

**Institution: University College London (UCL)**

**Unit of Assessment: 8 Chemistry**

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

### 1.1. Overview

Chemistry at UCL is vibrant and interdisciplinary justifying the departmental motto “*Inspiring the future*”. Our vision is simple: to generate world-leading chemical research characterised by innovation, insight and rigour achieved by our leading researchers across the breadth of the chemical sciences. We attract and retain highly talented staff by providing state-of-the-art facilities and high quality support to early career researchers enabling them to flourish. We embrace UCL’s interdisciplinary culture throughout the department to achieve the greatest breadth of impact for our research. The department has joint lecturer/professor appointments with Diamond/Harwell, London Centre for Nanotechnology (LCN) and Medicine and is the administrative home for the Institute for Materials Discovery (IMD), founded in 2014 to link materials research across UCL. The department has >300 active research collaborations with industry, UCL departments, other universities, national and international research centres.

### 1.2. Research strategy

#### 1.2.1. Structure

The department’s research strategy is led by the management working group (MWG, 6 academics) chaired by Head of Department (HOD, **Carmalt**), with input from the Director of Research (DOR, **Hailes**) and the Research Committee, in consultation with all academic staff and the Dean (**Parkin**) of MAPS (Mathematical and Physical Sciences) Faculty. External academics (e.g. Dobson, Oxford University; Walsh, Imperial College) and representatives from industry (e.g. Simon Hurst NSG; Phil Taylor AzkoNobel; Mark Storr AWE) further inform this strategy. The department’s research is divided into four sections for administrative purposes: Organic Chemistry and Chemical Biology (OCCB); Physical Chemistry and Chemical Physics (PCCP); Inorganic and Materials Chemistry (IM) including IMD; and Computational Chemistry (CC). Each section meets regularly to discuss objectives and to determine strategic priorities. MWG hold annual strategy meetings in research, undergraduate teaching, postgraduate teaching/research, safety/sustainability and EDI (equality, diversity and inclusion), with relevant colleagues attending to inform strategic directions (Figure 1). The annual research strategy meeting provides a yearly review of research in the department, informed by REF2014 recommendations, MAPS Faculty reviews and external advisors. Regular staff and PG surveys also contribute to the departmental strategy.

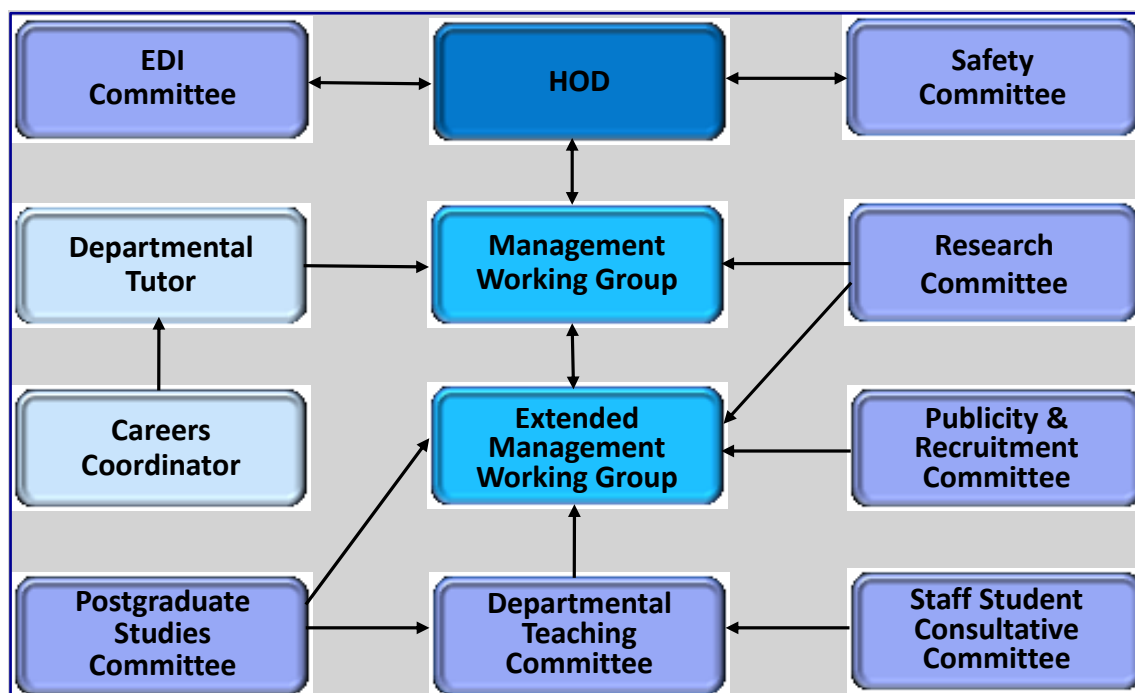


Figure 1. Departmental organisational structure, principal committees and reporting structures.

### 1.2.2. Strategic Aims and Vision

The department's vision is to achieve international excellence across major branches of chemistry including organic chemistry and chemical biology, chemical sustainability, computational chemistry, materials discovery and physical chemistry. In these areas we will sustain an internationally leading role to transfer results to inform policy makers, industry and the public. Our strategy for growth and sustainability is highlighted by forward planning to:

- Pioneer novel green chemistry strategies for molecular assembly, molecular recycling and materials construction.
- Address challenges of a zero carbon economy through sustainable approaches to energy storage.
- Develop new strategies for chemotherapeutics, personalised medicine and the Origins of Life.
- Develop new approaches to advanced instrumentation for fundamental and applied molecular science, notably in light mediated processes.
- Build on leadership in materials discovery and computational chemistry particularly in renewable energy, functional coatings and catalysis.

This will be achieved by:

- Maximising interdisciplinary research via existing strong collaborations, e.g. Harwell, and through new departmental interdisciplinary research themes.
- Supporting core activities by rewarding excellence of staff and making new appointments.
- Continuing to achieve a balanced funding portfolio from multiple sources and expanding support from industry (open days/networks/KT events).
- Continued allocation of internal resource to maximise quality and success in grant applications.
- Sustaining the quality and number of PDRAs, PhD and Masters students.
- Building on the excellent infrastructure and facilities to allow researchers to flourish and continuing as an equipment hub for UCL/neighbouring universities.
- Supporting high quality computer resources, locally and through access to extensive UCL and national/international facilities, and continuing leadership in high performance computing.

In the future OCCB will build on its existing strengths in biomedical imaging and biological therapeutics, deepening its interactions with UCL Medicine, School of Pharmacy (SoP) and the Francis Crick Institute. Research in the area of sustainable and green chemistry will be significantly expanded, taking advantage of the opportunities offered by UCL East, a £500M investment bringing together 8 UCL faculties to integrate research and education, theory and practice and connecting Experiments, Arts, Society and Technology (EAST). At UCL East 3 lecturer appointments, and the development of an MSc course in Chemical Sustainability will open up a range of new funding opportunities from UKRI and industry (lead **Hailes**). OCCB will continue contributing to cross-disciplinary research in the department, particularly in Light-Molecule interactions and organic materials. Objectives for PCCP include continuing to design, build and exploit innovative instrumentation for measuring and understanding the structure, properties and reactivity of molecules and solids in a range of environments; and to use this expertise to tackle problems in the priority areas of healthcare, quantum technologies, new materials and energy. The newly established Laser Science Centre (lead **Fielding**) will provide a focal point for many of these activities, helping to foster new collaborations across UCL. Future goals for IM and CC are to further integrate computational and experimental methods in materials research, expand research in materials for renewable energy and strengthen links with Diamond/Harwell through the Catalysis Hub, the X-ray Photoelectron Spectroscopy (XPS) National service and with the Faraday Institution (FI) through new battery technology research. New XPS methodology/data analysis will be introduced via development of methods for bulk materials and surfaces/interfaces in electronic devices using laboratory- and synchrotron-based spectroscopic methods. Chemistry staff work regularly at Harwell/Diamond (>10), including **Beale** (full time) and **Scanlon** (0.4FTE Diamond), and 20 UCL researchers are based there. Energy and Catalysis research will be further strengthened via close links with UCL Chemical Engineering. Links with Harwell will also be enhanced through engagement with the Rosalind Franklin Institute (RFI), of which UCL was a founding partner (**Tabor** UCL theme lead for Next Generation Chemistry; **Battaglia** UCL theme lead for Correlated Imaging).

Tackling the key research challenges will require collaborative, multidisciplinary approaches, bringing together multiple investigators with expertise in theory, computation, synthesis and measurement. To capitalise on our strengths, the department is developing 5 Research Themes: Chemical Sustainability; Chemistry and Light; Materials for the Future; Chemistry and the Environment; and Chemistry for Life to go beyond OCCB/PCCP/IM boundaries. These themes align with EPSRC priority areas/portfolios and UCL Grand Challenges (Sustainable Cities, Global Health, Human Wellbeing and Transformative Technology). For each theme, short/long term research strategy is being developed with regular meetings (formal/informal) and seminars to help drive forward future collaborations, grant applications and engage with end-users.

