Institution: The University of Leeds

Unit of Assessment: Chemistry (UoA 8)

a. Overview

The School of Chemistry (SoC) at the University of Leeds is a major UK chemistry department conducting the full continuum from fundamental through to exploitable and translational research. Evidence for excellence includes:

- since January 2008, SoC authors have published 924 journal articles, 13 book chapters, and 6 books. This work has received more than 7414 citations (Scopus) and includes 59 articles in *Science,* the *Nature* series*, PNAS, JACS* and *Angewandte Chemie*
- 47 patent applications in the Patent Cooperation Treaty or National Phase; currently, 11 patents are granted and maintained in the European and National Phase.
- 31% of staff returned in the REF5 have held a major fellowship during the REF period
- £26.8M research income (1/8/2008 to 31/8/2013), including £18.2M from RCUK. Current grants include two ERC Grants (at Advanced and Starting level), an EPSRC Leadership fellowship, and the recent award of a £3M contract from Sinochem of China.
- 77% of eligible staff have executed outstanding fundamental research (and are included in REF5) whilst the primary function of many other staff has been to translate and to exploit Leeds SoC research; the significant impact of this research is highlighted in the accompanying REF3a document.

The University has invested £18.2M in the School since 2008, including £3.5M to transform research at the interfaces of chemistry with medicine and chemical engineering.

Research is structured into five groups:

- *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**)

There is also a smaller sixth group, *Colour and Polymer Science*, which has primarily focused on exploitable research and is described in REF3a. The groups enjoy significant collaborations with researchers elsewhere in the Faculty of Mathematics and Physical Sciences, as well as in the Faculties of Biological Sciences, Earth and Environment, Engineering, and Medicine and Health. There are also very 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.

Three exemplar research highlights during the REF period have been: (1) the development of methods for preparing bioactive compounds of unprecedented diversity, now being translated and exploited through the €196M European Lead Factory (a platform for discovering leads for drug discovery); (2) the discovery of the importance of iodine in the chemistry of the Earth's atmosphere, using a combination of field measurements from the remote tropical oceans to the polar regions, and laboratory studies of the fundamental processes involved; (3) the development of a new approach to multidimensional many-body quantum dynamics, so that phenomena such as ultrafast photodynamics can be treated at the quantum level for the first time.

b. Research strategy

Research in the School is overseen by the Research and Innovation Committee, which is responsible for strategic planning, galvanising new research initiatives, promoting the translation and exploitation of fundamental research (REF3a), prioritising new instrument acquisitions, and management of the various research and analytical services. The committee meets monthly, and also organises two research strategy lunches per year to which all staff are invited.

The SoC's research strategy has been to focus on the distinctive themes of the five research groups. Following a review in 2011, some of the groups described in RAE2008 were reorganised to reflect growing strengths in new directions. The research themes are all at the disciplinary interfaces of chemistry with: physics, geology and biology (APC), biology and medicine (CBMC), physics and mathematics (CCCP), materials science and medicine (CDA), and chemical engineering (PRD). Three of the themes – atmospheric chemistry, chemical biology, and directed

assembly - were already judged to be very strong in RAE2008; since then, CBMC and CDA have grown substantially through new staff appointments (Section (c)). A further exciting change to the research base since RAE2008 has been the creation of the highly successful *Institute for Process Research and Development* (iPRD), described below. Their extensive industrial research collaborations, along with the strong industrial links in Colour and Polymer Chemistry and a number of spin-out companies, are an important dimension to the School's research portfolio.

The five research groups are listed below in alphabetical order. Membership of the groups (staff names in bold type) cuts across the traditional teaching sections - Inorganic, Organic and Physical - and staff are not restricted to being in a single group.

***Atmospheric and Planetary Chemistry*:** The vision of this group is to study the entire terrestrial atmosphere from the surface to the thermosphere, as well as the atmospheres of other solar system bodies (**Blitz, Heard**, **Pilling**, **Plane**, **Seakins**, **Whalley**). The UK is rated in the top two countries in the world in Atmospheric Chemistry (2009 International Review of UK Chemistry), and APC is a leading UK Chemistry department group judged by NERC grant income (in the top 4 during the REF period - current awards = £7.5M). In several areas - field observations of tropospheric radical species, laboratory gas kinetics, and chemistry of the mesosphere - the group is world-leading. There are close collaborations with colleagues in the *Institute for Climate and Atmospheric Science* (ICAS) within the School of Earth & Environment. There is also a strong synergy with the CCCP group, fostered by weekly internal seminars involving both groups.

The strategy of this group has been to use the full spectrum of atmospheric chemistry research techniques - observations (FAGE and DOAS measurements of tropospheric radicals; satellite retrievals of mesospheric metals); laboratory studies of elementary reaction kinetics and photochemistry, including simulations in a highly-instrumented atmospheric chamber (HIRAC); and modelling, in particular the *Master Chemical Mechanism* (MCM - developed at Leeds; see Impact Case Study 4), and the *Whole Atmosphere Community Climate Model* (WACCM – a US model with significant Leeds enhancements). The inclusion of four fellows from the *National Centre for Atmospheric Science* (NCAS) in the group provides a substantial boost to the research portfolio.

