, Gebze Institute of Technology, Turkey (**Coles**); Royal Society Dorothy Hodgkin Panel (**Reid**); EPSRC SATs (**Frey, Khalid**); Leverhulme Trust advisory board (**Khalid**); ExCALIBUR advisory board (**Khalid**); International Expert Panel for Canadian Innovation Foundation (**Reid**); International review – Trinity College Dublin and UCC (RoI) (**Reid**); Panel members for grant (e.g. Royal Society, EPSRC, ERC) and facilities access. 28 staff are members or associate members of the EPSRC peer review college and review for international funding bodies (e.g. NSF, IRC, SFI, Dutch, Finnish, German, Polish, Canadian and NZ national research councils); Expert reviewers for the ERC (**Mahajan**, **Day**, **Frey**, **Levitt**, **Nandhakumar, Kuprov**). **Smith** is Senior Independent Member of EPSRC's Council and board member of the Higher Education Funding Council for Wales.

Our academic staff's contribution to the community has been recognised through a number of awards and prizes during this REF period, including: **Smith**: awarded a CBE for contributions to research and HE; **Bartlett**: Alessandro Volta Medal of the Europe Section of the American Electrochemical Society (2014); Galvani Medal of the Electrochemistry Division of the Italian Chemical Society (2015); Giulio-Milazzo Prize of the Bioelectrochemical Society (2015); Luis Federico Leloir Award, presented by the Argentine Minister for Science (2016); Breyer Medal, Electrochemistry Division of the Royal Australian Chemical Institute (2017); Royal Society Wolfson Research Fellowship (2014-19); **Baud**: Roger Griffin Prize for Cancer Drug Discovery 2016 (BACR & Astex); **Birkin**: S-Lab Award Winner (2014); **L. Brown**: Eli Lilly OIDD Undergraduate Award (2014); **Goldup**: RSC Hickinbottom Award (2014); RSC Bob Hay Lectureship (2017); Royal Society Wolfson Research Fellowship (2019-24); Blavatnik finalist (2020); **Langley**: British Mass Spectrometry Society Lectureship (2016); **Levitt**: Russell Varian Prize in Nuclear Magnetic Resonance (2015); **Pileio**: BRSG-NMRDG Award for Excellent Contribution to Magnetic Resonance (2015); **Read**: National Teaching Fellowship (2017); **Tavassoli**: RSC Protein and Peptide Science Award.(2017) and European Peptide Society's Leonidas Zervas Award (2020).