Research activity on Covid-19, which will continue into the next REF period, has been initiated within the department. **Howorka** is leading a project delivering fast, portable, high-throughput and accurate antibody sensing by pioneering step-changing sensor nanopores. These will be integrated into memory-stick-sized-on-the-market kits by Oxford Nanopore Technologies (ONT) and clinically tested via collaborations with UCL Medicine. Covid-19 research activity also includes antiviral therapy and targeting activated macrophages to stop inflammation (**Battaglia**), a “cost effective” preparation of beta interferon- a naturally occurring protein that facilitates the body’s antiviral responses (**Macmillan**) and a computational effort to accelerate the development of antiviral drugs for Covid-19 by modelling proteins critical in the virus life cycle (**Coveney**).

To achieve our strategic aims the research committee, Heads of Section and HOD provide mentoring to staff to improve the quality of grant applications. All academic staff are expected to submit two grant applications a year as PI, with one to UKRI. This has led to a culture of collaboration and enhanced our total non-facilities grant portfolio to >£75M compared with ~£40M at the start of the REF period. This supportive culture will continue, as we strive to develop our funding portfolio, reflecting the collaborative ethos of UCL. The department recognises the key role that a large PhD cohort has on research outputs, and to maintain the number of PhD students, a departmental ‘matching scheme’ that provides a PhD studentship for ~£500K of UKRI income will continue as an incentive to staff, along with support for equipment. To enhance collaborations with industry and facilities, “impact PhD” studentships (50%UCL; 50%industry funded) will continue, e.g. 7 “impact PhD” students were supported in chemistry per year (2017-2020).

### **1.2.3. Achievement of Strategic aims set out in REF2014**

All key strategies defined during REF2014 have been advanced enabling the development of chemical approaches to address key scientific and societal challenges of the 21<sup>st</sup> Century. These included establishment of IMD; the Good Manufacturing Practice (GMP) radiochemical facility and the Laser Science Centre; enhancing links with Life/Medical sciences in Chemical Biology; expansion in sustainable chemistry and energy materials; growing leadership in computational methods for catalytic processes and crystal polymorph prediction. The QS world ranking shows UCL Chemistry rising from 43<sup>rd</sup> (2017) to 31<sup>st</sup> (2020).

The OCCB group, with its focus on the interface of organic chemistry and life/medical sciences, has played a key role in the development of next generation tools for fundamental and applied biomedical imaging. This development has been stimulated by major strategic investments by Cancer Research UK (CRUK) and EPSRC and multiple collaborations (e.g. UCL Medicine, UCL Cancer Institute and Centre for Advanced Biomedical Imaging) leading to: platform technology for radiolabelling of tracers for fluorine-18 imaging with positron emission tomography (PET) (**Årstad, Sander**); development of a GMP facility with production of injectable diagnostic agents for experimental medicine (**Årstad**); new liposome-based theragnostic nanoparticles for cancer imaging, with 3 patents licenced to Nanogenics Solutions (acquired by Ryboquin £4.5M) (**Tabor, Hailes**) and development of infraluciferin for *in vivo* near-infrared bioluminescence imaging (**Anderson**). **Powner** leads investigations in chemical origins of life, pioneering a new ‘Systems Chemistry’ approach showing how proteins could be synthesised in prebiotic solutions (£2M grant funding). New sustainable synthetic and biocatalytic strategies (**Hailes, Sheppard**) have allowed the synthesis of a range of chemicals from sugar beet pulp (EPSRC, £2M) and development of biocatalytic approaches to degradation of plastics in the UCL Designing Out Plastic Waste project (**Hailes**, £1M UKRI/EPSRC). **Howorka** has pioneered development of DNA and protein membrane nanopores (patent licenced to ONT). This led to the development of a new nucleic acid sequencing technology by ONT, contributing to the company revenue growing from £4.5M to £52M (2016-2019) and recently used in detecting rapid mutations of Covid. Furthermore, application in various sectors worldwide

improved disease prevention strategies in people and plants, improved crop yields and ensured safety and protected supply chains in the food industry. Other highlights since REF2014 include development of borate esters as efficient, green catalysts for direct amidation reactions (**Sheppard**; sold by Merck as the 'Sheppard Amidation Reagent') and antibody-drug conjugates (**Chudasama**) with 2 patents and the founding of a spin-out, *Thiologics* (**Baker, Caddick, Chudasama**). The novel orphan drug pitolisant (Wakik<sup>TM</sup>), developed by Emeritus Professor Ganellin in the department, is used for treatment of narcolepsy and Prader-Willi Syndrome, giving a significantly improved quality of life for people with rare diseases globally and saving 42% treatment costs for the NHS. The drug has generated >\$70M of sales revenue for *Bioprojet* and *Harmony Biosciences* over the past few years.

The PCCP section has made major contributions to developing and applying advanced instrumentation for fundamental and applied molecular science including the application of photoelectron spectroscopy (PES) to show how chemical substitution can determine the redox properties of green fluorescent proteins and development of liquid microjet PES (**Fielding**). An interdisciplinary research grouping brings together design, synthesis, photophysics and theory to investigate light-molecule interactions, focusing on two areas: organic/inorganic materials for solar cells (**Blunt, Bucar, Clarke, Schroeder, Worth, Ingle, Thornton**) and biologically relevant chromophores (**Anderson, Battaglia, Fielding, Hailes, Howorka, Wilden, Worth**), with a growing funding base (EPSRC £2.7M). Development of a new experimental route to generate 'pure' beams of molecular radicals (**SDPrice**) and investigating the phenomenon of stacking disorder in ice and the impact on the shapes of snowflakes (**Salzmann**) was achieved through >£3M funding (EPSRC, ERC, Leverhulme). **Battaglia** has developed a methodology for delivering macromolecules into live cells to probe cell dynamics and a unique Liquid TEM facility to visualise the dynamic nature of samples in their liquid form (>£4M funding). Based on this research, **Battaglia** has launched a spin-out company *SomaServe* to image live cells and improve their therapeutic viability. Gas sensitive semiconductor research from UCL Chemistry, previously led to the spin-out *Aeroqual* (**Williams, Parkin**), which has air quality monitors operating in 16 countries and an annual revenue increase from \$3.8M to \$25M (2013-2020). Expertise in analytical chemistry (**Caruana**) subsequently stimulated a new research masters course on Applied Analytical Science.

In the CC section, research on computational theory applied to solid-state chemistry and catalysis has extended its international standing. Leadership in materials and molecular modelling (MMM) is demonstrated by **Catlow** (1994-2018) and **Woodley** (from 2018) leading the Material Chemistry Consortium, managing 18% of resources on the national Tier 1 facility ARCHER, and comprising >80 academic groups for the application of supercomputing facilities in materials modelling. **Woodley** also leads the MMM Hub, which hosts the national Tier 2 High Performance Computing (HPC) facilities, THOMAS and YOUNG, for UK's MMM community (EPSRC £4M) and **Scanlon** leads the Tier 2 HPC facility, MICHAEL, for computational research within FI funded projects, established via £4.5M FI funding (>60 users). **SLPrice** leads in organic polymorph prediction (>£1.5M EPSRC, Horizon2020, Eli Lilly) supporting the development of computational methods for predicting organic crystal structures and their properties with >60 licensed bundles of DMACRYS code distributed to academic/industrial groups. The CompBioMedCentre of Excellence, funded by H2020 with 15 core partners (£1.5M) and >40 other partners, drawn internationally from academia, industry and healthcare is led by **Coveney** and is focussed on the development of computational methods for biomedical applications including the first full-scale 3D high-fidelity simulations of blood flow in the human vasculature. **Cora, Slater and Zwijnenburg** lead the computational work packages in the EPSRC Programme Grant "Integration of Computation and Experiment for Accelerated Materials Discovery" (PI: Rosseinsky £6.6M), where computational guidance has been key to the experimental discovery of materials, e.g. for solar hydrogen generation. Many in the CC section have developed software including the VECMA Toolkit (**Coveney**), open source (~50 users) QUANTICS for simulation of fundamental reaction dynamics (**Worth**), SUMO for automation of band structure and phonon band structure plotting (**Scanlon**), GALORE for production of simulated XPS spectra (**Scanlon**) and **Woodley** has developed software tools and a database to assist with the modelling of surfaces/interfaces.

The main goal set by the IM section during REF was to exploit expertise to develop new interdisciplinary projects. This fostered growth of transparent conducting oxides (**Carmalt, Parkin, Darr, Scanlon** >£3.4M funding) and new initiatives in battery technology including the EPSRC JUICED Energy hub and FI by focussing on new sustainable materials, e.g. aqueous Zn-ion batteries

and combinatorial and scale up methodology (**Darr, Cora, Parkin, Xu, Palgrave** >£4M funding). A national XPS centre at Harwell (**Palgrave**, £3.2M EPSRC with University of Cardiff) and UCL-wide activities in the use of carbon nitride graphenes as catalyst supports for electrochemical energy devices, funded by the EU Graphene Flagship (**McMillan, Sella, Cora**) were established. Nanomaterials for medical applications (**Davies, Lee, Parkin**), hydrogen storage, gas sensors, fuel cells, solar energy materials and self-cleaning surfaces (**Carmalt, Choy, Darr, Knapp, Parkin, Palgrave, Blackman, Dall'Agnes, Abdi-Jalebi**) received >£6.5M in funding, leading to 4 patents and co-funding with industry (e.g. Johnson Matthey (JM), NSG, Qinetiq, AzkoNobel, Altro). Notably, **Parkin's** research on coatings with NSG continued throughout the REF period (with **Carmalt**), which originally led to the world's first commercial self-cleaning window glass with ~2M sqm<sup>2</sup> of Activ<sup>TM</sup> coated glass now sold worldwide pa. **Beale** has developed new synchrotron-based "5-D" time, space and energy resolved tomographic techniques for materials characterisation, particularly of catalysts under reaction conditions. This research underpinned the spin-off company *Finden* and continued interaction with JM in heterogeneous catalysis has contributed towards the development of next-generation catalytic systems (**Beale, Catlow, Sankar**). Increased activity in IM provided expansion through two research masters degrees, *Materials for Energy and Environment* and *Advanced Materials Science* attracting >140 students each year.