Research highlights include: **Plane1** (*Nature*), which demonstrates the substantial influence of bromine and iodine chemistry on tropospheric ozone loss in the tropical marine boundary layer, impacting on the lifetimes of greenhouse gases; **Seakins1** (*Science*), which reports the discovery that vibrationally excited, non-thermalized species play an important role in the tropospheric chemistry of organic species, impacting on air quality; and **Whalley1** (*Atmos. Chem. Phys.*), which shows that the oxidation rate of globally important emissions of organic species from tropical forests is hugely underestimated.

Three areas were highlighted in RAE2008 for development and for which funding has been specifically sought. (1) *Heterogeneous chemistry*. Substantial advances have been made through grants from the NERC and Leverhulme Trust enabling the development of novel laboratory techniques for synthesising atmospheric nano-particles using photochemical and sol-gel techniques, studying the kinetics of ultrafine aerosol formation, growth and radical uptake (**Heard** and **Plane**). (2) *Interstellar and Planetary Atmospheres*. Major new laboratory programmes funded by the EPSRC and ERC (€2.5M Advanced grant) to study radical reactions using vacuum ultra-violet laser photo-ionization coupled with time-of-flight mass spectrometry; a pulsed Laval nozzle reactor to study reactions at ultra-cold temperatures; and a flowing afterglow system to study dissociative electron recombination reactions of ions in planetary ionospheres (**Blitz, Heard, Plane** and **Seakins**). (3) *Lidars*. **Plane** was a partner with QinetiQ and Hovemere Ltd in a consortium which won a major European Space Agency contract for a feasibility study for a satellite-borne lidar to measure winds and temperature in the upper atmosphere, and is now part of a task force at NASA Goddard Space Flight Center for a similar scoping study.

Significant aspects of the group's research portfolio links into major research directions of the Research Councils (e.g. energy, climate change, and air quality), and future plans include work in combustion/engineering issues related to carbon capture. The group also plan to increase their profile in planetary atmospheres (including explanets where higher temperatures allow synergies with combustion/pyrolysis work) and interstellar chemistry. They have published 213 papers since 2008 [1445 citations, 6.8 citations per paper] including publications in *Science*, *Nature*, *Nature Chemistry*, *Nature Geoscience* and the *Journal of the American Chemical Society (JACS)*.

***Chemical Biology and Medicinal Chemistry*:** The vision of this group is to develop and apply chemical approaches to understand fundamental biological mechanisms and to diagnose and treat disease. The group's research fully aligns with, and is funded by, a diverse range of funders including research councils, the EU, industry and biomedical charities. The group's research, at the interfaces with biology and medicine, is underpinned by expertise in the synthesis of novel, diverse small molecules (**AS Nelson**); medicinal chemistry (**Fishwick**, **Bon**); molecular recognition (**Wilson**); mechanistic enzymology (**Webb**); carbohydrate chemistry and biophysical chemistry (**Turnbull**); peptide chemistry (**Warriner**); nanoparticle diagnostics and therapeutics (**Zhou** and **Guo**); and biological colorants and photomedicines (**Sergeeva**). Research foci include: chemical probes of fundamental biological mechanisms; the development of drugs with novel therapeutic mechanisms; the directed evolution of proteins with valuable properties; and structural and mechanistic studies of enzymes. The *Astbury Centre for Structural Molecular Biology* (**AS Nelson** and **Wilson** served as Director (2009-2011) and Deputy Director (2012-), respectively) and the *Biomedical and Health Research Centre* (BHRC) foster interdisciplinary collaborations, most notably with the Faculties of Biological Sciences and Medicine & Health. There are strong synergies with the PRD group (in the area of bioactive small molecule synthesis) and the CDA group (in the area of targeted molecular delivery). EPSRC has explicitly cited the SoC as a major site for investment in chemical biology.

Chemical biology is underpinned by novel approaches for the preparation of diverse bioactive small molecules, including a synthesis of natural product-like molecules with unprecedented scaffold diversity that was highlighted in two *Nature* series journals, *Science, C&E News* and *Angewandte Chemie* (**Nelson1**). The extension of these synthetic approaches to diverse lead-like molecules is currently under vigorous development, and is being exploited in a recent €196M Innovative Medicines Initiative award to establish a European Lead Factory (€2M Leeds share – **AS Nelson**, **Marsden**). A major focus has been to develop chemical probes of biological mechanisms that are of direct value to biologists: for example modulators of protein-protein interactions (**Wilson2**), and stable mimetics of post-translationally modified proteins (**Bon1**, **Webb2**); remarkably, a protein kinase inhibitor was discovered that promotes the self-renewal of murine embryonic stem cells (**Nelson2**, featured in *Cell Stem Cell*), whilst resulting in the chemically-directed differentiation of human embryonic stem cells. A study into the nanomechanical detection of antibiotic mucopeptide bonding related to superbug drug resistance (**Zhou1**) received widespread coverage in the media.

