Institution: University of Leeds

Unit of Assessment: 8 (Chemistry)

1. Unit context and structure, research and impact strategy

The School of Chemistry (SoC) at the University of Leeds (UoL) is a major UK chemistry department conducting a wide spectrum of fundamental and applied research. The School's REF2014 strategy included: recruiting high-flying researchers at all academic levels (12 new positions, £2.2M investment); continued excellence in winning individual research fellowships (10 major fellowships since 2014); increasing large research grant income (14 grants >£1M); investment in research facilities (£4.1M); and bringing its research through to industrial exploitation (7 operating spin-out companies). This strategy aligns closely with that of the UoL (see REF5a). Since 2014, staff in the SoC have published 1249 peer-reviewed papers (>19,600 citations) and 11 patents.

Research is structured into five sections which cut across the traditional chemistry divisions (Inorganic, Organic and Physical):

- *Atmospheric and Planetary Chemistry* (**APC**)
- *Chemical Biology and Medicinal Chemistry* (**CBMC**)
- *Computational Chemistry and Chemical Physics* (**CCCP**)
- *Crystallisation and Directed Assembly* (**CDA**)
- *Process Research and Development* (**PRD**)

These sections enjoy significant collaborations with researchers in the Faculties of Biological Sciences, Earth and Environment, Engineering and Physical Sciences, and Medicine and Health, as well as strong links with a wide variety of industries. This range of fundamental and applied research activity is one of the most distinctive features of the School.

1.1 Research Strategy

Research in the School is overseen by the Research and Innovation Committee, which is responsible for strategic planning, galvanising new research initiatives, new instrument acquisitions and management of the various research and analytical services. The five research sections are described below (names in bold type indicate staff returned within UoA8).

***Atmospheric and Planetary Chemistry*:** this section studies the entire terrestrial atmosphere from the surface to the thermosphere, as well as the atmospheres of other solar system bodies and the interstellar medium. Atmospheric science at Leeds is rated 8th in the world (Shanghai Subject Rankings 2019), and the SoC is usually in the top 3 UK Chemistry departments for NERC grant income. In several areas - field observations of tropospheric radical species, laboratory gas kinetics, chemistry of the mesosphere, and whole atmosphere global modelling - the section is world-leading. There are close collaborations with colleagues in the *Institute for Climate and Atmospheric Science* (ICAS) within the School of Earth & Environment, the Astrophysics group in the School of Physics & Astronomy, and the *Priestley International Centre for Climate* (Deputy Director: **Plane** (2016-2020)) which was created by the University in 2016 with an investment of £10M (REF5a).

APC's strength is to use the full spectrum of atmospheric chemistry research techniques. Observations include measurements of tropospheric radicals, and lidar/satellite observations of the terrestrial and Martian atmospheres. Laboratory studies include elementary reaction kinetics and photochemistry in the gas phase, aerosol formation, and heterogeneous chemistry. Theoretical work makes use of electronic structure calculations and the *Master Equation Solver for Multi Energy-well Reactions* (MESMER) to develop chemical mechanisms. Atmospheric modelling includes the *Master Chemical Mechanism* (MCM), and the *Whole Atmosphere Community Climate Model* (WACCM – a model from the US National Center for Atmospheric Research (NCAR), with substantial Leeds enhancements). The inclusion of four senior scientists from the NERC-funded *National Centre for Atmospheric Science* (NCAS) (**Blitz**, Feng, Ingham and **Whalley**) in the section provides a substantial boost to the research portfolio.

Two areas were highlighted in REF2014 for development. (1) *Interstellar and Planetary Atmospheres*. Major new laboratory programmes funded by the ERC (Advanced, Consolidator and Early career grants) and STFC to study radical reactions using laser photo-ionization coupled with time-of-flight mass spectrometry, a pulsed Laval nozzle reactor for reactions at ultra-cold temperatures, and a reactor for dissociative recombination reactions of ions. (2) *Heterogeneous chemistry***.** Substantial advances have been made through NERC and ERC funding to develop novel techniques for studying the kinetics of ultrafine aerosol formation, growth and radical uptake.

Since REF2014, two tenure-track University Academic Fellows (UAFs – see REF5a) have been appointed: **Lehman**, who has developed a highly innovative laser frequency comb instrument for high resolution spectroscopy and kinetics; and **Stone**, who specialises in experimental studies of Criegee intermediates. An important strategic addition is **Marsh**, who holds a joint position between the UoL and NCAR in Boulder, Colorado, and is a world leader in the development of whole atmosphere chemistry-climate models.

Next 5 years: The Government's Clean Air Strategy (2019) will provide significant opportunities for research in air pollution and human health, mapping well onto APC's instrumental and modelling expertise and interests in emissions controls, combustion, the hydrogen economy, and indoor air pollution. We also plan to utilise the University Farm following significant investment (£4M, REF5a) for an atmospheric field observatory, and will continue to exploit GCRF funding in climate/atmospheric science. The field of exoplanet chemistry is expanding rapidly through new observations (e.g. ALMA, James Webb Space Telescope), which we will exploit through expertise in laboratory kinetics and whole atmosphere modelling, and links with the School of Physics & Astronomy.

Chemical Biology and Medicinal Chemistry**:** this section's vision is to understand fundamental biological mechanisms and to diagnose and treat disease. CBMC's research is underpinned by expertise in synthesis of novel, diverse small molecules for drug discovery; rational drug design; protein-protein interactions; protein engineering and synthetic biology; nanoparticle diagnostics and glycoscience; and chemical proteomics. Interdisciplinary collaborations with the Faculties of Biological Sciences and Medicine & Health are fostered through the *Astbury Centre for Structural Molecular Biology* (Deputy Director: **Wilson** (2012-2018), **AS Nelson** (2018-)). There are strong synergies with the PRD section in the area of bioactive small molecule synthesis and biotechnology and the CDA section in the area of targeted molecular delivery.

Areas highlighted in REF2014 for development were: (1) *Application of diversity-oriented synthesis to the creation of libraries of lead-like molecules for pharmaceutical discovery*. **AS Nelson** led the review of all innovative chemistry within the European Lead Factory (*impact case study 4*). A spin-out company Redbrick Molecular was established to bring these new scaffolds to end-users. Major EPSRC-funded programmes have supported work on fragment and lead-oriented synthesis, and autonomous discovery of functional small molecules by activity-directed synthesis. (2) *Novel chemical probes for understanding biological mechanisms and expanding the range of druggable targets*. An EPSRC Programme Grant (**Wilson**) has delivered new experimentally-validated computational tools to predict hotspot-regions at protein-protein interfaces, alongside synthetic methods for structural proteomics. Work in chemical proteomics has been strengthened by appointment of **Wright** as a UAF. (3) *Chemical/enzymatic modification of proteins for synthetic biology and industrial biotechnology.* Two EU consortia led by **Turnbull** have developed synthetic glycobiology to re-engineer proteins for applications in diagnostics and drug delivery, while a major Industrial Biotechnology Catalyst project has delivered enzymatic methods for synthesis of glycomimetics. (4) *Expand medicinal chemistry collaborations.* The Cheney Fellowship Scheme (REF5a) has brought world-leading researchers to Leeds, enabling major international collaborations in tuberculosis drug discovery (Chibale, Cape Town; host: **Fishwick**), phenotypic screening (Waldmann, MPI; host: **AS Nelson**) and protein-protein interactions (Hall, North Carolina; host: **Wilson**). Work on blood anticoagulants has led to spin-out company Lunac Therapeutics (**Foster**) to take a drug into the clinic (£5.8M venture capital/Biomedical Catalyst funding).