The close synergy between theory and experiment is a key feature of the department with significant overlap between research of the CC staff with that of the IM and PCCP staff (>10 projects, >£9M funding). **Catlow** with **Beale** obtained substantial funding for the catalysis hub at Harwell (£3M) to continue a major programme in catalytic science employing computational, synchrotron and neutron techniques. Application of computational techniques to energy materials, especially battery cathodes and design of new materials for a range of renewable energy applications links members of CC with IM. For example, **Scanlon** received funding from the FI for a theory/experimental project with **Palgrave** on Na-ion batteries. Within the JUICED hub **Cora** collaborates with **Darr** on new materials for Mg batteries and with **Parkin** on new electrocatalytic systems. **Battaglia** and **Gervasio** combine 4D imaging from Liquid TEM of protein structures, capturing dynamical motion in water, with molecular dynamic simulations. A Spectroscopy and Dynamics Group, established by the PCCP/CC section (**Fielding, SDPrice, Thornton, Worth**), provides a forum for researchers to share ideas, develop projects and host seminars. Indeed, a key strategy has been to develop a wide range of departmental collaborations and larger-scale research collaborations with other universities and UCL departments. This strategy has led to a myriad of new collaborations with the fields of medicine, life sciences, materials and physics (>50 over the REF period) both internal and external to the university. These links have established UCL as a key hub in many large-scale UK and international collaborations (Diamond/Harwell, FI, Graphene Flagship, CRUK, ILL, ESRF).

To enable successful grant applications in the evolving funding landscape, it is a continuing objective that all staff adapt as appropriate their research approach. For example, staff have translated their expertise to problems of applied interest in medicine and biosciences (**Fielding, Holt, McMillan**), electrochemistry (**Porter, Wilden**) and sustainability (**Hailes, Darr**). Overall, the department has published >1930 research papers during the assessment period (~1600 over REF2014), with ~320 papers pa. This publication rate is expected to grow further as new junior staff develop their research (11 lecturers within the first 3 years of appointment). Publications from the department have continued to be highly cited, with ~1.5x the average citations in the field. We have an active departmental seminar series reflecting the interdisciplinary nature of research in the department and joint seminars with the LCN, Thomas Young Centre (TYC), IMD and UCL SoP. A departmental weekly newsletter keeps staff informed of news, publications, seminars and funding.

UCL is committed to the *UK concordat to support Research Integrity* and a 4-level training framework in research integrity has been adopted. All PG research students are required to be trained to at least Level 2 "*Understanding Research Integrity*" prior to transfer from MPhil to PhD status (monitored via an electronic log system). All researchers are aware of procedures available to raise any concern regarding research practices, which would go via the HOD in the first place and be referred to the Research Integrity Unit within the Office of the Vice-Provost Research (OVPR) if necessary. UCL is committed to open access and all publications are made available through UCL Discovery - in Chemistry >96% of all publications accepted after 01/04/2016 and some software developed is also open access (Section 1.2.3). UCL Business (UCLB) provides support to staff for negotiating technology transfer arrangements (licensing/start-ups), to achieve commercial impact from their research, including proof of concept funding, e.g. *Thiologics* (£100K). Further support

through UCL Innovation & Enterprise, working closely with UCLB, is available through a dedicated team for innovation development and funding, such as Discovery-to-use (EPSRC projects), KT initiatives and early stage commercialisation (>£1.1M awarded to staff during REF period). Consultancies are arranged through UCL Consultants (UCLC) and overall consultancy income in the department was >£1M.

In summary, in line with our REF2014 strategic aims we have achieved the following:

- Targeted appointments (Section 2).
- Grant application success, balanced portfolio reducing EPSRC reliance (Section 3).
- Sustained/increased PDRAs and research students (Section 2).
- Equipment hub (Section 3).
- State-of-the-art computers (Section 3).

## 2. People

### 2.1. Staffing Strategy

The department has appointed **19** lecturers/professors since REF2014, with **10** staff retiring/leaving UCL, hence a net increase of 9 HEFCE-funded staff, showing continuing institutional support. The staffing strategy is set by MWG in consultation with the Dean and informed by sectional group meetings. We have enhanced interactions and joint lectureships with the LCN, Harwell and medicine and developed the IMD (a Director and 3 Lecturers). Our staffing strategy has been to maintain core staff numbers in each of the four research sections while expanding in key areas relating to the department's research vision and national initiatives. Expansion has involved an increase in staff numbers (Table 1) in materials chemistry; chemical biology; organic chemistry; nanoscale and soft matter and chemistry and light to enhance our strengths in these areas. Furthermore, appointments in electrochemical energy storage provide links with the FI initiatives.

**Table 1: New lecturers/professors appointed through the REF period**

2013-2015	2016-2017	2018-2019	2020
<b>Beale</b> (1/11/13) Functional materials used in catalysis and energy storage	<b>Worth</b> (1/7/16) Head of Physical Chemistry; Simulation of molecular reactivity	<b>Schroeder</b> (8/1/18) Functional materials for organic electronic applications	<b>Ingle</b> (4/1/20) Laser chemistry, spectroscopy & dynamics
<b>Choy</b> (1/2/14) Director of IMD; Multi-functional thin films	<b>Davies</b> (13/7/17) Design of novel nano-structured materials	<b>Dall'Agnes</b> (7/1/19) Electrochemical energy storage	<b>Simoncelli</b> (4/1/20) with LCN; DNA nano-technology
<b>Volpe</b> (1/9/14) Experimental and theoretical study of soft matter	<b>Sander</b> (1/9/17) with medicine; PET and Radiochemistry	<b>Xu</b> (1/4/19) Electrochemical energy storage	<b>Hele</b> (22/07/20) Theoretical chemistry; quantum mechanical motion
<b>Lee</b> (1/11/14) Nanomaterials and nanodevices	<b>Knapp</b> (1/10/17) Precursor design for the fabrication of materials	<b>Haynes</b> (3/6/19) Supramolecular chemistry linked to biology	<b>Colour codes:</b> Professor appointment Lecturer appointment Lecturer previous fellow
<b>Clarke</b> (1/3/15) Laser spectroscopy of organic materials		<b>Regoutz</b> (4/7/19) Materials and X-ray spectroscopy	
<b>Chudasama</b> (1/4/15) Chemical biology / protein bioconjugation		<b>Abdi-Jalebi</b> (1/11/19) Energy materials	

All academic staff that have left or retired during REF have been replaced. Exit questionnaires from this group were very positive about UCL Chemistry and the non-retirees departed for promotions (e.g. to take up a position as Pro Vice Chancellor) or a career change. The department has grown from 55 to 61.7FTE academic staff over the REF period, mainly appointing at lecturer level to bring in talented early career staff, respond to the national agenda (especially to priority areas set by UKRI, e.g. FI) and rebalance the career profile within the department. The department's/IMD's work is supported by 17 administrative staff and 22 technicians / research officers. During the REF period, 8 Lecturers (Teaching) have been appointed, who provide support in UG and PG teaching and lead on e-learning, student experience, innovations in laboratory classes and teaching. This includes development of a Citizen Science Project for 1<sup>st</sup> year chemistry UGs (received a RSC Higher

Education Technical Excellence Award and a UCL Provost Award). As well as enhancing the student experience the addition of 8 Lecturers (Teaching) alleviates pressure on academic staff ensuring there is sufficient time for research.

A number of staff hold/held fellowships in the department over the REF period: Ramsay (3 current: and 10 former; RSURF (1 current: and 2 former); Marie Curie (4 current and 5 former); NC3R David Sainsbury (1 former); NERC (1 former); ERC Starting Grant (**Scanlon, Bronstein**); ERC Consolidator Grant (**Battaglia, Salzmann**); RS Dorothy Hodgkin fellowship (**Simoncelli**); RS Industry (**Slater, Blackman**); Leverhulme (**Fielding**); EPSRC (current: **Clarke, Battaglia**; past: **Beale, Powner, Kerridge, Zwijnenburg**) and a UKRI Future Leaders Fellowship (**Schroeder**). Research fellows are strongly supported in applications for future positions and we have an excellent track record of appointing fellows to permanent academic positions through open recruitment processes.

