

Institution: University of Sheffield
Unit of Assessment: 8 - Chemistry
<p>a. Overview. Chemistry at Sheffield is thriving, with vibrant activity in all core areas and particular strengths in Polymers, Theory, Supramolecular Chemistry, Chemical Biology and Nanoscience. Cross-disciplinarity is a key feature of both our current research and future plans: this drives many fruitful interactions with our academic and industrial partners across the UK and internationally, with fundamental chemistry supporting our work in materials, energy and medicine. The unit is organised into four clusters that cover the full spectrum of core chemical science and also reflect our research strengths: Theory and Spectroscopy; Polymers, Surfaces and Materials; Chemical Biology; and Synthesis.</p> <p>Restructuring during RAE2008 has led to a step change in the quality of the research environment in the current REF period: highlights include the election of two members of staff as Fellows of the Royal Society, several major research grant awards (EPSRC Programme, Platform and Critical Mass grants; two ERC Advanced grants), with £10M of new grants awarded in the last 12 months. The major refurbishment programme of our laboratories is now complete and our plan to replace all major items of research equipment has been agreed with the University. During this REF period, six members of staff were promoted to professorships and seven to Readerships / Senior Lectureships. We have recruited six early-career researchers to balance our age and gender profile and ensure the long-term success of Chemistry in Sheffield. The substantial long-term grants held by the UoA will support internationally leading research activity through the next REF period, and we look forward to further growth in both volume and quality of our research outputs.</p>
<p>b. Research strategy</p> <p>Achievement of RAE2008 strategic aims. For RAE2008 we were organised into five clusters, which have been consolidated into four during the REF period: Theory and Spectroscopy; Polymers, Materials and Surfaces; Chemical Biology; and Synthesis. This structure reflects our strengths across core chemistry, whilst emphasising our interdisciplinary strengths in chemical biology and materials, which have represented a consistent strategic focus since RAE2001.</p> <p>A key goal of RAE2008 was to expand our staff complement from 35 to 40, which has been achieved <i>via</i> recent appointments in bioinorganic materials, chemical biology, synthesis, theory and catalysis (see part c). The addition of biological NMR (Waltho and Williamson), the appointments of Ciani and Staniland, and the promotion of Grasby and N Williams to personal chairs, reflects the growing strength of Chemical Biology. We have also raised the profile of Theory, developing the successful nucleus of Meijer, Pickup and Fowler established at RAE2008, as recognised by Fowler's recent election to FRS. Two new ECR appointments (Conte and Martsinovich) further strengthen Theory, and with the appointment of Hill in January 2014, we will boast one of the strongest activities in the UK in this area.</p> <p>Cross-disciplinary research was an important feature of RAE2008, and our strategy during the REF period has been to develop this activity. A particular goal was bioimaging, which has been developed as planned under the umbrella of the university-wide bioimaging initiative ('Imagine'): Leggett collaborates with Physics, using SPM and high-speed AFM techniques; Weinstein, Thomas and Armes collaborate with Biology on tissue engineering, luminescent compounds for cell imaging, and novel fluorescent polymers for intracellular delivery and labelling. There are many other strong, thriving collaborations within the University, such as:</p> <p><i>Physics:</i> Ryan on organic photovoltaics; Jones and Leggett on super-resolution microscopy; Leggett, Rimmer, Ryan, Fairclough and Armes on soft matter.</p> <p><i>Biology:</i> Leggett on photosynthesis; Thomas on imaging; Jones on protein ligands; Hunter on protein folding; Armes on stem cells; Grasby and D Williams on nucleic acids; N Williams and Waltho on enzymology; Armes on drug delivery; Waltho and Williamson on structural biology; Hippler on gas sensing.</p> <p><i>Engineering:</i> Armes, Weinstein and Fowler on imaging; Fairclough on polymer crystallisation; Ryan and Rimmer on tissue engineering; Armes on 3D printing; Leggett on self-assembly; N Williams on</p>

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self-assembling calixarenes to create bioactive surfaces; Brammer on CO₂ capture and utilisation.

Medicine: Jones and Coldham on imaging; Rimmer on antimicrobial and dental materials; Jackson on tools for protein analysis; Armes on hydrogels; Harrity on adrenomedullin antagonists.

Future strategic goals. We remain committed to the principle that the UoA will maintain activity in all areas of fundamental chemistry, which will support our work in materials, energy and medicine. Major research directions over the next REF period will include low-dimensional chemistry using biologically-inspired design principles, understanding non-covalent interactions in the condensed state and at interfaces, synthesis of complex molecular systems, polymerisation-induced self-assembly, and the interface between discrete mathematics and chemistry.