Next 5 years: CBMC members provide leadership in all four *Astbury Centre* research themes: The Dynamic Interactome (**Wilson**), Enabling Tools for Biological Discovery (**Wright**, **AS Nelson**), Communication at Cell Membranes (**Turnbull**) and Host-Pathogen Interactions (**Fishwick**). Substantial investment in the Astbury BioStructure Laboratory (£17M) and Wolfson Imaging Centre (£750K) will open new opportunities for structure-based drug design, and for investigatng dynamic biological systems in living cells. Having established the Rosalind Franklin Institute (RFI) Next-Generation Chemistry theme, **AS Nelson** is now Head of High-Throughput Molecular Discovery; UoL has established a formal partnership with RFI in autonomous molecular discovery which will be supported by 2 new UAF appointments (one based at Harwell). This partnership will accelerate work on interactions of intrinsically disordered proteins through a recent £5.4M BBSRC sLoLa award (**Wilson**). We plan further major investment in mass spectrometry equipment and expertise to support our growing programmes in chemical proteomics, which will also benefit from LeedsOmics that provides opportunities for collaboration with the Alan Turing Institute. We will tackle the global challenge of antibiotic resistance in collaboration with Professor Chibale (Cape Town) who leads one of the few fully-fledged drug discovery capabilities in Africa.

***Computational Chemistry and Chemical Physics*:** this section covers research in experimental and theoretical chemical physics. On the experimental side, velocity map imaging spectrometry has continued (**Whitaker**) and new directions are 2D terahertz spectroscopy and frequency-comb spectroscopy, achieved by appointing **Burnett** and **Lehman** (primary home in APC), respectively, as part of the REF2014 strategy. On the theory side, work includes: the application of novel methods of quantum dynamics for treating a large number of quantum degrees of freedom to simulate nonadiabatic chemical dynamics and intramolecular energy transfer (**Shalashilin**); developing efficient methods of classical dynamics which greatly extend the time scales of molecular dynamics (e.g., for the terahertz spectroscopy experiments)

(**Shalashilin**); molecular collisions and quantum stereodynamics (**Miranda**); and computational biophysics (**Auer**). In 2020 the group was joined by **de Leeuw** whose group works on simulations of chemistry in condensed phases and on surfaces, often of geophysical and astrophysical significance.

Next 5 years: Experimental work on 2D THz spectroscopy will continue in close collaboration with the School of Electronic & Electrical Engineering's THz group. Computational methods of quantum dynamics will be further developed, in particular ultrafast photochemistry. Developing collaborations with medicinal and organic chemists will involve performing simulations of protein and peptide dynamics. A new femtosecond soft x-ray experiment with beam time at the DESY Synchrotron (Hamburg) will be undertaken in collaboration with the Helmholtz-Zentrum, Berlin.

***Crystallisation and Directed Assembly*:** the construction of high-performance materials with properties optimised for their function demands control of composition and structure over length scales ranging from the atomic to the macroscale, and often requires the construction of materials with hierarchical structures. CDA addresses this challenge, with expertise spanning the full breadth of the topic. Biomolecular self-assembly is a key focus of the work on soft matter systems, where injectable hybrid hydrogels offer a promising treatment of back pain and in industrially-funded work hybrid vesicles are being used for drug delivery (**Beales**). Diverse work is carried out on hard matter and organic/ inorganic systems, encompassing crystallization, nanomaterial synthesis, supramolecular assembly and crystal engineering and nanocomposites. Topics range from fundamental research into crystal nucleation (**Meldrum**), the development of new classes of functional metallosupramolecular cages with entangled topologies (**Hardie**), and the first demonstration of the use of spin-crossover compounds as room-temperature coolants (**Halcrow**), to topics with immediate industrial applications such as the development of hierarchical inorganic aerogel materials for flow chemistry (**Menzel,** collaboration William Blythe) and fusion energy applications (**Menzel**, collaboration with AWE).

The diversity of the group supports innovative research collaborations, as exemplified by a project exploiting the principles of lipid self-assembly to develop novel toxicity detection platforms within microfluidic flow systems (**AL Nelson** and **Beales**). This formed the basis of the HISENTS HORIZON 2020 project and subsequent SABYDOMA project which is working with 6 companies to bring the technology through to commercialisation.

Research is supported by several University-wide research centres and their cutting-edge analytical facilities. The new *Bragg Centre for Materials Research* promotes interdisciplinary materials research, supported by dedicated PhD studentships and new UAF appointments. The *Leeds Centre for Crystallization* (Director: **Meldrum**) brings together the internationally-leading expertise in crystallisation at the UoL. Members of CDA also collaborate closely with the iPRD, particularly in the area of flow chemistry. Research at the chemistry/biology interfaces is supported by the *Astbury Centre*, including multi-scale modelling, evolving biomolecules to control material synthesis and nanomedicine (overlap with CBMC).

The REF2014 strategy was to broaden expertise in materials chemistry, which has been achieved through 2 new UAF appointments: **Chamberlain's** research on functional nanomaterials and heterogeneous catalysis complements existing expertise in homogeneous catalysis, while **Menzel's** research is industry-facing and focuses on inorganic nanostructures and hierarchical materials. Both have built substantial groups and brought new expertise in functional inorganic material and academic and industrial collaborations to the School.

Next 5 years: The *Bragg Centre* (Section 3) is a major new initiative that will bring many new opportunities to CDA by supporting existing research and fostering new collaborations. New opportunities for materials characterisation will be provided by the new *Bragg Building* (£96M investment, REF5a), which will offer a central location for new and existing analytical facilities including electron microscopy, scanning probe microscopy, XPS and a state-of-the-art cleanroom. The new EPSRC-funded Flo-XL facility in Chemistry will facilitate *in situ* analysis of crystallisation mechanisms and the synthesis of functional materials, and create new academic and industrial collaborations. New opportunities include the PoLNET3 network arising from the EPSRC Physics-of-Life grand challenge, and application of technology developed by coupling sensing platforms to continuous production lines for managing environmental pollution, climate change and the present pandemic. Large initiatives in the context of renewable energy vectors, and CO_2 capture and storage are expected to provide major opportunities for functional inorganic materials research over the next 5 years.

***Process Research and Development*:** research at the chemistry/chemical engineering interface is delivered through the *Institute of Process Research and Development* (iPRD). This was established in 2008 as a collaborative venture with the School of Chemical and Process Engineering (SCaPE) through a £2M University investment to underpin two chair-level appointments (**Blacker**, Muller, with >30 years' combined industrial experience) and two associate professors (**Nguyen**, Bourne), in order to build on strengths within the SoC in synthesis and catalysis and within SCaPE on particle technology/processing (Muller, Bourne returned in UoA 12).

PRD performs research aimed at providing innovative, economic and sustainable solutions to problems in the fine chemicals, pharmaceutical and novel materials industries. Work in this area is facilitated by a fully operational process laboratory (Section 3) believed to be unique in the UK university sector. The group operates a balanced portfolio of basic research (RCUK- and EU-funded), translational research (Innovate UK) and client/product-specific work (contract/consultancy-funded). Engagement with industrial partners is managed through an *Industrial Club* comprising 12 companies from the UK, EU, China, India and Switzerland, with interests from pharmaceuticals to equipment manufacture.

The REF2014 strategy was to expand focus to include process intensification through continuous technologies; closer integration with particle technology; and the processing and utilisation of sustainable feedstocks. The closer integration with particle technologies proposed at REF2014 led to the establishment of the £670K AstraZeneca Centre for Manufacturability at Leeds (see Section 4 on impact; outputs currently embargoed for commercial reasons). Expertise in continuous technologies has, *inter alia*, underpinned the development of autonomous reaction optimisation technologies (Bourne, **Blacker**; *Impact Case Study 2*), led to the commercialisation of 'fReactor' miniaturised CST reactors (**Blacker**; see below) and development of continuous electrochemical reactors (**Willans**, **Nguyen**). Advances in the use of sustainable feedstocks include the development of platforms for safe continuous oxidative biotransformations (**Blacker**) and the commercialisation of personal care products derived from food waste (**Rayner**, *Impact Case Study 3*). Novel catalytic technologies have been developed and commercialised (**Marsden**, **McGowan**, **Blacker**).