## 2.2. Staff Development

Following UCL's commitment to the Concordat to Support the Career Development of Researchers, the department promotes these guiding principles in employment, environment, culture, professional and career development. The department established annual staff surveys and issues identified are considered by relevant focus groups. Where appropriate, recommendations from the focus groups are incorporated into the departmental annual planning cycles, e.g. a staff appraisal checklist was introduced to encourage all appraisers to discuss career development, promotion and flexible working, which resulted in staff feeling their appraisal helped identify opportunities for career progression (86% vs. 56% in 2019 vs. 2015 staff survey). For staff development, a "mentor model" is adopted where each person is assigned an academic, unconnected with their research, providing careers support including CV development, grant applications and promotion. Staff are required to attend at least two training courses pa, for example fellowship/grant writing, PhD supervision, leadership and equalities training. Compulsory departmental training involves unconscious bias, harassment prevention and best practice in safety. Staff performance is monitored annually via staff appraisal (100% appraisal completion for all staff). Each year, measurable objectives are set for the following year and progress against these is assessed by the appraiser and used to identify training and requirements for promotion. Clear objectives are set for teaching, enabling, KT activity and research including number and quality of grant applications. The HOD and senior staff across the department provide support during the grant writing process, giving feedback on draft proposals, impact and the response to referees. OVPR Research Facilitators also provide support through training, mock interviews, proposal structuring and highlighting current calls. This has helped successful awards of ERC Starting/Consolidator grants and EPSRC/UKRI fellowship applications; FI large grants (**Scanlon, Palgrave**), large (>£1M) EPSRC grants (**Carmalt, Darr, Fielding, Hailes**) and catalysis hub application (**Catlow, Beale**). Colleagues also receive guidance, from senior academics within the department, in writing high-impact research papers, with staff often circulating draft manuscripts to others for comment prior to submission. Seminars and workshops continue to be organised in the department with, for example, the Nature Group, ACS and RSC publishing.

The staff development process has allowed a large number of fellows and PDRAs to progress to lectureships at UCL (9 staff) or other universities (**Bear** (Kingston); **Benhamou** (Le Harve Normandie); **Buckeridge** (London South Bank); **Crick, Lu** (QMUL); **Dunnill** (Swansea); **He** (Lincoln); **Kafizas** (IC); **Kerridge** (Lancaster); **Logsdail** (Cardiff); **Maruani** (Paris); **Peveler** (Glasgow); **Tartalini** (Coventry)). Our support has allowed all new lecturers to have success in expanding their research groups. Non-proleptic appointments, e.g. those on independent Royal Society, Ramsay, or EPSRC fellowships are not required to have a teaching load. However, many choose to do some limited teaching, including tutorials, demonstrating or lecturing to gain experience. New academic staff have a 33% teaching load in year 1, which increases to a full load (~30 lectures; ~200 contact hours) by the end of year 3. All new lecturing staff take an accredited HEA teaching qualification supported by UCL Arena (UCL's professional development pathway for teaching). New lecturers are given a minimum start-up fund of £30K in cash support, purchase of relevant kit (~£40K) and a PhD studentship to enable them to set-up their research group. New staff are able to recruit ~3 Masters students from the MSc/MRes courses to work in their group and are provided with laboratory space and given access to the extensive equipment portfolio and computer resources. As well as being supported by a senior academic mentor, new staff have monthly 1:1 meetings with the HOD to discuss progress and identify any further support required.

A workload model is used to monitor FTE, teaching commitments, departmental/institutional administrative roles and research supervision. Success in grant applications can be recognised through a reduction in teaching duties and staff can take sabbatical leave to develop new research or KT. While on sabbatical leave (20 staff over the REF period), staff are removed from all teaching/administration duties for a full year, and their workload is shared between other staff and trained PDRAs. Goals, agreed with the HOD, are set prior to any sabbatical and achievements are assessed against these goals. Successes from sabbaticals include **Fielding's** work on spectroscopic measurement on bioluminescence emitters leading to a £1.4M EPSRC grant and **Macmillan's** development of a biochemical toolbox for protein modification leading to funding from EPSRC/Leverhulme (£800K). The sabbatical programme will continue through the next REF period.

UCL introduced a new promotion framework in 2018 to support all academic career paths whether focused on research and education in equal measure, or on one or the other. The department puts forward cases for promotion based on merit and achievement through a well-developed promotion process, with no caps on promotion numbers. Candidates are encouraged, after consultation with their HOS and/or HOD, to submit their CV to a panel of professors, who consider applications, give advice and appoint a mentor to develop the case. The case is submitted to a Dean's committee and then to a Provost's committee for ratification. Through the promotion framework, Lecturers (Teaching) can progress to Associate Professor (Teaching) and Professor (Teaching). A departmental promotions workshop, organised by the departmental EDI committee (2016), significantly increased the number of staff who felt the promotion criteria were clear. These workshops were rolled out at Faculty level and are organised annually by MAPS to inform all academic staff about the promotions process. There have been 35 promotions since the start of 2013/14 academic year. Most female academics were probationary lecturers or at professorial level already, but the remaining gained promotions to Professor (**Holt** 2018) and Associate Professor (**Clarke** 2019; **Holt** 2013).

### 2.3. Research Students

UCL Chemistry has maintained a high number of students registered for PhD/EngD degrees (on 3 or 4 year courses; typically 200 students including those writing up). Funding for studentships was achieved via CASE, DTP, departmental and 'impact' studentships, the EPSRC CDT in Molecular Modelling and Materials Science (M3S), other aligned CDTs, strategic collaboration with international centres of excellence (A\*STAR, Singapore; JAIST, Japan), EU, charity, Wellcome Trust, and direct industry awards.

The department has a yearly intake of ~160 (234 in 2020) into its UG degree programmes, with student A-level scores averaging AAA or better. Of the 614 current UGs 256 are studying for MSci degrees and 358 a BSc. These students represent 32 different countries. Over the past 5 years, the F/M ratio of UG students has averaged 52.3% (national average on physical science courses 40.2%). The department also plays a pivotal part in the teaching of the Natural Sciences BSc/MSci degrees (162 UGs). Recruitment of UGs underpins the department's financial position and provides exceptionally well-trained graduates for the research school. A success is the department's PG school, which now has 187 students on MSc/MRes courses (Table 2), including an increase in %F (49% 2019; 29% in 2014). There are 6 masters courses (MSc/MRes) in the department covering materials chemistry, organic chemistry and drug discovery, applied analytical chemistry, molecular modelling and chemical research. The department admitted 64 new PhD/EngD students over the 2019/20 academic year. The EPSRC M3S CDT is developing into a self-sustained centre maintaining an intake beyond the funded period through "impact PhD" studentships, CSC scholarships and A\*STAR studentships, as well as a MSc course in Molecular Modelling. The EngD students have an industrial sponsor and spend ~6 months in industry (>40 companies). The department has played a leading role in two flagship PhD programmes: the Wellcome Trust 4-Year PhD Programme in Structural, Computational and Chemical Biology (co-director **Tabor**) and the BBSRC London Interdisciplinary Doctoral Programme (LIDo), fostering interdisciplinary research between Chemistry and Life Sciences. The department also enjoyed success in several recently funded collaborative CDTs, e.g. **Hailes** Co-I on "Transformative Pharmaceutical Technologies" with University of Nottingham and **Thornton** Co-I on "Advanced Characterisation of Materials" with LCN and Imperial College. The newly funded Wellcome Trust Optical Biology PhD programme (2020–2029) includes supervisors from Chemistry (**Baker, Fielding, Tabor**).



**Table 2: Research student FTE, by academic year**

	2013/14	2014/15	2015/16	2016/17	2017/18	2018/19	2019/20
PhD/EngD	166	179	189	174	162	172	169
MSc	27	37	43	44	110	106	162
MRes	16	21	23	22	25	26	25
<b>Total PG</b>	<b>209</b>	<b>237</b>	<b>255</b>	<b>240</b>	<b>297</b>	<b>304</b>	<b>356</b>

The current PhD/EngD students come from 17 countries (5 from outside the EU). The students are attracted to UCL by its international reputation, current students, Open Days, a significant web presence, active departmental Twitter account and a dedicated full-time administrator. Guidelines are provided to academics for advertising PhD positions and interviewing (ensuring students of high quality and EDI is taken into consideration). PhD submission rates within a year after end of funding remain high (>95%). In the past few years there has been a shift to increasing numbers of 4-year funded studentships rather than 3-years. The Graduate Tutor (**Anderson**) monitors PG progression. PhD students are initially registered for an MPhil degree and transfer to full PhD registration during their second year. A secondary supervisor is assigned to each student, who participates in assessment milestones and provides support. These milestones include: in 1<sup>st</sup> year a presentation introducing their research topic and a 20-page report, assessed by the secondary supervisor and discussed with the student during a viva. In 2<sup>nd</sup> year, a 40-page report including a timetable for PhD completion and an assessment of the student's progress by the primary supervisor, which is reviewed by a panel. This culminates in a viva to ratify an upgrade from MPhil to PhD. In the case of failure, the student is permitted a second attempt to upgrade 18-24 months from their start date. During 2<sup>nd</sup> year students give a poster presentation and in 3<sup>rd</sup> year a 25-minute seminar. EngD students follow these requirements but have a range of additional training since they follow an MRes degree in their 1<sup>st</sup> year. These students complete lecture courses, a dissertation, poster presentations, industrial days, schools events and can take training from the Project Management Institute (receiving the Certificate of Project Management). Some EngD students are employed by their sponsor after graduation (~30%). All PhD/EngD students are able to contribute to teaching (e.g. demonstrating) and outreach events.

UCL Graduate School provides further support and training opportunities for students, as well as maintaining the electronic Research Student Log, which all PG students must complete at regular points through their degree. This is monitored by supervisors and records scheduled formal supervisory meetings, academic and discipline-specific key skills obtained. Through this log PG students can plan, assess, and monitor their progress and manage their continuing professional development for their future career. The department introduced a successful thesis-writing workshop (2019) and students obtain support for job applications (application forms, CVs) from supervisors and UCL Careers Service, as well as from graduate school courses on career planning. Career events are provided both departmentally and faculty-wide. Students log attendance for non-structured activities including conferences, external training, teaching and extracurricular activities.