Translational research has been greatly enhanced through institutional investment in the BHRC, which is a partnership between the University's four STEM faculties and the Leeds Teaching Hospitals NHS Trust. The BHRC was established through £13M investment (£10M from the University's Transformation Fund; Chemistry share: £1.2M). BHRC has invested in three technology groups and 16 Senior Translational Research Fellows (including **Bon** and **Beales**). The University's Medicinal Chemistry & Chemical Biology group (Director: **Fishwick**) exploit the outstanding research infrastructure for research at the interface with biology, and have expertise in synthesis, medicinal chemistry (including structure-based drug design) and high-throughput screening. They collaborate on drug discovery programmes in a wide range of therapeutic areas in collaboration with colleagues from the Faculties of Biological Sciences and Medicine & Health. In addition, lead-like small molecule scaffolds are being commercialised following a licensing deal with Albany Molecular Research Inc. The group has published 245 papers [2148 citations, 8.7 citations per paper] since 2008 including papers in *Nature Chemistry, Nature Genetics, Nature Chemical Biology, Nature Nanotechnology*, *Angewandte Chemie* and *JACS.*

***Computational Chemistry and Chemical Physics*:** This group covers research in chemical physics and mathematical chemistry: gas-phase chemical dynamics, including coherent control (**Nix** and **Whitaker**); oscillatory and autocatalytic reactions (**Taylor**); and theoretical treatments of gas- and liquid-phase dynamics (**Pessoa de Miranda** and **Shalashilin**). There is a strong overlap with the APC group in areas such as photochemistry. During the REF period this group have made important experimental (**Nix1**, **Whitaker1**) and theoretical (**Pessoa de Miranda1**, **Shalashilin2**) contributions to gas-phase reaction dynamics. Significant work in this area is planned to continue with further developments in velocity map imaging spectrometry (**Whitaker**), multidimensional quantum mechanics (**Shalashilin**), and the rigorous quantification of dynamical reaction mechanisms (**Pessoa de Miranda**). The group's vision for the next 5 years is to apply these

techniques to study much more complicated reactions and processes, such as condensed phase chemical physics and protein dynamics, through building links with biology and quantum physics. **Taylor** already has a strong track record in experimental studies and mathematical modelling of complex chemical kinetics in solution. A highlight is her paper **Taylor1** (*Science*), which explains how the communication between unicellular organisms becomes coordinated with increasing cell density. The group has published 91 papers since 2008 [430 citations, 4.7 citations per paper], including papers in *Science*, *Physical Review Letters*, and *Angewandte Chemie*.

***Crystallisation and Directed Assembly*:** The vision of this research group is to apply assembly-based approaches, operating over length scales ranging from atomic to macroscopic, to generate new functional materials. An overarching goal is to gain understanding of the physico-chemical interactions which govern these mechanisms, and the materials range from hard inorganic materials, through soft bio-related molecules, to nanoscale supramolecular assemblies. The ability to design and synthesise functional materials through self-assembly is a complex problem whose resolution demands a long-term approach, as recognised by the adoption of the theme "Directed Assembly of Extended Structures with Targeted Properties" as an EPSRC Grand Challenge. Self-assembly is also an important component of the Grand Challenge "Systems Chemistry: Exploring the Chemical Roots of Biological Organisation".

This challenge is being met at Leeds through two University-wide research centres. First is the *Centre for Molecular Nanoscience* (CMNS). The research interests of the SoC members of CMNS include: liquid crystals (**Bushby**), self-assembly of peptides (**Aggeli**); nanotoxicology (**Beales**, **LA Nelson**); nanostructures, membranes and polymers (**Beales**, **Bushby**, **LA Nelson**, **Thornton**); multi-scale modelling (**Auer**); and nanomedicine (**Beales**), which overlaps with the CBMC group (in particular **Wilson**). Second is the *Leeds Centre for Crystallization* (established in 2012; Director: **Meldrum**), which enables this group to profit from the huge expertise available in crystallisation at Leeds. Focusing on the production of new materials, SoC members of the Crystallisation Centre synthesise metal-organic molecular-crystals which exhibit valuable switching properties (**Halcrow**), and metal-organic framework compounds with potential catalytic and separation properties (**Gould** and **Hardie**). Bio-inspired approaches are used to control crystal nucleation and growth, and to generate new materials with hierarchical structures (**Meldrum**).