Next 5 years: Extensive cross-campus collaborative expertise within iPRD will be further strengthened by creation in 2019 of a unified Faculty of Engineering and Physical Sciences. We will continue to leverage this in the development of novel continuous reactors and processes,

particularly in meeting the needs of emerging areas such as flow biocatalysis and non-traditional product processing (e.g. polymers). As "Industry 4.0" becomes a priority for companies, we will exploit our leading position in autonomous optimisation platforms and cognitive manufacturing, strengthened by recent major RCUK awards (including a partnership with IBM to develop new algorithms). Both align with the recently awarded EPSRC CDT "Molecules to Product" (Deputy Director: **Blacker**) hosted at Leeds.

1.2 Impact Strategy

The School actively supports the embedding of impact throughout the research process from inception to delivery. At the very earliest stages, we support project co-development with end-users through a variety of mechanisms, including facilitating *consultancy* (all staff are entitled to perform 12 days of consultancy per year by right, with the potential to extend with HoS agreement); hosting sub-discipline-specific *industry "clubs"* and *advisory boards* (e.g. iPRD and *Astbury Centre*), with regular thematic meetings leading to proposal (co-)development; and extended *secondments* and *placements*, both outgoing (e.g. **Rayner**, 50% FTE secondment to spin-out C-Capture 2017-1818 – *Impact Case Study 1*; Bourne, RAEng Industrial Fellowship 2015-16, Senior Research Fellowship 2019-, both with AstraZeneca – *Impact Case Study 3*) and incoming (e.g. workers from Ono Pharmaceuticals, Biome, Esseco and AstraZeneca to iPRD).

Once collaborative or commercially-relevant projects are established, the Faculty of Engineering and Physical Sciences has three dedicated R&I Development Managers who provide expert advice on potential sources of support for different impacts e.g. for activities to be costed in research grant applications or to access funding such as RCUK Impact Acceleration Accounts. These can provide staging funding to drive research outputs towards market. Examples include the EPSRC IAA funding facilitating commercialisation of patented hydrogen transfer catalysts (**Marsden**, **Blacker**, **McGowan**) and ERC/STFC IAA funding to **Plane** for NO_x catalyst commercialisation. Alternatively, the funding has been used to provide project support for major collaborative ventures such as the £670K *AstraZeneca Centre for Manufacturability* at Leeds, wherein AZ partnered with the iPRD to apply Leeds expertise in product processing and characterisation to develop science-led solutions to common problems in pharmaceutical manufacture.

The R&I Development Managers provide a conduit to the Commercialisation team within Research and Innovation Services at Leeds, who provide support and funding for patenting, commercialisation and spin-out development. Recent successes include *C-Capture*, a company exploiting novel low-energy CO_2 capture technology developed at Leeds by **Rayner** with a current turnover of >£1M pa (*Impact Case Study 1*); *Keracol,* a sustainable personal care products company which markets products through international brands such as Marks and Spencer and Estée Lauder, as well as their own Dr Craft product range (**Rayner** – *impact Case Study 2*)); and *Redbrick Molecular*, a new spin-out jointly owned by Leeds and the University of Sheffield, which commercialises bespoke building blocks for drug discovery (**Marsden**, **AS Nelson** – *Impact Case Study 4*)). The 2019 opening of the £40M NEXUS business engagement facility (REF5a) supports not only the growth of University spin-outs (e.g. Keracol is now located there), but also incoming businesses seeking to collaborate with the University.

Impact is also derived from non-commercial platforms such as software, open-access tools and databases. MESMER (https://www.chem.leeds.ac.uk/mesmer/introduction.html) is an open source programme developed in the SoC for kinetics simulations and is used by groups worldwide, with >6000 downloads since 2014 (**Blitz** and **Seakins**). **Shalashilin** (with Martinez at

Stanford) has contributed the *Ab Initio* Multiple Spawning module method to the MOLPRO quantum chemistry package. The LLAMA program (https://llama.leeds.ac.uk/) has been developed by **AS Nelson** and **Marsden** as an open access web-based tool for the creation and analysis of virtual compound libraries for drug discovery, with ~950 users worldwide (>20 countries) from industry and academia (>30 companies/research institutes; >100 Universities).

Next 5 years: We will continue to encourage colleagues to develop impact from their work through expert support in proposal development, facilitating co-creation of projects (e.g. through pump-priming consultancy and short-term projects), supporting researcher mobility, and buy-out of time for impact-related purposes. Specific opportunities include our leading positions in cognitive chemical processing, chemical biology (including probe molecules), sustainable technologies and atmospheric composition studies.

1.3 Open Research Environment and Research Integrity

Staff in the SoC are required to deposit author-accepted versions of papers in the White Rose open access repository (>92% compliant since April 2019). There is also funding available through the UoL Library for making UKRI-funded papers "gold" open access. SoC policy is for data on which research papers are based to be deposited in a secure, backed-up facility e.g. the UoL Library data repository https://archive.researchdata.leeds.ac.uk/ for data-sets up to ~1 Tb and the PETAL (Petabyte Environmental Tape Archive for >1 Tb data-sets). Making data open access is an important aspect of research integrity/replication. In addition, all first-year PhD students in the SoC take a short course in "How to keep a lab notebook" which covers open access and integrity, as well as University-level training in research ethics.

2. People

2.1 Staffing Strategy and Staff Development

At the heart of the development of all staff is the *Staff Review and Development Scheme* (SRDS), www.leeds.ac.uk/hr/development/srds.htm. SRDS helps staff achieve their full potential by providing a two-way review of progress, identifying key objectives, providing constructive feedback, and identifying and planning appropriate development (REF5a). All staff are expected to go through probation if they have not already done so for their current or similar role. Early career members of staff have a reduced teaching load (typically starting at 60%, ramping up over 5 years). Their research progress is mentored on a regular (at least quarterly) basis through meetings with a designated senior member of staff.

In the SoC, all research grant applications are reviewed internally by two independent members of staff. Proposals to EPSRC are then formally evaluated by an internal panel of 4 members. NERC proposals are evaluated before submission by a University-wide panel. Staff are required annually to enter onto a database their planned grant applications over the following 18 months, to ensure workload support for major applications. The implementation of these plans is then reviewed during an *Annual Academic Meeting* between each staff member and the Head of School, Director of Research & Innovation, and Director of Taught Student Education. The meeting is also used to examine the staff member's workload balance including specific research-related matters e.g. success with PhD student recruitment, research facilities, and timely production of research outputs.

The age distribution in the School reflects a vibrant, well-balanced department (33% of staff are under 45), guided by a cohort of more experienced colleagues (57% are 45-60, and 10% are

over 60). During the REF period, one permanent staff member moved to the U. Sheffield, and 12 new staff have been added across the 5 research sections.

Current staff are listed below according to their primary research section (section leader underlined). Many staff contribute to the activities of other research sections, significant examples are described elsewhere in this document. The letters in parentheses denote status [P = Professor, R = Reader, AP = Associate Professor, EO = Experimental Officer, L = Lecturer, SL = Senior Lecturer, RF = Research Fellow, UAF = University Academic Fellow, * = Emeritus Professor].

APC Staff summary: Blitz (RF), Heard (P), Lehman (AP), Marsh (P), Plane (P), Seakins (P), Stone (AP), Whalley (RF). **New staff:** Lehman, Marsh, Stone. Currently there are 13 PDRAs and 12 PGRs.

CBMC Staff summary: AS Nelson (P), Fishwick (P), Foster (AP), AS Nelson (P), Sergeeva (L), Taylor (P), Turnbull (P), Warriner (SL), Webb (AP), Wilson (P), Walco (L), Wright (UAF), Zhou (P). **New staff:** Foster, Taylor, Walco, Wright. Currently there are 22 PDRAs and 45 PGRs.

CCCP Staff summary: Burnett (UAF), de Leeuw (P), Miranda (L), Shalashilin (P), Whitaker (P). **New staff:** Burnett, de Leeuw. Currently there are 5 PDRAs and 5 PGRs.

CDA Staff summary: Ansell (SL), Auer (L), Beales (AP), Bushby (P), Chamberlain (AP), Halcrow (P), Hardie (P), Kee (R), Kulak (EO), Meldrum (P), Menzel (AP), AL Nelson (P), Thornton (L). **New staff:** Chamberlain, Kulak, Menzel. Currently there are 14 PDRAs and 35 PGRs.