#### 2.4. Equality and Diversity

UCL Chemistry has an excellent record of supporting all members of the department with systems in place that encourage a family-friendly, inclusive and supportive culture; this culture was recognised by the department being awarded a Silver Athena Swan award (April 2020). The HOD actively promotes candidates for institutional/external awards, career and leadership development programs with input from MWG. The department provides financial support for in-house training, e.g. unconscious bias and improved awareness of harassment. It is mandatory for staff to attend "Where do you draw the line?" training (a harassment prevention approach developed by UCL, Universities of Cambridge, Manchester and Oxford), which is also being offered to PhD students. The department is ensuring that the equality culture is owned by all in the department, which is led by the active EDI committee which has representatives from all staff groups (academic, technical, professional services, research associates) as well as students (UG, Masters, PhD). The HOD is Co-Chair of the EDI committee, ensuring that all actions have full departmental support. The department has improved its representation of diversity during a recent redesign of the departmental webpage. In July 2019, Dr Sean McWhinnie (Oxford Research & Policy) provided guidance on data presentation and instigated surveys and focus groups for staff and students. The surveys are updated and run annually to monitor the impact of actions and inform our strategy to achieve equality. The department now has

a LBGTQ+ Champion and “Out@UCL” and “Friends of Out@UCL” stickers are “opt out” rather than “opt in” for all staff. LBGTQ+ visibility lanyards are commonly worn by staff and we have reviewed our staff handbook to include what we do to support the LBGTQ+ community. “Out@UCL” training is available for staff and some departmental toilets have been refurbished to be gender neutral. To further support staff and students we have a Student Support Officer and a Wellbeing Champion within the department and three staff were trained as mental health first aiders. We also have a BAME Champion and have recently agreed departmental Race Pledges through a faculty initiative aligning to the 2020-2023 Faculty strategic EDI plan and the 2020-2021 UCL EDI strategy. These pledges represent a basic level commitment to advance race equity by addressing local specific challenges. The department’s mentoring scheme, a review of student recruitment practices to increase diversity across our student body, recruitment of a BAME Champion and proactively targeting BAME researchers for future academic positions are examples of initiatives here.

UCL Chemistry has established a PDRA Support Network, a LBGTQ+ Network and a PhD Network. These networks enhance general wellbeing via initiatives such as: coffee mornings, lunches, careers advice, external speakers of relevance and specialised events (e.g. LinkedIn workshop, CV advice service, thesis writing workshop). We recognise that one of the significant attrition points in the academic career trajectory for chemistry is the transition from PDRA to lecturer. Consequently, we have appointed a PDRA Tutor in addition to the network to support PDRAs in the department. Staff support is also available from UCL’s Employee Assistance Programme and for students from Student Support and Wellbeing. We actively promote UCL’s Report to Support, a tool to report bullying, harassment and sexual misconduct.

Established policies are in place to support career breaks. The department provides extra funds for staff on maternity leave, including PDRA funding to provide support in overseeing research groups and a sabbatical upon returning to work. Support is provided for paternity leave and two male academics have recently benefitted from shared parental leave; if required PDRA funding is provided to oversee the research group during the leave. An active university wide parents and carers together (PACT) network provides support for new parents and within the department 50% of new parents (83% new mothers) have attended PACT events since 2014. Departmental meetings are held within core hours of 10am-4pm to facilitate carer responsibilities. All staff can work flexible hours as required, and ~50% of staff work offsite ~1 day per week. The department has a local “Work from Home” code that clearly defines expectations and support. In addition, staff can work away from UCL for extended periods, particularly valuable for staff using central facilities for research. Cover for supervision of students and safety whilst staff are offsite is coordinated within each section. For staff and students based at Harwell we have set up a UCL@Harwell network and organised a staff away day there. Our new “Harwell Integration” project (budget £6K p.a.) covers travel costs for staff and students to improve integration between the two sites.

UCL Chemistry has actively sought to reward and support all staff, and has a particularly strong record in the promotion of women in science. **Carmalt, Davies, Fielding, Holt** and **SLPrice** have been active nationally at “Women in Science” events (RSC, IOP) and **Haynes** has developed a “Women in Supramolecular Chemistry” mentoring network. The department has recruited 7 female lecturers in the past few years following positive action through the recruitment process. Here, the HOD or HOS personally lead searches to identify applicants and target female researchers. Job specifications and shortlisting criteria have been developed to be as general as possible. More women have been appointed to senior roles in the department/UCL including HOD, HOS, DOR and MAPS faculty Vice Dean (Education). All interview panel members have unconscious bias training and all panels are gender mixed (at least 33% female). Staff are encouraged to attend conferences, most funded via grants, although additional funds at Faculty level are available for staff with caring responsibilities (MAPS Caring Fund). Support towards travel for PhD students is provided by the department and researchers also apply for funding from the RSC. For the past 3 years the department has encouraged and funded PDRAs who want to attend the RSC Joliot-Curie Conference, an event supporting the aspirations of early career researchers. Female PDRAs have been encouraged to attend but funding is open to all.

Outputs for REF were selected from submissions from individual staff, by a group of senior staff (all received training in EDI) including members of MWG, DOR and the Research Committee. The draft and final selection of outputs were circulated to all academic staff in the department for comment and input. A panel with equal gender balance reviewed the provisional output list, were provided with

data, including the F:M ratio, %Early Career and %BAME (for staff vs. output) and ensured that there was no unconscious bias applied to the output selection (Table 3).

**Table 3: Summary of staff and output selections against 3 characteristics**

Characteristic	Category	Proportions	
		HESA 3 staff FTE	Selected outputs
Gender	Male	76.94%	77.48%
	Female	23.48%	22.52%
Ethnicity	White	84.80%	82.12%
	BAME	10.13%	13.91%
Age	Under 45	49.23%	52.98%
	45 or above	51.13%	47.01%

Extra support was arranged for remote working through the Covid-19 pandemic. Departmental meetings were held virtually, along with research seminars. Weekly staff meetings, chaired by HOD, were held to keep everyone informed of developments and maintain a connected department. Guidance for working from home effectively and looking after mental health were provided regularly as were funds to purchase home-working equipment. Line managers had regular contact with staff to discuss their well-being, workload and working arrangements, suggesting refocused activities and flexible working patterns. Academic staff provided support to PhD students and PDRAs through 1:1 and group virtual meetings. A 'Covid-19 Measures' section on the PhD internal webpage provided information and a communication channel to the Graduate Tutor. Every effort was made to ensure that PhD research could continue remotely with students developing new skills applicable to future research. RCUK funded students could receive up to 6-months paid extensions and UCL provided 3-month extensions for all funded PhD students in their final year with a possible 3-months additional funding on a case-by-case basis; the UCL hardship fund was increased to £3K per individual. UG teaching moved online and innovative lab kits and data analysis/computational research projects were developed. The department was chosen as a pilot for re-opening (June 2020), and the Covid safety working arrangements (strict social distancing, online access monitoring, occupancy numbers) was held up as an exemplar across UCL and documents/arrangements were shared with other departments.

### 3. Income, infrastructure and facilities

#### 3.1. Income

The department receives extensive grant funding. EPSRC income over the REF period for research projects remained high (£45M). Based on previous strategic reviews, we have diversified grant income with a markedly greater proportion now coming from non-EPSRC sources (from 2013/14 to 2019/2020) including EU government bodies (£1.56M to £14.6M), MRC (£186K to £6.7M), BBSRC (£3M), InnovateUK and Knowledge Transfer Partnerships (£1.9M), Royal Society (£2.5M), Leverhulme (£2.2M), and UK industry including studentships (£5.6M). Total grants administered in the department has increased from 200 (2012) to >400 (2019). The significant uplift in EU funding was achieved through award of 2 ERC consolidator grants, 2 ERC starting grants, an ERC Advanced Grant, H2020 grants and 8 Marie Curie fellowships over the REF period. Funding increases also included co-investigators on large EPSRC grants, e.g. **McMillan, Parkin, Hailes** and **Catlow** (>£4.5M). Additional grants awarded included: Leverhulme (21 grants); Wellcome Trust (4 grants); MRC (9 grants); BBSRC (13 grants); NERC (3 grants and a fellowship) and the European Commission (48 grants) that contributed a further £33.5M of support. These grants support the work of ~70 PDRAs at any one time as well as 5 senior research fellows. The department has ~50 companies, across a wide cross-section of UK industry, who sponsor PhD studentships. Research expenditure on grants over the REF period was >£60.3M (up from ~£55M for REF2014), dominated by research council, charity, EU and industrial funding. Awarded funding for central facilities usage included Diamond (£6.6M), ESRF (£219K), ISIS (£3.4M) and ILL (£932K), with a total of > £11.5M.

Future departmental strategy will continue the policies that have developed our substantial funding portfolio, including sabbatical leave, extensive internal review of grants, enhancing industry links and further collaborative applications with other institutions (especially at programme grant level). UCL/MAPS faculty has invested >£11M in chemistry/IMD equipment and infrastructure over

the REF period and is committed to future improvements. Plans involve further developing chemistry's presence at the Harwell Campus, UCL East and FI.