At the core of what we do is an increased emphasis on sustainability, and the 'energy' societal theme puts chemistry at the heart of the University's research strategy. Our research in photophysics and photochemistry benefits from close alignment with "Project Sunshine", an overarching theme across the Faculty of Science that provides pump-priming funding. Work on photovoltaics (Martsinovich and Ryan), photophysics and light-harvesting (Ward and Weinstein), energetic compounds (Portius) and biofuels (Fairclough) has benefited from this initiative.

Research in the **Synthesis** cluster will underpin research activity across many different areas. The UoA has strength in this key discipline, which feeds into a number of major research programmes. Important themes will include synthetic methodology for total synthesis and medicine, fundamental aspects of homogeneous and heterogeneous catalysis, design of crystalline materials and self-assembly of materials with novel light-harvesting, luminescence, guest-binding, gas separation, or catalytic properties. The **Polymers, Materials and Surfaces** cluster will concentrate on synthesis and processing of polymeric materials for nanotechnology and photonics applications, with the construction of solar cells in collaboration with physicists and the design of novel biomaterials with engineers and biologists. The cluster will use self-assembly and surface patterning to investigate interfacial phenomena, including tribology, adhesion and biocompatibility. The **Chemical Biology** cluster will focus on developing new chemical tools to tackle important problems in biology and medicine, and on unravelling the underpinning molecular processes of catalysis and recognition in biological systems. The NMR groups led by Waltho and Williamson will continue to play a leading role here. The appointment of Staniland will establish a new research area at the interface of biology and materials chemistry on biogenic synthesis of magnetic nanoparticles. The **Theory and Spectroscopy** cluster will build on its strong foundations in fundamental theory, calculation, simulation and modelling, with new appointments adding to our strengths in molecular properties, aromaticity, basis set design, dynamics, interfacial chemistry and physics, large-scale *ab initio* computation, and simulation of devices and materials.

The Krebs Institute for mechanistic biology will continue to provide a focus for collaboration with biologists and medics within the University. The Kroto Research Institute will provide a similar focus for collaboration with engineers, physicists and cell biologists. These structures map well onto our cluster organisation, and have been particularly fruitful in developing applications of synthetic chemistry in new collaborations with the Medical School, and Biology (Jackson, Coldham, Harrity and Jones).

Promoting and sustaining an active research culture: We foster our vibrant research culture through a Research Committee that rapidly identifies emerging themes and challenges, and a programme of seminars and half-day symposia with speakers nominated by each research cluster. This programme facilitates exchange and dissemination of ideas both within the UoA and with visitors from around the world. Research Away-Days are held regularly, at which members of staff discuss issues such as research collaboration, IP protection and exploitation, best practice in PhD student supervision, and identifying new research and funding opportunities. The heads of each research cluster provide leadership and make decisions on research investment *via* the Executive Committee; they are also involved in major decisions concerning infrastructure improvements, bids for large-scale equipment, and allocation of space. Research council DTA resources are deployed strategically to stimulate research activity in key areas. Importantly, the involvement of many staff in national (RCUK) / international (EU / FP7) funding and policy bodies (part e) ensures that we are at the forefront of formulating and responding to new initiatives.

Our new appointments in catalysis (Conte), bioinorganic materials (Staniland) and theory (Conte,

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Martsinovich; Hill from 2014) reflect the research priorities identified above and will open up new lines of research and collaborative opportunities. Existing grants will support our research activities well into the next assessment period (e.g. 5-year Platform, Programme, Critical Mass and ERC awards). Long-term stability is ensured by the breadth of our funding portfolio and the balanced age profile of our staff.

c. People

Staffing strategy. Our academic staffing strategy reflects our long-term research plan to maintain a wide research base covering all core areas of chemistry, whilst maintaining critical mass in key interdisciplinary areas. An expansion of our academic staff complement was a goal identified in RAE2008, and the number has grown from 35 to 40, as planned. Early in the REF period, we recruited two new lecturers, one in chemical biology (Ciani) and one in synthesis (Portius). This year we have made four more appointments: in bioinorganic materials (Staniland), catalysis/theory (Conte), and theory (Martsinovich, and Hill from 2014). We have also increased the number of University Teachers to five to enable researchers to maximise their effectiveness. More than half of our academic staff are mid-career: the six new appointments made during the REF period have balanced our age profile, which puts the UoA in a strong position to maintain its vibrant research activity for the foreseeable future.