PRD Staff summary: Blacker (P), Marsden (P), McGowan (P), Nguyen (L), Rayner (P), Willans (AP). Bourne (AP) and Muller (P) are returned through UoA 12. Currently there are 9 PDRAs and 28 PGRs.

Support for interdisciplinary research. In addition to encouraging participation at senior level through the University-wide *Astbury* and *Priestley Centres* (Section 1), there are 5 joint appointments (ca. 50:50) with other Schools: **Marsh** (Physics & Astronomy); **Blacker**, Dr Richard Bourne, Dr Sean Collins, Professor Frans Muller and **Nguyen** (Chemical & Process Engineering).

Study leave arrangements. While there is no automatic study leave entitlement, staff are encouraged to apply for personal fellowships and we have a good track record of success during the REF period:

ERC Advanced Grant Fellowships (**Meldrum** and **Plane**).

ERC Early Career Fellowship (**Wilson**).

EPSRC Leadership Fellowship (**Meldrum**).

EPSRC Established Career Fellowship (**AS Nelson**).

EPSRC Fellowship (**Burnett**).

Marie-Curie Individual Fellowship, ERC Early Career Fellowship (**Lehman**).

Additionally, Bourne (50% SoC, returned through UoA12) held RA Eng Industry (2015-16) and Senior Research (2019-) Fellowships, and **de Leeuw** an AWE William Penny Fellowship (2014).

Flexible/remote working. In the last 5 years, 9 members of staff have made formal flexible working requests which have all been granted. Advertised posts include wording to encourage applicants who would require flexible working or job share arrangements. The School also supports informal requests for flexible or remote working arrangements e.g. approving requests for one day a week to be kept free from timetabled teaching activities to allow for a research day. For the benefit of researchers at all levels, research seminars are organised within core working hours (10 am - 4 pm).

Career pathways for part-time staff. Policy in place to encourage part-time staff to consider splitting/sharing major leadership roles, in order to gain leadership experience which is important for promotion.

Research support for staff with caring responsibilities. A policy is in place to allow staff or research students with caring responsibilities to apply for funds to support childcare costs associated with attending conferences/training events (e.g. the SoC paid for **Wright's** partner to accompany her with young baby to a conference).

Support for staff returning from leave. A policy is in place to support staff taking planned family leave to arrange suitable cover for their research activities and to allow momentum to be maintained (**Wright** and **Willans** have benefitted). This includes providing support to researchers in the section, undertaking experimental work and preparing data/first drafts of papers and grant applications. There is an option for fixed-term cover to be extended beyond an individual's return to allow them to focus on rebuilding research activity before resuming teaching and administrative duties. Individuals returning to work from either family or ill health leave can apply for additional funds from the SoC to support registration fees/travel/childcare costs associated with research activity.

Rewarding research success. Additional workload release is available for any individual with more than 40% of their time externally funded. Individuals performing exceptionally across the breadth of their roles can be recommended for a salary increase or one-off payment.

2.2 Post-Doctoral Research Associates

There have been 165 PDRAs in the School of Chemistry between 2014 and 2020, of which 11 have been Marie Curie Fellows. All new PDRAs employed in the School receive a comprehensive induction and are subject to a probationary period, which provides structure and support to establish and work towards a set of objectives, identifying any training and development needs. Once the probationary period has been successfully completed, researchers join the SRDS Scheme (see above). The UoL offers a wide range of training activities through its *Organisational Development and Personal Learning* service. This includes a suite of courses developed specifically to support early career researchers (e.g. applying for funding, academic career skills, introduction to academic leadership) as well as more general courses (e.g. developing digital practice, writing skills, using social media, organisation and personal effectiveness, project management). We offer PDRAs teaching opportunities (including lecturing), and support for HEA accreditation. Coaching and mentoring happens informally through the research sections in the School, but there is also a mentoring programme run across the University where researchers can be matched with a mentor from outside of their subject area to provide career guidance.

2.3 Postgraduate Research Students

The SoC recognises that PGR students make a major contribution to the research programme of the School and University. We have ambitious plans to increase the number and enhance the quality of our postgraduate intake, against the prevailing funding and demographic trends of declining PGR provision, by increasing numbers of international PhD students. Currently, the number of registered PGRs in the SoC is 97. These students are funded by EPSRC (29), NERC (8), STFC (1), University and SoC Scholarships (17), industry (2), overseas sponsors (22), ERC (5), Charities (4), BBSRC (4), MRC (3) and alumni donations (2). This diverse range of funders is regarded as an important strategic strength. Currently, a further 20 PGRs are registered outside Chemistry but supervised primarily by SoC staff (these students are funded by NERC/BBSRC/MRC DTPs or EPSRC CDTs that are housed in other Schools at the UoL).

During the REF period the School has been a major stakeholder in graduate programmes within the University including the *Astbury Centre's* Wellcome Trust 4-year PhD programme; the BBSRC-funded White Rose Doctoral Training Partnership (with York and Sheffield); five EPSRC CDTs (Molecules to Product, BioEnergy, Complex Particulates, and Soft Matter & Interfaces 1 & 2); and NERC SPHERES and PANORAMA DTPs. 17 studentships have been collaborative with industry.

Recruitment. Studentships are advertised on the School of Chemistry website and FindaPhD.com. An Open Day is also held in January each year. All applicants are interviewed by a panel of three members of staff drawn from at least two Sections to maintain a common standard of admission. A written report on the interview performance informs the final admission decisions, which are taken by the Director of Postgraduate Studies.

Training, Support and Monitoring. The University's new Graduate Record of Achievement and Development (*GRAD*) electronic system records all aspects of a PGR's career, from admission through to final examination, ensuring a consistent experience for all PGRs. This includes student training plans, which are first agreed with the supervisor within one month of starting, then continuously updated by the student during their programme of study as required. *GRAD* is also used to record supervision meetings and training courses attended; at least ten minuted, one-to-one supervision meetings per year are mandatory for each student. PGRs are required to submit the following pieces of work during their degree: a literature report after 4 months; a transfer report, which is examined by a *viva voce* exam after 11 months; and two further research reports at 22 and 34 months. Submission, examination (for transfer) and provision of student feedback for these milestones are also undertaken through *GRAD*. Students are interviewed one-on-one by the Progression tutor during each year of their degree to monitor general progress. Students present a poster in year 2 and give a talk in year 3 at the School's annual postgraduate conference, where prizes for best talk and poster (voted by both students and staff) are awarded. The School has an excellent record of successfully delivering PhD training: the completion rate of PhD students during the REF period has averaged 93%, with 100% of those submitting within 4 years of registration (cf. with 85% in the REF2014 period).

All PGRs have the opportunity to engage in mentoring and teaching through involvement in undergraduate practical work demonstration and final year, MChem, project supervision. In addition, PGRs are expected to hone their communication skills by disseminating their research at departmental seminars and international conferences, with many winning awards for their contributions.

2.4 Equality and Diversity

Three members of the Equality and Inclusion committee sit on the School's Management Committee, where decisions about all aspects of research, funding, rewards and leadership are made. Two members of the E&I committee also sit on our Rewards Committee.

Seven members of the academic staff are female (3 are Professors). The gender balance has remained 16% female, although 33% of UAF appointments during the REF period have been female. At postdoctoral level the balance has increased from 29% female in 2014 to 43% in 2020 (consistently 1-2% higher than the Russell Group benchmark), and that of research support staff has increased from 15% to 40%.

The PGR gender balance has been (39±3)% female over the REF period. Offers to female PGR applicants have increased from 27% to 51%, reflecting an increase in the quality of applications received. This has coincided with changes to our on-line marketing material placing greater visualisation of the engagement of women in chemistry (https://physicalsciences.leeds.ac.uk/info/4/school_of_chemistry).

3. Income, infrastructure and facilities

3.1 School Level

The total research income between 2014 and 2020 is £37.5M, averaging £5.7M per annum.