Research highlights of CDA include: **Auer2** (*Phys. Rev. Lett.*), which addresses the common tendency of peptides and proteins to assemble into fibrillar aggregates, important because such oligomeric aggregates are associated with degenerative diseases such as Alzheimer's; **Meldrum1** (*Nat. Mater.*) which describes the formation of inorganic/organic composites with properties comparable to native biominerals; and **Hardie1** (*Nat. Chem.*), which describes a new form of molecular knot which is one of the most topologically complex, mechanically interlocked molecules that has yet been reported. The group has published 214 papers since 2008 [1929 citations, 9.0 citations per paper] including papers in *Nature Chemistry, Nature Materials, Advanced Materials, Advanced Functional Materials, Angewandte Chemie*, *and JACS*, and hold 5 granted and maintained patents.

***Process Research and Development*:** The vision of this group is to provide novel solutions for the sustainable and economic manufacture of fine chemicals, pharmaceuticals and new materials. Interactions in the key area between chemistry and chemical engineering are managed through the iPRD. This was established in 2008 as a collaborative venture with the School of Process, Environment and Materials Engineering (SPEME) through extensive University investment (a £2M Transformation Fund project), and is underpinned by four joint appointments between the two Schools within the REF period – **Blacker** (ex-ICI/Avecia/Piramal) and Frans Muller (ex-Syngenta/AstraZeneca) at chair level, and **Nguyen** and Richard Bourne at fellow level (Muller/Bourne are returned under UoA12). **Blacker** and Muller were appointed from industry with over 30 years' experience. The Institute builds on expertise in synthesis (**Marsden**) and catalysis (**Blacker**, **Marsden**, **McGowan**, **Nguyen**, **Willans**). These activities, focused through the iPRD, are achieved through a balanced portfolio of basic research (RCUK and EU-funded), translational research (e.g. TSB-funded) and client/product-specific work (ERDF and contract/consultancy-funded). In all cases, industrial partnership and, where appropriate, co-funding of research, is key to ensuring the end-user relevance. This is managed through an *Industrial Club* comprising 15 companies from the UK, EU and beyond (China, India, Switzerland). Their interests range from pharmaceuticals to equipment manufacture.

The development of hydrogen transfer chemistry exemplifies the integrated research/innovation approach. Building on a catalyst developed for amine racemisation by **Blacker** at Avecia/Piramal, **Marsden** and **Blacker** secured EPSRC funding for a collaborative project (with Prof Jon Williams, Bath and Piramal) to develop novel hydrogen transfer chemistries of amines. This in turn led to two consecutive TSB-funded projects to develop immobilised variants of the catalysts (**Blacker**, **McGowan** – with AstraZeneca, Pfizer, Reaxa, Yorkshire Process Technology (YPT)), a licensing deal to exploit the UoL-held IP generated (with Yorkshire Process Technology), two industrially co-sponsored studentships (AstraZeneca) and an EPSRC/KTS project with GlaxoSmithKline.

The group's strong record of collaboration with industry is evidenced by participation in 8 TSB grants supporting supply chains in the process chemistry sector (see REF3a for details). The commercial exploitation of technologies developed in the iPRD is a key part of the strategy, and has been realised through the establishment of University spin-outs (Keracol, C-Capture) and licensing deals (YPT, Albany Molecular Research Inc). The iPRD is a major partner in a recent €26m Innovative Medicines Initiative award in Sustainable Pharmaceutical Chemistry (CHEM21) [€1.5m Leeds share – **Blacker**, **Marsden**, **AS Nelson**]. In the next 5 years the PRD group will focus on process intensification through continuous technologies, closer integration with particle technology (SPEME at Leeds) to underpin holistic approaches to the development and production of new commercial entities, and the processing and utilisation of sustainable feedstocks.

Research highlights include: a novel catalyst system for producing coloured polymer materials in a single step (**McGowan1**, *Angew. Chem.*), which has received world-wide coverage - the "Black Dress" created using the process is now on display at the Science Museum; and a new catalytic method for synthesis of complex amines by activation of simpler amines (rather than previously-used alcohols) using a "borrowing hydrogen" approach (**Blacker2**, *Angew. Chem.*). The group has published 161 papers [1462 citations, 9.1 citations per paper] since 2008, including papers in *Nature Chemistry, Angewandte Chemie* and *JACS*, and hold 6 granted and maintained patents.

c. People, including:

i. Staffing strategy and staff development

Staff are listed below in their primary research group, although many staff contribute to the activities of other research groups. Status is indicated in parentheses: AP = Associate Professor, L = Lecturer, P = Professor, R = Reader, RF = Research Fellow, RP = Research Professor, SL = Senior Lecturer. The names of ECRs are italicized, and group leaders are underlined.

APC Staff summary: Blitz (RF), Heard (P), Pilling (RP), Plane (P), Seakins (P), Whalley (RF). Currently there are 11 PDRAs and 16 PGRs.

CBMC Staff summary: *Bon* (RF), Fishwick (P), *Guo* (RF), AS Nelson (P), *Sergeeva* (L), Turnbull (AP), Warriner (SL), Webb (L), Wilson (P), Zhou (SL). **New staff:** Bon, Guo, Sergeeva. Currently there are 18 PDRAs and 44 PGRs.