Career Development Support. We aim to create an environment that supports and promotes success, encouraging staff to achieve and excel. Our staff development strategy provides clear mechanisms for facilitating progression of staff (including research assistants) at all stages of their careers. These mechanisms include the use of mentoring, probation, CV reviews and promotion advice, staff review, and research planning. In the annual appraisal, progress over the previous 12 months is examined and realistic targets are agreed for the next 12 months. This is a supportive and constructive process, which allows staff – especially those less experienced – to discuss research plans and grant application strategies with senior colleagues. All staff are members of at least one research cluster to foster collegiality, encourage the development of collaborations, formulate joint bids for shared equipment, and provide a framework for training and development of PhD students and PDRAs. The success of our staff development process is illustrated by our two EPSRC Advanced Research Fellows (Portius, Weinstein), who have successfully established independent research groups and were appointed to lectureships (Weinstein is now SL).

Newly appointed members of academic staff are individually mentored by a senior colleague during a 3-year probation period. This develops research skills, including writing proposals and papers, planning and supervision of research, identifying funding opportunities, and developing collaborations. Teaching and administrative loads are kept low initially to allow new staff to develop their research programmes. New members of staff are supported with start-up funding, allocation of PhD studentships, access to a pool of shared equipment, funds for international travel and reduced teaching loads, as well as mentoring from senior colleagues.

The success of our strategies for ensuring career development of staff at all levels is shown by the fact that during the REF period six members of staff were promoted to professor and two others have accepted chair appointments elsewhere. In addition, seven members of staff have been promoted to Senior Lecturer / Reader, and two were elected Fellows of the Royal Society.

Teaching Relief and Study Leave. The increased complement of University Teachers means that academic staff teaching loads have been managed so as not to have an impact on research capacity in the REF period. We provide targeted teaching relief for staff to take sabbatical leave to work in another institution and develop new research expertise: our study-leave policy prioritises staff secondments to industrial or university laboratories to build new collaborative links and learn new skills.

Research Fellowships. Research activity in the UoA has been boosted by the award of seven prestigious research fellowships, which are a clear indication of the quality of our research environment. Two members of staff were awarded Leverhulme Senior Research Fellowships (Ward, Fowler), three held EPSRC Research Fellowships [one Senior (Hunter) and two Advanced (Portius and Weinstein)]. Harrity was awarded a Royal Society Industry fellowship to work with Peakdale Molecular, and Coldham was awarded a Leverhulme Study Abroad Fellowship to work

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with collaborators in the US and Sweden.

External Visitors. Our stimulating research environment attracts research visitors from other organisations, which in turn strengthens our collaborative links with industry and universities worldwide. Eighteen academics from the US, Australia, Japan, Asia and Europe have worked here during their sabbatical leave in the REF period. Eight industrial scientists (from QuantuMDx, Murata Manufacturing, Advanced Manufacturing Research Centre Malaysia, Cytec and DSTL) have been seconded to the UoA for extended periods (>2 years in some cases).

ECR Integration and Career Development. Post-doctoral researchers (RAs) make a significant contribution to research in the UoA, and we have effective arrangements for managing their career progression. In 2012 the University was awarded the HR Excellence in Research award from the European Commission and we are committed to applying the 7 principles of the UK Concordat for the Career Development of Researchers and supporting the University's action plan. All RAs receive tailored inductions that highlight a range of Researcher Professional Development (RPD) and career development opportunities to fit their career tracks. Induction events facilitate networking across disciplines and RAs are supported by a researcher mentoring programme. All RAs are integrated into the staff review process, with the same opportunities as permanent staff, including guidance on career progression. PIs provide mentoring support to encourage and guide RAs in applications for independent funds (e.g. fellowships) to facilitate the transition to independent researcher. RAs are given the opportunity to undertake appropriate teaching duties as preparation for their independent academic careers. Our success in career development is evidenced by the number of Sheffield-trained chemists successfully gaining academic positions, with more than 20 researchers who worked in the UoA during this REF period now in permanent academic posts at universities throughout the world.