Major grants (>£1M):

EU "Synthetic biology of carbohydrate-binding proteins: engineering protein-carbohydrate interactions for diagnostics and cell targeting" (£3.6M – **Turnbull**)

EPSRC Programme grant "Crystallisation in the Real World: Delivering Control through Theory and Experiment" (£2.5M - **Meldrum**)

EPSRC Programme grant "Integrated computational and synthetic tools to drive the discovery of orthosteric protein-protein interaction inhibitors" (£2.2M – **Wilson**, **AS Nelson**)

ERC Advanced grant "Dynamical Control of Mineralisation" (£2.0M - **Meldrum**)

ERC Advanced grant "Cosmic Dust in the Terrestrial Atmosphere" (£1.9M - **Plane**)

ERC Early career grant "Highly Instrumented Low Temperature Reaction Chamber" (£1.5M – **Lehman**)

EPSRC Leadership fellowship "Crystallisation in Confinement - A Biological Perspective" (£1.9M - **Meldrum**)

EPSRC Platform Grant "New Strategies for Controlling Crystallisation" (£1.4M - **Meldrum**).

EPSRC Established Career fellowship "Autonomous Discovery of Functional Small Molecules" (£1.2M – **AS Nelson**)

EU "HISENTES" (£1.2M – **AL Nelson**)

EPSRC Fellowship "Dynamics, Control and Energy Transfer at Terahertz Frequencies" (£1.1M – **Burnett**)

EPSRC "Cognitive Chemical Manufacturing) (£2.0M – **Bourne**, **Chamberlain**, **Muller**)

EU "European Lead Factory (EUC²LID)" (£1.0M – **AS Nelson**)

BBSRC "Deciphering the function of intrinsically disordered protein regions in a cellular context" (£5.4M - **Wilson**)

EPSRC Strategic Equipment bid "A Platform for Chemical Probe Identification and Optimization Facilitating Interrogation of Biological Mechanisms" (£1.5M – **Warriner**, **Wilson**, **Wright**).

Research within the School is underpinned by 8 support staff including 6 research officers. The principal instrumental services - 6 NMR spectrometers (up to 600 MHz, and cryoprobe capability), 4 mass spectrometers, X-ray crystallography, optical spectroscopy, electron microscopy, thermal analysis, particle size analysis, robotic liquid handling, a biological chemistry suite, and HPLC - are each operated by a senior technician or research officer who is also responsible for the training of postgraduate students and PDRAs. The "core" equipment was replaced in 2013 with a £1.4M grant (£1M from EPSRC, £400K from the university). The electronic and mechanical workshops (2 technicians) provide general repair services but, more importantly, they design and build a range of instruments, primarily for the APC and CCCP sections. All support staff are encouraged to keep abreast of new developments by attending courses and conferences.

The University has also funded a Priestley Centre Chair in Comparative Planetary Atmospheres (£230K, shared with Physics & Astronomy, **Marsh**) and 6 University Academic Fellowships which are 5-year tenure track appointments (£2M).

3.2 Research Section Level

APC have five very well-equipped laser laboratories (a total of 280 m^2 divided into 14 experimental bays). There are world-leading facilities for studying neutral, ion-molecule, particle nucleation, heterogeneous and photochemical reactions relevant to the atmospheres of Earth and other planets. These include a large collection of pulsed nanosecond lasers, time-of-flight and quadrupole mass spectrometers, a frequency-comb spectrometer, a surface science UHV chamber, pulsed Laval nozzle reactor, grating, cavity and Fourier transform spectrometers, a Meteoric Ablation Simulator and ultra-fine particle sizing equipment. The HIRAC atmospheric chemistry simulation chamber operates over a wide range of temperatures and pressures, with unique in situ radical detection. There are also wet chemistry facilities for inorganic & organic astro- & geo-chemical research. Since 2014, the UoL has provided £400K funding for high performance laser systems. APC also has a block grant for cosmic dust analysis at the Diamond I08 Scanning X-ray Microscopy beamline. An extensive range of field apparatus is available for the detection of radical species by laser-induced fluorescence (the FAGE technique, which operates from ground/ship-based and airborne platforms). The section is also an extensive user of the MCM, which was developed in the SoC and which is internationally recognised as the leading computer model of organic reactivity in the atmosphere, as well as the MESMER program for kinetics simulations (see above). APC has 120 dedicated cores on the university's massively parallel High Performance Computers, which are used to run whole atmosphere chemistry-climate models such as WACCM for the terrestrial atmosphere and the LMD-Mars model for Mars.

CBMC has excellent infrastructure for research at the interfaces with biology and medicine: three biological containment laboratories (Category 1 and 2) equipped for genetic manipulation, protein expression, purification and biophysical characterisation; a suite for the synthesis and purification of small molecule libraries; a small molecule screening facility, with dehumidified ligand storage; Hamilton 8 channel and 96 channel robotic liquid handling;

fluorescence/luminescence/absorbance high-throughput screening in 384-well plate format. The section additionally benefits from its participation in the *Astbury Centre for Structural Molecular Biology* which provides access to all major structural biology and biophysical techniques. Recent major institutional investment in the £17M Astbury Biostructure Lab provides us with access to a suite of electron microscopes including two Titan Krios instruments for high resolution cryo-EM and tomography with facilities for correlative fluorescence/EM microscopy and time-resolved EM; protein NMR spectroscopy facilities at 600-950 MHz; and binding analysis instrumentation, including surface plasmon resonance, isothermal titration calorimetry, microscale thermophoresis, and a suite of 10 mass spectrometers optimised for protein analysis including ion mobility and HDX/FPOP footprinting. These facilities are transforming our ability to study small ligands binding to very large and very dynamic macromolecules, including studies in living cells.

CCCP has access to the Leeds THz Photonics Laboratory, one of the largest, best-equipped university THz research facilities in the world, which includes: eight optical bench-based systems, with five femtosecond oscillator-based pulsed imaging and spectroscopy systems, including ultra-broadband, pump-probe, and both freespace and guided-wave apparatus; and QCL-based imaging and spectroscopy systems. The facility also includes an 8 mK cryogen-free dilution refrigerator, with fibre-optic and microwave access, 1.2 K optical access cryostats, including cryogen-free systems, and magnetic fields up to 12 T. Research also benefits from: two state-of-the-art MBE growth chambers focused on III-V semiconductors; and a nanotechnology class 100 fabrication facility (which will soon be upgraded as part of the new *Bragg Centre*). CCCP has a laser laboratory of 83 m^2 equipped with a number of femtosecond and nanosecond lasers, a very high resolution velocity map imaging spectrometer, and a frequency comb spectroscopy system, together with a newly refurbished computational office suite of 72 m^2. The computational group is among the biggest users of the University's High Performance Computer facilities, and also has a dedicated cluster designed for efficient *ab initio* quantum dynamics calculations.

CDA is supported across a number of laboratories, with a range of analytical equipment including Raman microscopy, BET, TGA and DSC, DLS, an electrochemical analyser and a FEG-SEM with integral EDX, as well as synthetic laboratory suites and a single crystal X-ray diffractometer with a micro-focus dual wavelength X-ray source. The section also makes extensive use of the School NMR suite and accurate mass ESI-MS, and has been supported by a block allocation grant at the small molecule crystallography station I19 at Diamond. There is also access to significant additional instrumentation through the *Royce Institute* (REF5a). A new facility has been established through the award of a £1.1M EPSRC Strategic Equipment Grant in 2019: Flow-XI- A New UK Facility for Analysis of Crystallisation in Flow Systems. Flow-XI uses X-ray diffraction and Raman spectrometry to study crystallisation in flowing plugs or continuous flow, enabling users to conduct *in situ* studies of crystallisation mechanisms and pathways with unprecedented reproducibility and time resolution. Essential access to electron microscopy facilities is provided through university centres located in Engineering and Biology. The well-established LEMAS Centre (4 academics and 6 support staff with over 400 users) in SCaPE houses 2 TEMs, including a new £2.4M analytical cryo-TEM optimised for low dose analysis, 7 SEMs and a new £1.2M cryo-FIB-SEM. Powder XRD is available in the Schools of Chemistry and Chemical Engineering. The two state-of-the-art Titan Krios microscopes in the Astbury Biostructure Laboratory are equipped with direct electron detectors (DED) for high resolution imaging and electron tomography of samples under cryogenic conditions. The SQUID magnetometer in Physics is used to investigate the properties of spin-crossover compounds.