CCCP Staff summary: *Nix* (L), Pessoa de Miranda (L), Shalashilin (SL), Taylor (SL), Whitaker (P). **New staff:** Nix. Currently there are 4 PDRAs and 7 PGRs.

CDA Staff summary: Aggeli (L), Auer (L), *Beales* (RF), Bushby (RP), *Gould* (L), Halcrow (P), Hardie (P), Meldrum (P), LA Nelson (P), *Thornton* (L). **New staff:** Auer, Beales, Gould, Meldrum, Thornton. Currently there are 15 PDRAs and 19 PGRs.

PRD Staff summary: Blacker (P), Marsden (P), McGowan (R), Willans (RF), *Nguyen* (RF). **New staff:** Blacker, Willans, Nguyen. Currently there are 12 PDRAs and 30 PGRs.

Eleven out of 36 returned staff have held major **fellowships** during the REF period: EPSRC Advanced Fellowship (2004-2009, **AS Nelson**); EPSRC Leadership Fellowship (2010-15, **Meldrum**); ERC Advanced Grant Fellowship (2012-2017, **Plane**), ERC Early Career Fellowship (2010-2015, **Wilson**); RCUK Academic Fellowships (2005-2010, **Taylor**; 2008-13, **Auer**); Royal Society Dorothy Hodgkin Fellowship (2009-2017, **Willans**); Royal Society Industry Fellowship (2008-10, **Marsden**); Royal Society University Research Fellowships (2001-2010, **Aggeli**; 2005-2013, **Turnbull**); Wellcome Trust Career Re-entry Fellowship (2012-2016, **Guo**).

There is an even distribution of experience: 15 research fellows and lecturers; 6 senior lecturers/readers/associate professors; and 15 professors. During the REF period, excluding retirements, only one permanent staff member has left (Murray, who moved to the School of Earth and Environment in the University and is still closely involved with the APC group). Nine new staff

have been added; these are mostly in CBMC, CDA and PRD, reflecting the University's investment through its Transformation Fund. The next new staff appointment is planned to be at the lecturer level in atmospheric chemistry, in one of the areas highlighted for growth in section (b).

Eight members of the academic staff are female (20% of staff, 2 are Professors), compared with just 4 in RAE2008, while the gender mix at other levels is broad (43% at postgraduate level and 25% at postdoctoral level). The Faculty of Maths and Physical Sciences was awarded an Athena SWAN Silver award in 2012. Further details of the faculty equality and diversity policy can be found at www.maps.leeds.ac.uk/.

All staff are supported by the *Staff and Departmental Development Unit* (SDDU), which provides an integrated training and development service. The University has a *Next Generation Researcher* programme, which has been developed in line with the Concordat to Support the Career Development of Researchers and the national Researcher Development Framework (RDF).The implementation of the programme has, with the ending of ring-fenced Research Councils UK (RCUK) Careers Development and Skills Training (Roberts) funding in 2011, led to the creation of a faculty training hub to provide training and development for research students and research staff. In 2010, Leeds was awarded the HR Excellence in Research Award by the European Commission in recognition of its commitment to career development for researchers.

At the heart of the development of all staff is the *Staff Review and Development Scheme*, which helps staff achieve their full potential by providing an annual two-way review of progress, identifying key objectives, providing constructive feedback, and identifying and planning appropriate development. All staff go through probation if they have not already done so for their current or similar role. Early career staff in the SoC have a reduced teaching load (typically starting at 20% and ramping up over 3 years), and their research progress is mentored on a regular (at least quarterly) basis through meetings with a designated senior member of staff. Staff members are also fully supported in making grant applications. Research proposals are reviewed internally by two independent members of staff before submission. Staff also enter annually onto a database their planned applications for the following 18 months, typically in consultation with their research group leader. The implementation of these plans is then reviewed during an annual meeting between each staff member and the Head of School and Director of Research & Innovation.

ii. Research students

The 107 PGR students in the School (at 30/09/2013) are funded by EPSRC (52), NERC (14), University and SoC Scholarships (14), overseas sponsors (7), ERC (6), industry (6), charities (3), BBSRC (1) and MRC (1). The School is a major stakeholder in graduate programmes within the University including the Astbury Centre's Wellcome Trust PGR programme (recently renewed to 2018), the BBSRC-funded White Rose Doctoral Training Partnership (with York and Sheffield), and the EPSRC-funded Molecular-scale Engineering, Tissue Engineering, and Energy CDTs. More than 60 studentships have been collaborative with industry. Studentships are advertised on the School of Chemistry website and FindaPhD.com, and an open day is held in Jan/Feb each year. All applicants are interviewed (in person, or via Skype for most overseas applicants) by a panel of three staff members drawn from across the School to maintain a common entry standard. 88% of incoming PGRs have a Master's degree (2011-2013 intake).