### 3.2. Infrastructure

The Chemistry department currently operates over 4 sites. The main site, the Christopher Ingold Building (CIB; 9000 m<sup>2</sup>), houses all UG teaching and the majority of the department. A smaller site exists in the Kathleen Lonsdale building (KLB; 800 m<sup>2</sup>) where computational, synthetic organic, radiochemistry and flow chemistry take place. IMD is based in the Roberts building and comprises a core team of academics and researchers focussing on delivering the next generation of advanced materials. The department led a successful EPSRC bid for a research facility for catalytic science, located within the research complex at Harwell (2013-2018) and played a key role in the renewal (2018-2023) with staff located at Harwell. UCL Chemistry (**Palgrave**) was also a partner in the EPSRC National XPS facility with the main laboratory based at Harwell. The department is a major user of central facilities, particularly at Diamond. It has joint laboratories in the LCN, especially for PCCP measurements.

The department has seen substantial investment in infrastructure since 2014. To underpin its research goals, the department has sought to provide the best laboratory space, state-of-the-art instrumentation, and a dedicated support infrastructure of workshops, glassblowers and instrument specialists. The 3<sup>rd</sup> floor synthetic laboratories, which house the IM section, have been refurbished and new low velocity fumehoods (£1M) have been fitted. A new laboratory dedicated to initiatives in battery research was part of the refurbishment and supports research from **Parkin, Carmalt, Xu and Darr**. Laboratory space in the Roberts Building was refurbished to house IMD (£1M). UCL also provided significant investment of £3.5M to establish a new UCL Laser Science Centre in the basement of the CIB (350 m<sup>2</sup>) providing a focal point for inter-departmental research and to foster interdisciplinary collaborations. The basement lab space was selected due to low vibrations and the environment has been specified to a very high standard (temperature control  $\pm 0.5$  °C). This investment is enhanced by an EPSRC equipment grant bid (**Fielding**, £1.4M) to provide state-of-the-art femtosecond lasers. The new Laser laboratories provide space for chemistry groups (**Fielding, Clarke, Volpe, Ingle**) and a group from Physics. The GMP laboratory was developed (£3.4M) as part of a wider refurbishment of the KLB to support the latest techniques for medical imaging of diseases, such as cancer and dementia, and production of PET tracers to detect and map how a disease progresses (**Årstad**), currently supporting 5 hospitals/medical schools.

In 2019, the departmental mechanical workshop was merged with the Department of Mechanical Engineering to provide an enhanced service with state-of-the-art equipment. Two full-time technicians from Chemistry work in the facility and provide advice, guidance, and a bespoke service for equipment manufacture. The department's glassblower provides a high standard of work, consultation and design services and an electrical support group (3 technicians) provides routine/preventative maintenance as well as construction of equipment. Close interaction between academic staff and the workshops means that apparatus can be quickly optimised or upgraded. In computational science, 6 local computer clusters are maintained by 3 support officers. In computing, £4.5M was invested in hosting the national MICHAEL Supercomputer (**Scanlon**) and the departmental cluster, used by students for teaching and research projects, was upgraded (£100K). The department has taken a leading role in reducing our environmental footprint and fully adopting a "green agenda". This activity, coordinated by **Sella**, is part of UCL's Carbon Accountability Scheme pilot and LEAF (Lab Efficiency Assessment Framework) is reviewing laboratories to improve sustainability. All windows (~600) in the CIB were replaced (2016, £1.2M) due to poor performance of the buildings original single glazed windows. The new windows are comprised of self-cleaning glass, Pilkington Activ<sup>TM</sup>, developed from underpinning research in UCL Chemistry (**Parkin**). The new windows have resulted in a reduction in maintenance and a significant decrease in heat loss. Redundant corridors on the 2<sup>nd</sup>/3<sup>rd</sup> floors have been converted into student breakout spaces to enhance interaction between PG students; the UG common room was also refurbished.

### 3.3. Facilities

Departmental facilities have been significantly enhanced during the REF period. The UCL budget is organised by faculties, with each given a target for its contribution to central costs. UCL chemistry has hit (or exceeded) its targets each year resulting in significant inward investment in new open access instrumentation. This investment allows the department to act as an equipment hub for other

UCL departments and multiple external users including other universities, hospitals and industry. For example, external groups using NMR: 18 UCL departments, 12 industrial users/other universities; mass spectrometry: 8 UCL departments; TEM/SEM: 6 UCL departments, 4 other universities; XRD: 11 UCL departments, 2 other universities; Figure 2). The department now has 8 mass spectrometers, 5 high field NMR instruments, 3 SEMs, 3 TEMs, 2 XPS, 2 Raman instruments, 7 powder diffractometers and 1 single crystal diffractometer. EPSRC equipment bid success allowed for the purchase of a 700 MHz broadband cryoprobe and high-field NMR spectrometer (**Aliev**, £1M), used in a range of studies, including the origin of life (**Powner**), material precursors (**Carmalt, Knapp, Parkin**), polymers (**Schroeder**) and catalysis (**Bakewell**) and other NMR instrumentation. UCL RCIF funding provided upgrades to mass spectroscopy facilities (High Resolution UPLC-Q-Exactive Orbitrap Mass Spectrometer £336K), the Stoe Cu diffractometer (£150K) and XPS (£18K), an optical microscope (£80K), battery testing facilities (£100K) and a high-speed centrifuge (£42K).

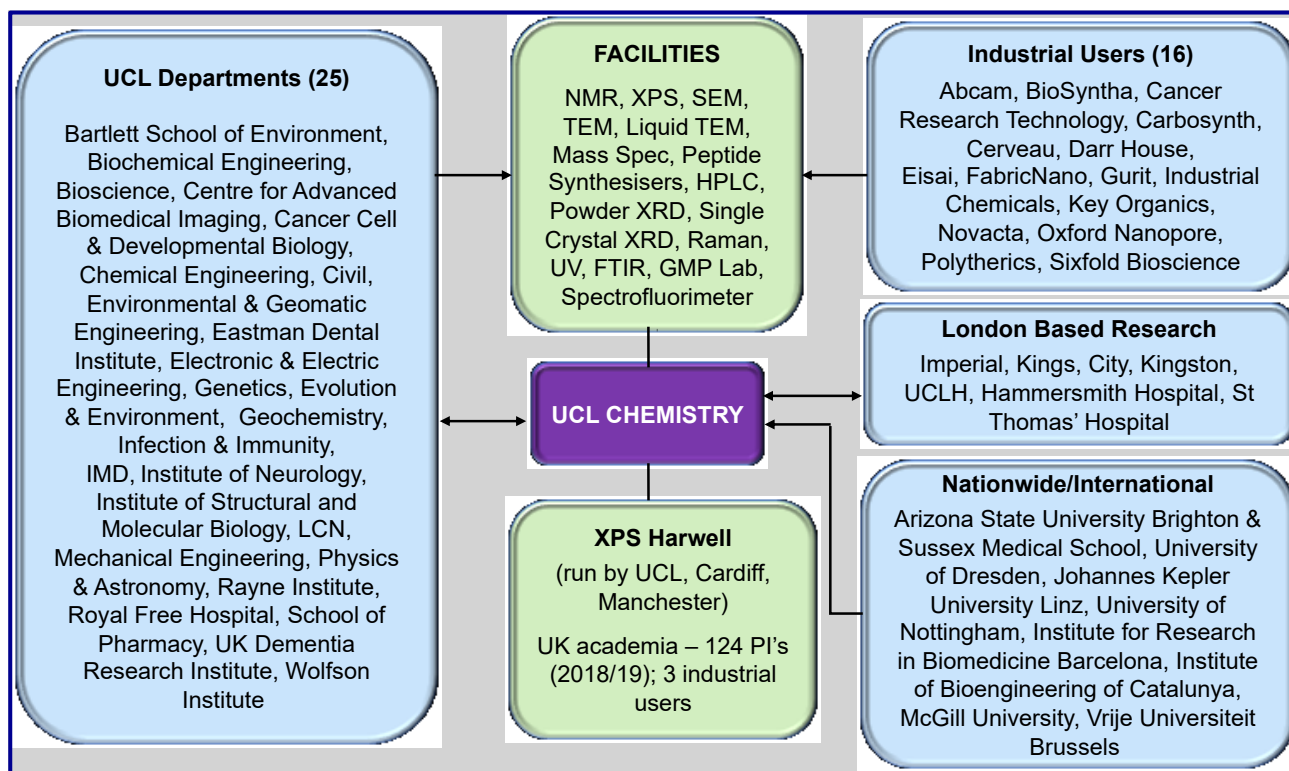


Figure 2. Selection of external users of facilities and collaborations.

UCL Chemistry has also developed the EPSRC/Jeol Centre of Liquid Phase Electron Microscopy with the world's first liquid TEM capable of looking at the formation and evolution of structures in flowing liquids, including soft materials, cells and catalytic nanoparticles, funded by EPSRC (**Battaglia**). XPS facilities have been upgraded via the purchase of a Photoelectron Spectrometer (EPSRC £780K, **Palgrave**) to join our existing UCL-funded multi-user XPS facility, which has >200 users. The new capabilities of the PES instrument (ultraviolet PES, simultaneous angle resolved data collection and *in situ* sample heating and cooling) has significantly extended the breadth and depth of science we support. These capabilities have also been expanded with the national XPS facilities at Harwell (£3.2M), of which UCL is a partner (**Palgrave**), enabling further investigation of material composition. These facilities have also been enhanced with the recent purchase of an FT-Raman (£100K), a Spectrofluorometer with Near-Infrared (£75K) and a X-ray Fluorescence Spectrometer (£55K).