Elemental analysis (ICP) is available in Earth Sciences, and in Engineering there is a powder diffraction offering hard and soft X-ray photoelectron (XPS) with X-ray emission spectroscopy (XES), and sample characterisation with environmental control.

PRD is based around a fully operational process laboratory (originally established through a £4.5m investment from the Regional Development Agency and the European Regional Development Fund 2009-2012). The laboratory houses a wide variety of pilot-scale batch (up to 50 litre) and flow process scale-up equipment (including a 10 bar trickle bed reactor, continuous polymerisation, continuous electrochemistry, and continuous liquid-liquid extraction), much of which has been developed in house (e.g. 'fReactors' for small-scale continuous batch processing, now commercialised with Asynt; 53 units sold worldwide in 22 months). A broad range of analytical techniques have been introduced since 2013, including real-time mass spectrometry, normal and near IR, ultrafast (U)HPLC, and NMR. Most distinctively, five self-optimising reaction platforms have been funded which include novel reactors, novel analysis methods and novel algorithms, many of which have been developed in conjunction with industry (e.g. AstraZeneca, GlaxoSmithKline, IBM). The lab operates to the highest standards of safety with a dedicated laboratory manager responsible for the running of the facility. Process development work has assisted several companies towards commercial manufacture of products (see section 2).

3.3 Sustainability

Chemistry at Leeds, which is one of eight Schools within the Faculty of Engineering and Physical Sciences, is amongst the most research active and vibrant Schools within the University. The University has made clear its intention to continue strong support for the School, both near and medium term. In particular, as part of a continuing programme of major capital investment in the Faculty which most recently has included the creation of the Sir William Henry Bragg Building to house the School of Physics & Astronomy and the School of Computing (£96M, due for completion in late 2020), the University is planning a major building and refurbishment programme for the School of Chemistry (starting in 2022). The re-developed School of Chemistry, which will be adjacent both to the Bragg Building and the major Engineering Schools within the North-East quarter of the University campus, will create a world-leading integrated campus for Engineering and Physical Sciences (REF5a). This physical infrastructure will facilitate and build upon the already existing very strong research links between the Chemistry APC, CCCP and PRD sections and the Schools of Physics & Astronomy and Chemical & Process Engineering, which includes significant collaborative research grant portfolios as well as joint appointments (3 research Chairs, 2 associate professor/lecturers, and 2 University Academic Fellows).

Additionally, the University continues to underline its commitment to maintaining an internationally-leading profile in structural molecular biology/science at the biology-chemistry interface, with the £17M capital investment in the Structural Molecular Biology suite within the *Astbury Centre* (see above and REF5a). As a major stakeholder School within *Astbury* (e.g. substantial joint grant portfolio with members of CBMC), the School of Chemistry is set to benefit greatly from this investment and, as part of the current planning towards the major refurbishment of the School, will be taking full advantage of the opportunity to create an integrated international centre of excellence for science at the chemistry-biology interface.

High Performance Computing is essential for activities in the APC and CCCP sections, such as global atmospheric modelling, electronic structure theory calculations and molecular dynamics.

The University has invested over £1.5M during 2019 in the latest HPC cluster at Leeds, which provides a Linux-based service with 5960 standard compute nodes at a clock rate of 2.0 GHz. Planned investment in HPC over the next 5 years is planned to exceed £1M pa.

A particularly exciting future development that is set to cut across all five research sections is the development of Artificial Intelligence (AI). The SoC is set to take a leading role in this area, both within the UoL and externally through the University's partnerships with the Alan Turing and Rosalind Franklin Institutes (REF5a), and is planning major investments in both staff and infrastructure.

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

4.1 Academic Collaborations

The SoC supports visits from potential research collaborators in two ways. First, staff can bid against an International Academic Mobility Pump-priming Fund to cover travel and accommodation costs for visitors. Second, each staff member is allocated 12 "visitor months" every two years, where the costs of office space, IT and library access for the visitor are covered by the SoC.

During the REF period there have been 72 **visiting academics** (35 of whom stayed longer than 6 months and 37 for between 1 and 3 months). 32 visitors were from Asia, 25 from Europe, 6 from South America, 5 from North America and 4 from Africa.

49% of papers published by SoC staff during the REF period had international co-authors from the following countries (number in parentheses): US (168), Germany (138), France (71), China (61), Spain (38), Italy (32), India (28), Japan (24), Switzerland (20), and rest of the world (220). 48% of papers had UK authors outside Leeds, and only 25% of papers were authored solely at the UoL. 10% of papers involved collaborations with corporations.

Significant collaborations are listed below by research section.

APC: Leading involvement in NERC-funded atmospheric field campaigns with multiple UK collaborators e.g. AIRPRO (**Heard**, **Whalley**). ERC Advanced project CODITA involved 9 partners in the US and 3 in Germany (**Plane**). NERC INFAMOS development of novel atmospheric spectroscopic probes with Oxford (**Heard, Seakins, Whalley**). Chemistry around AGB stars via the AEROSOL ERC project with Leuven and Queens Belfast (**Heard, Plane**). EU EUROCHAMP chamber network (**Seakins**). Professor Heather Lewandowski (U. Colorado, Boulder) spent 6 months at Leeds supported by the UK-US Fulbright University of Leeds Distinguished Chair award.

CBMC: EPSRC programme grant POPPI on perturbation of protein-protein interactions (led by **Wilson**, **Nelson**) with Bristol. Coordinator of ERASynBIO consortium "SynGlycTis" and H2020 MSC-ITN "synBIOcarb" (**Turnbull**) with partners in 5 EU countries. Chair of COST Action CM1102 "MultiGlycoNano" (**Turnbull**) with ~60 participating groups from 21 countries. European Lead Factory consortium with ~30 partners from academia and pharma (**Nelson**, **Marsden**). Royal Society-funded collaboration on antibiotics discovery with Professor K. Chibale, Cape Town (**Fishwick**).

CCCP: Collaboration with Imperial, Bristol and Cardiff within an EPSRC programme grant on "Chemistry and Mathematics in Phase Space CHAMPS"; NSF/EPSRC-funded international

collaboration with Stanford U. to develop new methods of quantum dynamics and their implementation (**Shalashilin**).

CDA: Collaboration with UCL, Warwick and Sheffield within an EPSRC programme grant on "Crystallisation in the real world", and Bath, Nottingham and Strathclyde on the EPSRC Strategic Equipment Grant "Flow-XI: A New UK Facility for Analysis of Crystallisation in Flow Systems"; participation in EU-FP7 collaborative research project (SMILEY) (**Meldrum**). COST action CM1305 "Explicit Control over Spin-states in Technology and Biochemistry" (**Halcrow**). European COST action TD1308 "life-ORIGINS" work group leader (**Kee**). EPSRC project "An integrated biophysics approach towards realisation of a new class of membrane-active anticancer therapies" with Sheffield, Durham and York (Beales). HORIZON 2020 grants HISENTS (**AL Nelson**, **Beales**) involving 11 international partners, and SABYDOMA with 19 international partners (**AL Nelson**). Collaboration with Sao Paulo State University under a FAPESP funded research visit, leading to subsequent EPSRC funding (**Beales**).

PRD: Significant activity within the EPSRC Catalysis Hub (co-I **Blacker** in Phases 1 & 2); EPSRC Dial-a-Molecule network (co-I **Marsden** in phases 1 & 2).