Research students agree a training plan with their supervisor within one month of starting. The University's Postgraduate Development Record System (PDRS) provides a training needs analysis tool, and is also used to record supervision meetings and training courses attended. PGR students in Chemistry are required to submit the following pieces of work during their degree: literature report (after 3 months); research reports at 6, 21 and 30 months; and a transfer report which is examined by a *viva voce* exam after 11 months. Students are interviewed one-on-one by the Progression tutor during each year of their degree to monitor general progress. Students also 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 prestigious Wellcome Trust-funded PhD scheme at Leeds has an external scientific advisory board who act as mentors to the students; recent members have included the Nobel Laureate Sir Tim Hunt, and the Max Planck Institute Directors Prof. Ulrich Hartl and Prof. Herbert Waldmann. It is notable that in the 2013 Postgraduate Research Experience Survey the School's PGRs rated the progression and monitoring procedures 10% above the Russell Group chemistry average.

PGR students have distinguished themselves at international conferences. Examples since 2010 include oral presentations at: the International Carbohydrate Symposium, Tokyo (M. Fascione); International Conference on Chemical Kinetics, MIT (R. Shannon); Faraday Discussion 147 on Chemistry of the Planets (C. Whalley); AGU Fall Meeting, San Francisco (P. Edwards); International Gas Kinetics Symposium, Boulder (J. Lockhart); and ACS meeting, New Orleans (V. Azzarito). Poster competition prizes include: XIX EuCheMS conference on organometallic chemistry, Toulouse (S. Lucas, top 2 out of 400 posters); ISSOL-Bioastronomy conference, Montpellier (K. Marriott); RSC H. A. Skinner prize at Faraday Discussion 153 (J. Milkiewicz); ANZMAG meeting in Victoria, Australia (K. Evans); 63rd Nobel Laureate Meeting, Lindau (C. Macrae); 6th RSC Medicinal Chemistry symposium (K. Long); 8th International Conference on Chemical Kinetics (N. Howes and R. Caravan). In March 2012, four PGR students were selected to present their work at the SET for Britain event at the House of Commons, making the SoC the best represented chemistry department at the event.

PGR students have also progressed to prestigious research careers during the REF period: Christopher Cordier (PhD 2008) secured a Herchel Smith fellowship (Cambridge) and is now a Royal Society University Research Fellow (Imperial); Martin Fascione (PhD 2009) holds a Marie Curie International Outgoing Fellowship at the University of British Columbia/University of York; Anoop Mahajan (PhD 2009) is now a staff scientist at the Indian Institute of Tropical Meteorology; Roisin Commane (PhD 2009) is at Harvard University; Fred Campbell (PhD 2009) is a Marie Curie Fellow in Leiden; Iain Wilkinson (PhD 2010) is at the Steacie Institute for Molecular Sciences, Ottawa; Peter Edwards (PhD 2011) is at the National Oceanic and Atmospheric Administration, Boulder; Lei Song (PhD 2013) is at Oxford University; Bram Cantaert (PhD 2013) is at the Nanyang Technological University, Singapore.

The SoC has ambitious plans to maintain the number and quality of our postgraduate intake, recognising that these students make a major contribution to the research program of the School and University. Between 2008 and 2012, the number of registered PGRs in the SoC increased from 86 to 115. Currently, a further 39 PGR students are registered outside Chemistry but supervised primarily by SoC staff. The School has an excellent record of successfully delivering PhD training: the completion rate of PGR students during the REF period has averaged 94.5%, with 85.0% of those submitting within 4 years of registration. Looking forward, besides the continuing BBSRC DTP, Wellcome Trust scheme and EPSRC CDTs referred to above, SoC research groups are involved in a number of new doctoral training programmes in the following strategic areas across the university: atmospheric chemistry (NERC DTP SPHERES), biofuels (EPSRC CDT in Bioenergy), and polymers (EPSRC CDT in Soft Matter Functional Interfaces).

d. Income, infrastructure and facilities

Since 2008, the University has invested £2.0M to create the iPRD and £1.2M for BHRC Research Fellows within the SoC. Other investments include £10.9M to refurbish several of the major research laboratories within the School; £1.6M for cost-sharing equipment purchase; and £1.0M for four University Research Fellows.

Research within the School is underpinned by 17 support staff including 4 research officers. The principal instrumental services - 6 NMR spectrometers (up to 600 MHz), 4 mass spectrometers, X-ray crystallography, optical spectroscopy, electron microscopy, thermal analysis, particle size analysis 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 refreshed in 2013 with a £1.7M grant (£1.0M from EPSRC, £0.7M from the University). The stringent safety needs of the School are provided for in part by two technicians, and the Chair of the Safety Committee sits on the School’s Management Committee. The School’s extensive IT requirements are served by 9 faculty staff. The electronic and mechanical workshops (2 technicians) provide general repair services but, more importantly, they build a range of instruments, primarily for the APC and CCCP groups. All support staff are encouraged to keep abreast of new developments by attending courses and conferences.