The department covers maintenance contracts on selected equipment with the rest maintained by a team of in-house technicians. These technicians train the researchers and the ethos is that all researchers should acquire their own data from instruments, overseen by lab managers. Training involves problem classes and hands-on sessions. Support for learning data analysis, e.g. XPS, is available via online in-house courses, which researchers can work through independently. Technicians are active in research and regularly co-author papers. The aim is for facilities to break even on a cost basis and be efficient on instrument usage, deriving maximum value from our public investment. A key aim is to support all research work and no academic has been prevented from

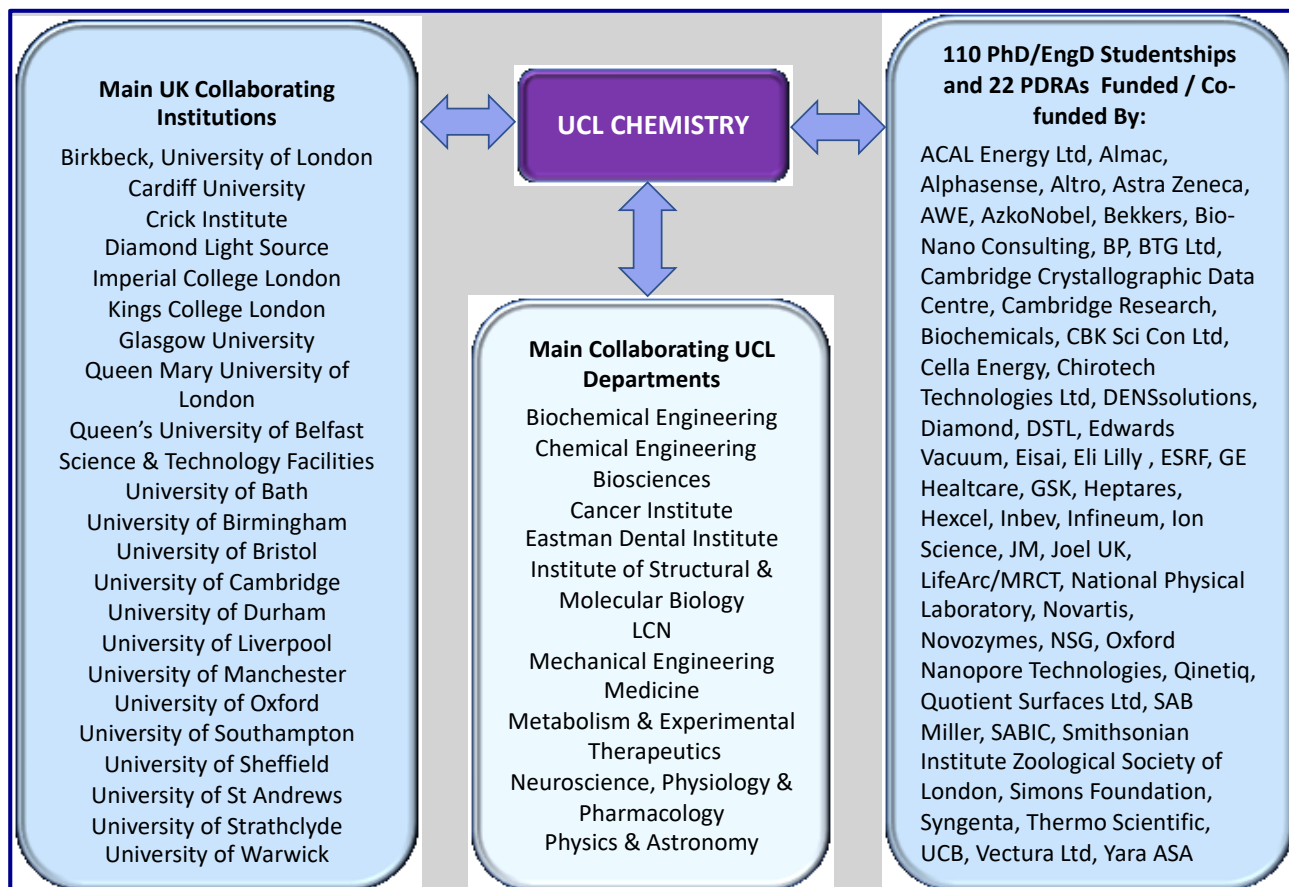
doing research for lack of funds. Staff without external funding are provided with advice on grant proposals and financial support for consumables and facilities access.

The department uses a system to track chemicals in the department (Quartz), which is a web-based labelling system which reduces duplication, and enhances sharing, thereby reducing waste. UCL has outstanding library facilities with online access to >1900 chemistry journals and makes extensive use of the British Library (5 minutes from the department). The department also funds Bibliotech ebooks, providing online access to a range of Chemistry textbooks, which are extremely popular with students and have been vital during Covid-19 remote learning.

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

##### 4.1. Collaborations

The department strongly supports collaboration, which is enhanced through the new departmental research themes. Collaborations are developed through Away Days, industrial days, sectional meetings, workshops and networking events. Industrial days provide opportunities for staff to explore industrial connections with invited companies. These showcase our research with presentations from academics and industry, poster presentations, idea pitching and developing possible areas for collaborations. External researchers from academia and industry regularly use our facilities and departmental staff are involved in collaborations with ~25 other UCL departments (Figure 2). Interaction with UCL Engineering has increased over the REF period which led to >240 publications, 25 joint research grants (>£25M). Departmental research has been well funded by industry, including >100 PhD studentships and 22 PDRAs from ~50 different companies. There are also substantial links with other UK institutions/industry (50) and international institutions (145) through collaborative projects, programme and EU grants (Figure 3). In total, 762 different national and international partner universities appear in joint publications in the review period, with, for example 1200 papers with other UK institutions, 419 with US institutions, 133 with France, 170 with Germany and >100 with industrial partners. 72.7% of all our publications have at least one international co-author.



*Figure 3. Key collaborations including industrially funded projects.*

In addition to our key role in the UK Catalysis Hub and the National XPS centre at Harwell, the department plays a lead role in the TYC, one of the largest assemblies of computational chemists,

physicists and materials scientists in the world (>80 active academic groups in the London area). The TYC supports an extensive programme of conferences, visits and seminars, as well as providing a valuable platform for community engagement. **Battaglia** and **Tabor** are members of the UCL@Crick Academic board. In addition, **Scanlon** is UCL PI on 3 large FI consortium grants on energy storage (>£4.8M); and **Coveney** is the coordinator of 3 EU grants (>£3M UCL component). **Powner** is a PI in the Simons Collaboration on the Origins of Life, aiming to advance understanding of the processes that led to the emergence of life. The collaboration comprises investigators in diverse fields from across the world, and PDRAs chosen through an annual competition. This scheme has funded 6 PhD students and 5 PDRAs in **Powner's** group, and a further 2 studentships have been funded through the Volkswagen Stiftung, "Life programme". OCCB section staff are involved in a collaboration in Yamaguchi, Japan involving joint research projects and visits. **Tabor** also leads on extensive collaborations through the CRUK-funded City of London Major Centre and **Volpe** organises the UCL Soft Matter Network (>80 PI's).

UCL Chemistry staff have played leading roles both in industry and the legal field. **Slater** and **Blackman** held RS-industry fellowships and **Catlow**, **Beale**, **Sankar** and **Schroeder** play a lead role with JM collaborations and, for example, arranged a UCL-JM industry day, covering green chemistry, catalysis, energy and healthcare. **Scanlon** is the Director of the AWE-UCL Centre for Computational Materials Science, which fosters connections between UCL and AWE through funded PhD studentships and for UG students for 8-week summer projects on materials chemistry issues of interest to AWE. **Cockcroft** has been an expert witness in pharmaceutical patent disputes for law firms in USA, worth ~\$100m to the winning side and potential impact on drug sales. **Clarke** and **Schroeder** are UCL Chemistry representatives in the Centre of Advanced Materials for Integrated Energy Systems, a £2.1M EPSRC network between the universities of Cambridge, Newcastle, Queen Mary and UCL; workshops in London have provided PhD students with a platform to promote their research and introduce them to grant writing, fellowship schemes and seed funding. Staff in the department also contribute to chemistry in developing countries. **Darr** co-founded a networking charity UP-SIGN (UK-Pakistan Science Innovation Global Network) to address the economic and social challenges of Pakistan, coordinating academics and professionals from both countries. **Catlow** played a leading role in establishing a materials modelling centre in South Africa. The M3S EngD researchers led in the establishment of a local computational research group at the Kwame Nkrumah University of Science and Technology in Ghana, via multiple visits, delivering a series of lectures/workshops and working closely with local researchers to implement the techniques into their projects. Overall, UCL chemistry staff have >150 international research collaborations and use central facilities in ~15 countries, especially for diffraction (NIST, Oakridge, ILL, ESRF) and large laser usage.

Research outputs have been published on departmental and college websites, video and podcast, and through television, radio and newspapers. **Sella**, the department's publicity coordinator, champions UCL Chemistry's media exposure (Section 4.2). Examples of research covered in the media include **Carmalt/Parkin's** work on superhydrophobic materials (published in *Science*), **Powner's** work on the origins of life (published in *Nature*), **Coveney's** modelling of HIV-protease viral sequence to predict personal medicine (published in *Journal of Chemical Theory and Computation*) and work on clay composites (published in *Advanced Materials*), and **Rowley's** work on CFC's (published in *PCCP*).