4.2 Research Collaborations with Research Users

The School has been particularly successful in building projects with industry:

Funded directly or jointly with Innovate UK: *Centre for Manufacturability Design* (AstraZeneca - **Blacker**); CelluPAT and OPTOMS (Innovate UK/Fiberight - **Blacker, Bourne**); MSW-IndUK (BBSRC/Innovate with UK partners Fiberight, AMT, Defiant Renewables, S.Amit&Co., ICT, NEERI and VIT - **Blacker**); Ligpoly (Innovate UK/Biome - **Blacker**); HMF-Scale (Innovate UK/Biome - **Blacker**) with a patent application for a bioprocess to make sustainable and biodegradable polymers.

EU-funded industrial collaborations include: IMI European Lead Factory consortium (7 large pharma companies and 10 SMEs - **AS Nelson**, **Marsden**, **Foster**); IMI Sustainable Pharmaceutical Chemistry (CHEM21) consortium (partners GlaxoSmithKline, Pfizer, Orion, Bayer, Johnson & Johnson, Sanofi - **Blacker**, **Marsden**, **AS Nelson**), TASPPI ITN (5 industrial partners - **Wilson**).

Industrial collaborations with the following SMEs: Reaxa (TSB); YProtech (TSB); Critical Processes (TSB); DyeCat (TSB); Avantium (TSB); Specialty Glycans Consortium funded by BBSRC/Innovate UK Industrial Biotechnology Catalyst (partners GSK, Prozomix, Carbosynth, Dextra, Ludger); SynBIOcarb EU Marie Sklodowska-Cuire ITN (partners GlycoSeLect, Elicityl, GLYcoDiag, enGenes) (co-ordinated by **Turnbull**).

Industrial funding of PhD students: AstraZeneca (13 CASE), Novartis (1 CASE), Pfizer (2 TSB, 1 KTS), GlaxoSmithKline (2 CASE, 1 KTS), Syngenta (TSB, 1 CASE/CDT), Imerys (CASE), Bod Ayre (TSB), Body Shop (TSB), Knauf (IUK), Nestle (1 CASE), Syngenta (0.25 FTE), AMT (IUK), Biome (1 CASE), Fiberight (2 PhD), YPT (1 CASE), UK Met Office (1 CASE); Atomic Weapons Establishment (1 CASE), William Blythe Ltd.(1 PhD); Redbrick Molecular (2 CASE).

EPSRC-funded collaborations with the following industrial project partners: Astex, AstraZeneca, Domainex, GlaxoSmithKline, Johnson Matthey, Novartis, Syngenta, NI Cancer Research (**Blacker**, **Chamberlain**, **Marsden**, **AS Nelson**, **Nguyen**, **Wilson**); Redbrick Molecular (**Marsden, AS Nelson**); Sterling Pharma solutions, Asynt, Concept Life Sciences, Dr Reddy's (**Blacker**, **Nguyen**); IBM, Promethean Particles and Swagelok (**Chamberlain**).

4.3 Leadership and Recognition in the Academic Community

Major Research Awards and Prizes

Elected Member of Academia Europaea (2017), Fellow of the Learned Society of Wales (2016) (**de Leeuw**)

RSC Environment Prize (2017) (**Heard**)

RSC Interdisciplinary Prize (2017) (**Meldrum**)

European Federation of Medicinal Chemistry UCB-Ehrlich Award (2018) (**AS Nelson**)

EGU Bjerknes Medal for Atmospheric Science (2017); elected Fellow of the American Geophysical Union (2017) and Fellow of the Royal Society (2020) (**Plane**)

Shell Springboard Award (2016) and Business Green Award, Breakthrough of the Year (2019) (**Rayner**, company C-Capture)

RSC Norman Heatley Award (2016) (**Wilson**)

ACS Infectious Diseases Young Investigator Award (2019) (**Wright**)

Plenary/medal Lectures

24th International Symposium on Gas kinetics and Related Phenomena, York, 2016 (**Blitz**)

RSC Faraday Discussion Meeting, Cape Town, 2017; 7th conference of the Federation of African Societies of Chemistry, Gaborone (Botswana), 2019; National Conference on Materials Physics, Bengaluru (India), 2020 (**de Leeuw**)

14th International Conference on Molecular Magnetism, St Petersburg (Russia), 2014 (**Halcrow**)

13th International Conference on Materials Chemistry, Liverpool, 2017; Royal Australian Chemical Institute Inorganic Chemistry Meeting, Wollongong, 2019 (**Hardie**)

US Department of Energy - Chemical Sciences, Washington DC, 2016 (**Heard**)

6th European Conference on Crystal Growth, Varna (Bulgaria), 2018; 9th International colloids conference, Barcelona, 2019 (**Meldrum)**

52nd International Conference on Medicinal Chemistry, Caen (France), 2016 (**AS Nelson**)

UCB-Ehrlich Award Lecture, XXV European Federation of Medicinal Chemistry International Symposium of Medicinal Chemistry, Llubljana (Slovenia), 2018 (**AS Nelson**)

6th EuCheMS Chemistry Congress, Seville (Spain), 2016 (**Nguyen**)

Vilhelm Bjerknes Medal Lecture, European Geosciences Union, Vienna, 2017 (**Plane**)

International Conference on Chemical Kinetics, Ghent (Belgium), 2015 (**Seakins**)

Joint Iberian meeting on Atomic and Molecular Physics, Barcelona, 2017 (**Shalashilin**)

29th International Carbohydrate Symposium, Lisbon, 2018 (**Turnbull**)

Ischia Advanced School of Organic Chemistry, Ischia (Italy), 2014 (**Wilson**)

Journal Editorship (editorial board member or guest editor)

Physical Chemistry Chemical Physics; *Advances in Biomembranes and Lipid Self-Assembly* (**Beales**)

Synthesis and Catalysis (**Chamberlain**)

Scientific Reports (**Fishwick**)

Journal of Chemical Biology and Drug Design (**Foster**)

CrystEngComm; *Supramolecular Chemistry* (**Hardie**)

Atmospheric Chemistry & Physics; *Atmospheric Measurement Techniques*; *Chemical Society Reviews* (**Heard**)

Journal of Atmospheric and Solar-Terrestrial Physics (**Marsh**)

MRS Bulletin; *International Materials Reviews*; *Chemical Society Reviews* (**Meldrum**)

Journal of Atmospheric Chemistry (**Plane**)

Atmospheric Measurement Techniques (**Whalley**)

ChemistryOpen (**Willans**)

Computational and Structural Biotechnology Journal; *Sensors* (**Zhou**)

SoC staff are advisory editorial board members for a further 12 international journals.

Committee Membership (Learned Societies, International Scientific Councils)

Society for Molecular Imprinting (**Ansell**)

EU Softcomp network for self-assembling and biomimetic systems (**Beales**)

IOP Molecular Physics Group (**Lehman**)

Consultant to Wellcome Trust Seeding Drug Discovery Programme (**Fishwick**)

SCI Fine Chemicals, Society of Chemical Industry (**Foster**)

RSC Supramolecular and Macrocyclic Chemistry Group (**Hardie**)

RSC Faraday Division Council (**Heard**)

President of the Astrobiology Society of Britain; Chair, RSC Coordination and Organometallic Chemistry Interest Group (**Kee**)

RSC Spectroscopy & Dynamics Group; IOP Molecular Physics Group (**Lehman**)

International Commission on the Middle Atmosphere (President), Scientific Committee on Solar Terrestrial Physics (SCOSTEP) (**Marsh**)

RSC Dalton Division Awards panel (**McGowan**)

Materials Research Society, Board of Directors; RSC Prize Committee (**Meldrum**)

Chemistry theme lead, Rosalind Franklin Institute (**AS Nelson**)

EGU Atmospheric Sciences Medals panel chairman; AGU Macelwaine Medal committee (**Plane**)

RSC Gas Kinetics Group (**Seakins**)

RSC Carbohydrate Interest Group (Chair) (**Turnbull**)

RSC Chemistry-Biology Interface Division Council (**Webb**)

RSC Applied Catalysis Group (**Willans**)

RSC Chemical Biology and Bioorganic Group (**Wilson**)

RSC Carbohydrate Group (**Zhou**)

Funding Panel Membership

UKRI Future Leaders Fellowship panel; EPSRC Strategic Advisory Team; Royal Society Challenge Grants and Newton International Fellowship panels; NSF and DoE panels (**de Leeuw**)

ERC Starter Grant PE5 panel; Royal Society Newton International Fellowships Committee (**Hardie**)

NERC Discovery Science and Independent Research Fellowship panels chair (**Heard**)

International Funding Panel Member, NASA Exobiology Programme (**Kee**).