APC: This group has four very well-equipped laser laboratories (a total of 280 m^2 divided into 12 experimental bays) for studies of neutral, ion-molecule, particle nucleation and photochemical reactions. Equipment includes a wide variety of pulsed nanosecond lasers, time-of-flight and quadrupole mass spectrometers, a surface science UHV chamber, pulsed Laval nozzle reactor, grating and Fourier transform spectrometers, 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. 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) and absorption spectroscopy (the DOAS technique). The group is also home to the MCM, which is internationally recognised as the leading computer model of organic reactivity in the atmosphere. The group has 192 dedicated cores on the university's massively parallel high performance computer (POLARIS), which are used to run whole atmosphere chemistry-climate models.

CBMC: Superb research infrastructure at the interfaces with biology and medicine was provided through £7.5M JIF and £1.5M SRIF3 funding just before the REF period. Facilities include two Category 2 biological containment laboratories equipped for genetic manipulation, protein expression, purification and biophysical characterisation; and a suite for the synthesis and purification of small molecule libraries and peptides (1.0 FTE support for HPLC). A small molecule screening facility, with dehumidified ligand storage, robotic liquid handling, high-throughput screening and a laboratory informatics management system (1.5 FTE support), is exploited in ligand/drug discovery projects. Access to all major structural biology and biophysical techniques is available through the Astbury Centre.

CCCP: The APC and CCCP groups have between them access to one of the best equipped laser facilities in a UK chemistry department, with continuous wave, nanosecond and femtosecond sources from the deep IR to vacuum ultraviolet. This group also has a very high resolution velocity map imaging spectrometer. A newly refurbished laboratory (45 m^2) houses the complex chemical kinetics group. The computational group have sole access to an 80 node Beowulf cluster, and the group as a whole also make extensive use of the university's ARC1 high performance computer.

CDA: This group is supported across a number of laboratories including a newly-refurbished space for Meldrum's group (300 m^2), with a wide range of analytical equipment including Raman microscopy, BET, TGA and DSC, and a benchtop SEM, as well as synthetic laboratory suites. A new high resolution FEG-SEM with integral EDX, and a single crystal X-ray diffractometer with a microfocus dual wavelength X-ray source, were purchased in 2013 through the EPSRC Core Capability Scheme. The core members of CMNS have recently moved to a suite of new laboratories, which include space for electrochemistry, biochemistry, and chemical synthesis. Essential access to electron microscopy facilities is provided through university centres located in Engineering (a national EM facility run by Prof. R. Brydson) and Biology. SoC staff also have access to a bio-imaging facility (Biology), dynamic light scattering, powder diffraction and zeta-potential particle measurements (Engineering), and a SQUID magnetometer (Physics).

PRD: Through a £4.5M investment from Yorkshire Forward and the European Regional Development Agency (2009-2012), the Institute has built a fully operational process laboratory which is believed to be a unique facility in an academic host institution. The laboratory houses a wide variety of pilot-scale batch and flow process equipment in a safe environment that is suitable for both academic research and industry support. A dedicated laboratory manager is responsible for the facility. The lab enables safe scale-up of chemical processes up to 50 litre reactor and to make 10's kg of product, and has been used to help many SMEs and large international companies improve process performance and make material for testing.

e. Collaboration or contribution to the discipline or research base

Significant external collaborations are listed below by research group.

APC: leading involvement in NERC/EU-funded atmospheric field campaigns - RONOCO, OP3, COBRA, ClearFlo, SHIVA, CHABLIS (**Heard**, **Plane**); PI of EU HotPay multi-national suborbital rocket (**Plane**). The ERC CODITA project involves 9 partner institutions in the US and 3 in Germany (**Plane**). The HIRAC chamber is part of the EUROCHAMP network (**Seakins**, **Pilling**).

CBMC: PPI-net, a EPSRC/MRC/BBSRC-funded chemical biology network focusing on protein-protein interactions (**Wilson**, **AS Nelson**); EU COST action working groups "Multivalent ligands for cholera toxin inhibition and sensing" and "Multivalent Glycosystems for Nanoscience" (2011-) (**Turnbull**); EU COST action working group "Foldamers" management committee member and working group leader (**Wilson**, 2009-); leadership within the IMI-funded European Lead Factory consortium (EU funded, partners: Bayer, J&J, Sanofi, AstraZeneca, Merck, UCB, Lundbeck and 5 SMEs) (**AS Nelson**, **Marsden**). Professor Rob Liskamp (Univ. Utrecht) hosted at Leeds in 2012.

CCCP: EU ITN training networks ICONIC and LaserLab Europe (**Whitaker**). **Shalashilin's** new Ehrenfest approach to computational molecular dynamics is being included within the *MOLPRO* quantum chemistry program suite and his boxed accelerated classical molecular dynamics (BXD) has been added to the CHARMM package. He also holds a major NSF/EPSRC grant on nonadiabatic dynamics with Stanford University.