#### 4.2. Contribution to the Research Base, Economy and Society

UCL chemistry staff have given >1100 invited lectures over the assessment period in >37 different countries and >100 plenary/keynote lectures, including **Parkin** and **Davies** at eMRS in France, **Cora** at ZMPC2015 in Japan, **Salzmann** at XXIII IUCr International Conference in Canada and **Fielding** at 7<sup>th</sup> EuChMS Chemistry Congress in USA. Staff have been on the advisory boards and organising committees for >120 international conferences/workshops. They are also editors/board members for >30 international journals, including *J. Mater. Chem.*, *J. Peptide Science*, *Faraday Trans.* and *Crystal Growth & Design*, and **Gervasio** and **Woodley** have both edited books. **Cora** was a contributor to quality assessment of Italian Universities (equivalent to REF) in 2017. Furthermore, 10 staff currently hold visiting professorships, for example **Coveney** holds a Chair by Special Election at University of Amsterdam (30 such visiting professorships held by chemistry academics over the REF period).

Chemistry staff have played a leading role in examining >300 UK PhD theses and 100 international theses in >15 different countries during the REF period. They have also refereed proposals for >30 international research councils and charities, including the US National Science Foundation; US

Department of Energy; ESRF; Dutch Research Organisation; Finland Academy of Science; Irish Research Council; New Zealand Marsden grants; Russian Research Council; European – H2020, ERC consolidator, Marie Curie and ITN programme; and the US-Israel Science and Technology Foundation. Over 30 staff in the department have refereed for EPSRC in the last year as college members and referee for other grant funding bodies including MRC, BBSRC, NERC, Wellcome Trust, Leverhulme Trust, Royal Society and UKRI fellowships.

Staff contribute directly to UK learned societies, including **Fielding** (RSC Council and Chair of RSC Publishing Board 2012-16), **SLPrice** and **Holt** (RSC Faraday Council (2012-15 and 2015-18)), **Caruana** (RSC Analytical Division Council), **Tabor** (Chair of the RSC Protein and Peptide Science Group), and **Davies** (RSC Materials Chemistry Council). Departmental staff also sit on SCI, IOP and IOM committees. **Parkin**, **SLPrice**, **Volpe** and **Sankar** are evaluators for Royal Society Newton fellowships; **Carmalt** chairs the Ramsay Fellowship panel and was a jury member of UK Blavatnik Awards; **Bell** chairs the British Zeolite Association and the Structure Commission of the International Zeolite Association and **Sheppard** was Chair of SCI Young Chemists panel (2014). **Tabor** and **Carmalt** currently serve on RSC division awards committees.

Chemistry department staff were awarded >20 national and international medals and awards, including 9 individual RSC awards (Table 4). **Chudasama** was highlighted in the Forbes List in Science and CNN News as a future leader in chemistry, while **Thornton** received a Royal Society Wolfson Research Merit Award. **Coveney**, **McMillan**, **SLPrice** and **Parkin** were all elected as Members of the Academia Europea. **SLPrice** was elected Fellow of the Royal Society in recognition of her outstanding contributions in the development of quantum mechanics to quantify the forces between molecules and their application in computing the structures and properties of organic solids. Fifteen academic staff (**Beale**, **Carmalt**, **Caddick**, **Catlow**, **Coveney**, **Howorka**, **Parkin**, **Price**, **Marson**, **McMillan**, **Salzmann**, **Scanlon**, **Thornton**, **Wills**, **Worth**) are listed in the PLoS databases of the 100,000 most cited researchers (<https://doi.org/10.1371/journal.pbio.3000384>).

Chemistry staff also play a major role in shaping government policy and in administration of key initiatives/evaluations. **Catlow** was elected Vice President and Foreign Secretary of the Royal Society in 2016 and Vice-President European Academies, Science Advisory Council Co-Chair, Inter-Academy Partnership – Policy. **Catlow** was also a Member of the STFC panel developing the strategy for UK participation in X-FEL science and Chair of the Science Advisory Committee for the ISIS UK spallation neutron source. **Coveney** is a member of the Advisory Council for the Institute of Advanced Study and a Member of Scientific Advisory Board for the Hartree Centre. **Coveney** also contributed to multiple strategy documents in HPC for the European Union, leading to expanded funding in HPC and creation of a new funding agency EuroHPC. This was enhanced by **Coveney** being co-author of the UKRI Science Case for UK Supercomputing and a Member of the UK Government E-Infrastructure Leadership Council (2012-17). **Slater** was a member of the e-infrastructure advisory panel to enable recommendations for investment into computer hardware/software and **Woodley**, with the UK Materials Modelling Sector, co-authored a White Paper in 2019 for Exascale Supercomputing. **Woodley** is now leading UKRI's MMM Design and Development Working Group as part of the Excalibur Project that aims to ensure the UK is ready to exploit the next generation of supercomputers. **Gervasio** is Director of the JC Maxwell CECAM node dedicated to the promotion of fundamental research on advanced computational methods. **Hailes** helped develop strategy for UK Chemical Biology via RSC Chemical Biology Interface Division and **Powner** is an Executive Council Member, International Society for the Study of the Origins of Life, which sets overall Society policies. **McMillan** was on the Physical Science and Engineering Advisory Panel for STFC (2012-2017) while **Beale** is a member of the STFC panel advising UKRI infrastructures road map. **Salzmann** was Chair of molecular spectroscopy user group at ISIS (2015-2018) and **Sankar** is on the Scientific advisory council for the ESRF.

Staff have also been on the advisory panels for other UK universities including **Catlow** for a review of science departments at Durham University (2015) and **Fielding** on the Cambridge University Chemistry Department Scientific Advisory Panel (2019), the External Advisory Board for School of Chemistry, University of Cardiff (2017) and Disciplinary Reviewer for University College Cork Research Quality Review (2014-15). **Holt** was external peer for the Faculty of Natural and Mathematical Sciences at Kings College London while **Tabor** was on the 2019 Oxford Recognition of Distinction Committee. In addition, **Holt** is involved with assessment of chemistry degree programme quality as part of the RSC Committee for Accreditation; **Wills** was a committee member of RSC Educational Council (2016-2019) and **Lewis** was a member of RSC Education Division



reviewing school examination provision (2014), is a member of RSC SE Regional Steering committee and contributed to the Heads of Chemistry UK initiatives on recruitment with **Carmalt**. **Chudasama** ran a Translational Skills training event for PhD students (2017) in London, which included training in presentation skills, science communication, IP and technology transfer.

**Table 4: Summary of staff awards and prizes:**

Royal Society of Chemistry Awards & Prizes		
Name	Prize	Year
Scanlon	Harrison-Meldola Medal	2015
Battaglia	McBain Medal	2015
SLPrice	Interdisciplinary Prize	2015
Parkin	Tilden Prize	2016
Fielding	Award for Service	2017
Powner	Harrison-Meldola Medal	2019
Carmalt	Applied Inorganic Chemistry Award	2019
Regoutz	Joseph Black Award	2020
Catlow	Faraday Lectureship Prize	2020
Other Prizes or awards		
Parkin	Royal Society Armourers & Brasiers' Company Prize	2014
Thornton	John Yarwood Medal	2014
SDPrice	SASP Schrodinger Medal	2014
Catlow	Gerhard Ertl Prize Lecture	2014
Thornton	Tabor Medal	2015
Parkin	IOM <sup>3</sup> Griffith medal	2015
Powner	Bürgentstock JPS Fellow	2015
Caruana	Martin Fleischmann Lecture	2015
Blackman	PW Allen award	2016
Chudasama	GSK Emerging Academic	2017
Chudasama	Howard Prize Lecture	2018
Catlow	CNR Rao Prize Lecture	2020

Chemistry staff play a leading role nationally and internationally in the public understanding of science through the media, including Pint of Science (8 staff), schools lectures (18 staff) and public talks. This is championed by **Sella**, who was a member of STFC's Public Engagement panel. **Sella** has made >150 appearances on TV/radio during REF, from offering expert advice to BBC on nerve agents, poisons and plastics, contributions to CrowdScience BBC World Service and expertise on ammonium nitrate explosion, Lebanon. He also writes a monthly column in Chemistry World (>50k circulation) on the use of chemical apparatus and is on the advisory board for Cheltenham Science Festival. **Powner** also contributed to the Cheltenham Science Festival on "How Did Life Begin?" and to events such as RSC North-West Regional Organic Outreach meeting and lectures for Prince's Teaching institute. The department has displayed stands at Royal Society Summer exhibitions (2017, 2019) highlighting Smart Surfaces (**Carmalt, Parkin**), Catalysis (**Beale, Catlow**) and XPS (**Palgrave**). Since 2015, >90 schools have visited UCL Chemistry to take part in our outreach days. Contributing to the national effort, **Sella** led a team synthesising >400 L of hand sanitiser (2020), which was distributed to UCLH and care homes across London, along with unused PPE from the department, to help address shortages in the early weeks of the Covid-19 crisis. Finally, we were delighted with the news that **Catlow** received a Knighthood in the 2020 Queen's birthday honours for services to leadership in science and research.