EPSRC Capital and Equipment Strategic Advisory Team, Strategic Equipment Panel (**Marsden**)

EPSRC Responsive Mode and Programme Grant panel chairs (**Meldrum**)

EPSRC Healthcare Technologies Strategic Advisory Team, EPSRC Physical Sciences panel chair, CRUK programme grant panel (**AS Nelson**)

UK Space Agency Aurora Science panel; ERC Advanced Grant PE10 panel (**Plane**)

ERC Starter Grant PE5 panel (**Hardie**)

NERC Discovery Science; EPSRC Responsive Mode; NSF and DoE panels (**Seakins**)

IBCarb BBSRC Network in Industrial Biotechnology, Newton International Fellowship Physical Sciences Committee (**Turnbull**)

Royal Society Newton Fellowships and Research Grants (Biological) panels (**Webb**)

STFC Life Science panel (**Whitaker**)

EPSRC strategic advisory team (physical sciences), Inaugural New Horizons panel and Responsive Mode panel; EU Marie Curie Fellowships panel (**Wilson**)

Scientific advisory board membership:

UK Catalysis Hub (**Blacker**)

Wellcome Trust Seeding Drug Discovery Programme (**Fishwick**)

UK National Crystallographic Service (**Hardie**)

UK Met Office Space Weather Research (**Marsh**)

Scientific Advisory Board, Plateforme Intégrée de Criblage de Toulouse; Chemistry theme lead, Rosalind Franklin Institute (**AS Nelson**)

Scientific Advisory Board, Max Planck Institute for Chemistry, Mainz; National Center for Atmospheric Research, Boulder (**Plane**)

Leadership of International Programmes

Leader, International Space Science Institute International Team on “Quantifying Hemispheric Differences in Particle Forcing Effects on Stratospheric Ozone"; Co-leader, SCOSTEP Working Group on “Trends in the MLT"; International Space Science Institute Team on “Quantifying Hemispheric Differences in Particle Forcing Effects on Stratospheric Ozone" (**Marsh**)

Chair, Innovation working group of the EU Nanosafety Cluster (**AL Nelson**)

Leader, Chemical Transformation Cluster of EPSRC CO2Chem network (**Nguyen**)

Scientific Conference Leadership

Chair, Royal Society Theo Murphy meeting on “The artificial cell: biology-inspired compartmentalization of chemical function” (2018) (**Beales**)

Theme Chair, Goldschmidt Conference 2017 International Program Committee (**de Leeuw**)

Chair, Whole Atmosphere Modelling Workshop “Developments in the context of space weather”, Tres Cantos, Spain (2018); Chair, 12th International Workshop on Layered Phenomena in the Mesopause Region (2015) (**Marsh**)

Chair, British Association of Crystal Growth (2014); Chair, Royal Society Theo Murphy Meeting on “Nucleation: past and future challenges for experiment, theory and simulation” (2016); Chair, Faraday meeting (2021) on “Understanding Crystallization in Complex Systems: Recent Advances and Future Challenges” (**Meldrum**)

Chair, Gordon Research Seminar on Atomic & Molecular Interactions (2014) (**Lehman**)

Chair, Royal Society Theo Murphy International Meeting on “Synthetic Glycobiology” (2018) (**Turnbull**).

International Workshops on Aromatic Foldamers (Philadelphia 2016 & Seoul 2017) (**Wilson**)

Patents

‘*Catalysed Dye Systems*’ (**Rayner**, **McGowan**). Australian Patent 2010268006 (2016), European Patent 2448545 (2016), Chinese patent 102470080 (2017), European Patent

3111915 (2017). Describes a new system of hair dyeing which avoids particularly hazardous components used in current commercial systems; led to the UoL spin-out Dyecat.

'*Methods for the Capture and Release of Acid Gases*' WO2015/092427 A2, PCT/GB2014/053786 (2014), granted in US, EU and Japan. '*Aqueous system for the capture and release of acid gases*' (**Rayner**). PCT/GB2018/052209 (2018). Describes the use of amine free, carboxylate salt-based CO_2 capture processes; now being commercialised by UoL spin-out C-Capture (Impact Case Study 1).

'*Natural Hair Dyes*' (**Rayner**). Australian Patent 2010247136 (2016), Canadian Patent 2835316 (2018), European Patent 2477597 (2018). Describes the use of natural anthocyanin-based colorants in hair coloration, now commercialised by UoL spin-out Keracol under their Dr Craft brand (Impact Case Study 3).

'Personal care composition comprising a natural film-forming biopolymer and methods of making the same' (**Rayner**). Australian Patent 2013369087 (2018), European Patent 2934682 (2018). Describes the use of natural biopolymers for use in hair care applications such as hair sprays; commercialised by UoL spin-out Keracol (Impact Case Study 3).

'*Metal Complexes*' (**Marsden**, **McGowan**, **Blacker**). PCT Int. Appl. WO 2017103623A1 (2015). Describes highly active and robust homogeneous catalysts for redox-neutral alkylation of amines for use in fine chemical synthesis. Technology licensed under royalty to Umicore N.V.

'*Heterocyclic urea compounds*' (**Fishwick**). PCT 9060515 (2015). Describes the invention of a new class of antibacterial agents for use in combating infections involving Gram-positive bacteria.

'*Modulators of androgen synthesis*' (**Taylor**), US Patents US 9072743 (2015), US 9375433 (2016), US 9585887 (2017), US 9585890 (2017) and US 9808462 (2017); Australian Patent AU 2013322612 and NZ Patent NZ 706067 (2017). Describes using the compound VAL401 to treat lung cancer, and pancreatic and prostate adenocarcinomas; the compound has successfully negotiated phase II clinical trials and is being developed by ValiSeek Ltd.

'*BIOSENSOR*' (**AL Nelson**). European Patent EP 2 176 654 B1 (2017). Describes the first genuine robust toxicity sensor which can be used in water and Pharma screening.

'*Provision of Microbacterial Growth in Sugar-Solutions*' (**Blacker**). Application W&R Ref: P753012GB - UOL 16016/GB/P1 (2019). Describes the automated control of microbial infection in sugar solutions derived from municipal solid waste.

'*Catalytic Converter*' (**Plane**). PCT Int. Appl. WO 2020148522 (2020). Describes a new low-cost catalyst for the removal of NO_x in engine exhausts.

Outreach Activities

The School of Chemistry offers free-to-access MOOCs (Massive Open Online Courses) through FutureLearn. Five courses in Medicinal Chemistry (**Willans, Foster**, **Taylor**), Global Challenges and Chemical Products (**Fishwick, Marsden, Rayner, Turnbull**), Atmospheric Chemistry (**Heard**) and Planetary Chemistry (**Lehman**) have attracted a total of 103,075 registrations since 2017, of which 43,300 are active learners

(https://www.futurelearn.com/subjects/science-engineering-and-maths-courses/chemistry).

The Superposition (https://www.thesuperposition.org/) is an open collective of science and arts people in and around Leeds who do creative work at the science/art interface (founded by **Whitaker** with an RSC grant). **Beales** commissioned a kinetic sculpture as part of EPSRC grant EP/M027929/1 (https://www.youtube.com/watch?v=W4WmQs6q6t0).

The *Astbury Conversation* is a biennial international conference (since 2016) at the interfaces between chemistry, biology and physics, which embeds a public lecture, a public exhibition attended by >300 people, and a laboratory masterclass for Year 12 and 13 school students.

Public lectures include: Cafe Scientifique (**Beales**, **Hardie, Turnbull**), Pint of Science (**Beales, Lehman, Turnbull, Wilson**), Bolton Lecture in Astronomy (**Plane**).