CDA: A team of 4 UK universities with an EPSRC Critical Mass grant on switchable molecular crystals (led by **Halcrow**). A team of 5 UK Universities within an EPSRC programme grant on hard/soft interfaces (**Meldrum**); 2 UK universities and 2 USA universities in a joint EPSRC/NSF Materials World Network grant (**Meldrum**); an EU FP7 network in nanotoxicology (**LA Nelson**).

PRD: Leading members of the IMI Sustainable Pharmaceutical Chemistry (CHEM21) consortium (EU funded, partners GSK, Pfizer, Orion, Bayer, J&J, Sanofi) (**Blacker**, **Marsden**, **AS Nelson**); Industrial collaborations with large companies: AstraZeneca (5 CASE, 2 TSB), Pfizer (2 TSB, 1 KTS), GSK (KTS), Syngenta (TSB), Bod Ayre (TSB), Body Shop (TSB), and SME's: Reaxa (TSB, Host of RS Industry Fellow - **Marsden**), YPT (TSB), Critical Processes (TSB), DyeCat (TSB), Avantium (TSB).

Leadership and Recognition in the Academic Community

Research awards: Royal Society Brian Mercer Award (**LA Nelson**). RSC Corday-Morgan medal (2008) (**AS Nelson**). RSC Corday-Morgan medal (2011) (**Hardie**). RSC Supramolecular Annual Bob Hay Lectureship (2012) (**Wilson**). RSC Carbohydrate Award (2013) (**Turnbull**).

Journal editorship: Editor, *Atmos. Measure. Tech.* (**Heard**). Editor-in-Chief, *J. Atmos. and Solar-Terr. Phys.* (**Plane**). Editorial Board membership: *Chem. Soc. Rev.* (**Heard** and **Meldrum**); *Polyhedron* (**Halcrow**); *MRS Bulletin* and *Int. Mater. Rev.* (**Meldrum**); *Cryst. Eng. Comm.* (**Hardie**), *J. Atmos. Chemistry* (**Plane**), *Org. Biomol. Chem.* (**Turnbull**).

Committee membership: Chair, RSC Faraday Division on Conferences (**Heard**). RSC Biomaterials Group, British Association of Crystal Growth, Board of Directors of the Materials Research Society (**Meldrum**). RSC Chemistry Biology Forum Executive and Chair, RSC Bioorganic Group (**AS Nelson**). Chair, RSC Gas Kinetics Discussion Group (**Seakins**). Chair, RSC Supramolecular Chemistry Group (**Wilson**). Chair, RSC Coordination Chemistry Discussion Group and member of Dalton Council (**McGowan**).

Scientific leadership: Co-I and Leader of the Catalysis Theme, Dial-a-Molecule EPSRC Grand Challenge (**Marsden**). Steering committee, European Research Course on Atmospheres (**Plane**). Chair of the CM1102 COST network with 60 research groups from 18 European countries (**Turnbull**). Co-I, PPI-net network in chemical biology (**Wilson**).

Funding panel membership: Chair, EPSRC Physical Sciences (Chemistry) panel, 2008 and 2012 (**Halcrow**). Chair EPSRC Bright Ideas Awards 2013 (**Meldrum**). EPSRC Strategic Equipment Panel, 2011- (**Marsden**). Materials Science Grants Review Panel, Academy of Finland, 2013 (**Meldrum**). Netherlands Organisation for Scientific Research funding panel (**Hardie**, L**A Nelson** and **Wilson**). Chair, EPSRC Organic Studentships Panel (**AS Nelson**). Deutsche Forschungsgemeinschaft review panel (2009-2011), ERC Advanced Grant proposal review panel (2008-2012), NASA Heliophysics senior review panel, 2013 (**Plane**). NASA grant panel, 2012 (**Seakins**). Newton International Fellowship Physical Sciences Committee, 2012- (**Turnbull**).

Scientific advisory board membership: Forschungszentrum, Jülich (**Heard**). International Advisory Board for "Fusion Materials" grant (Japan); EPSRC Physical Sciences Strategic Advisory Team (**Meldrum**). Independent Review Committee for Utrecht Institute for Pharmaceutical Sciences (**AS Nelson**). Max Planck Institute for Chemistry, Mainz (**Plane**).

International Scientific conference leadership: Scientific steering committee, RSC–IUPAC Congress, Glasgow (2009) (**Heard**); Chair, Faraday Meeting 159 (2012); Co-chair, Materials Research Society meeting, Mexico (2013) (**Meldrum**). Chair, IUGG - Layered Phenomena in the Mesopause Region (2013) (**Plane**). Chair, Atmospheric Chemistry Mechanisms Conference, UC Davis (2011) and International Gas Kinetics Symposium (2008 and 2010) (**Seakins**). Session leader, Gordon Research Conference on Nonlinear systems chemistry (2012) (**Taylor**). Chair, Faraday Discussion 153 (2010) (**Whitaker**).

Visiting Professorships: Visiting Associate Professor at Nagoya University, 2009 (**Halcrow**). Vielberth Foundation visiting Professor, University of Regensburg, 2012 (**Whitaker**).