Equality and Diversity. We are committed to equality and diversity in all aspects of staffing; we recruit the best academic and research staff regardless of their race, gender, nationality, sexual orientation, or religion. A key diversity challenge for us, and for the profession as a whole, is to attract, retain and develop excellent female staff. The Faculty of Science is committed to being a place of choice for women to work and has established a Faculty Equality and Diversity Committee, chaired by Prof. Jane Grasby (Chemistry). Prof. Grasby has also been seconded for two days a week to the EPSRC Developing Leaders scheme to promote gender equality across the Faculty of Science. The University operates a Women Academic Returners Programme, which offers flexible funding to women returning after a break to ensure that they are able to focus on research, and from which two members of staff in the UoA have benefited. Five members of staff have taken maternity or paternity leave in the REF period. The UoA takes a flexible attitude to part-time contracts, and two academics have had part-time contracts to facilitate childcare arrangements, with a guarantee of a return to a full-time contract.

Research students

Postgraduate research students enrolled on doctoral programmes

Year	2008/09	2009/10	2010/11	2011/12	2012/13
Total FTE	121.8	116.8	104.3	103.5	108.8

(a) Funding. PhD students in the UoA are supported by a wide range of sources, which is important for ensuring the sustainability of the research student population. In the REF period, studentships have been funded by the EPSRC, BBSRC, EU, industry (see below), research charities and overseas governments (46 students from 10 different countries in the REF period). Additional long-term support from the University has allowed the UoA to fund 11 PhD studentships from its core budget. University support has also been provided through two White Rose studentship networks (with York and Leeds). A programme of 'A*Star' studentships (jointly funded by the University and research institutes in Singapore) has given several students the chance to spend two out of four PhD years in Singapore.

(b) Centres for Doctoral Training. Members of the UoA have played leading roles in establishing and managing 4 EPSRC interdisciplinary CDTs: Leggett was director of the Life Sciences Interface CDT and is co-director of the Molecular Scale Engineering CDT; Rimmer is co-director of the Tissue Engineering and Regenerative Medicine CDT; Ward is deputy director of the E-futures

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CDT. The recently announced chemistry-led CDT in Polymers, Soft Matter and Colloids (50 CASE studentships) will support collaborations with physicists, cell biologists and engineers. A substantial philanthropic donation has allowed the Faculty of Science to establish the Project Sunshine CDT, with three students based in Chemistry, and more to come as this area grows. Several members of the UoA are involved in the BBSRC White Rose Doctoral Training Partnership on Mechanistic Biology in collaboration with Leeds and York. These collaborative PhD networks now form an important part of our strategy for recruiting talented students into chemistry. **(c) Industry Collaborations.** The UoA has strong collaborations with the chemical industry, and 41 different companies – including all of the major UK pharma, agrochemical and polymer companies – have funded PhD student research in the UoA in the REF period. In addition to 27 EPSRC/BBSRC Industrial CASE awards, industrial collaborators provided support for 45 fully-funded and CASE-type studentships. These interactions have led directly to commercial exploitation: for example, collaboration with AstraZeneca on virtual co-crystal screening led to software, which has now been licenced to other companies by the University; collaboration with GSK developed synthetic routes to compounds that are now sold by Peakdale Molecular Ltd.

(d) Recruitment. PhD candidates must hold a minimum of a 2.1 Masters level degree in chemistry or an equivalent qualification; all UK PhD applicants are interviewed by at least two members of staff. The CDT schemes in which we participate are advertised nationally and attract very high quality applicants. The department provides matched funding from the DTA to encourage industrial collaboration; these studentships also attract excellent applicants. A new mechanism for allocating PhD studentships has been put in place, which allows us to advertise early and make sure that we recruit the highest-quality students.

(e) Research Training. The Department's Postgraduate Committee coordinates PhD training, including the University's Doctoral Development Programme (DDP), management of mentoring and progress, and pastoral care. All research students receive a thorough induction with different elements covered at University, Faculty and Department level. In addition to their primary supervisor, each student is assigned an independent advisor as an impartial mentor. The recent influx of students on 4-year programmes associated with CDTs has led to the development of a particularly thorough professional skills development package, which has been adopted for all PhD students. New students have a tailored "Training Needs Analysis" to identify which DDP modules and other activities are required to provide appropriate training both in transferable professional skills and subject-specific skills. Presentation of a written literature review (6 months), a research cluster seminar (9 months), a research report (12 months), a poster (24 months) and an outline thesis plan (30 months), all with formal assessment, are compulsory. Students attend research group seminars, departmental seminars and give regular presentations to their research group. In the third year, a talk is given as part of a research cluster symposium; students are also expected to give presentations at national or international conferences. PhD students can acquire teaching skills by acting as laboratory demonstrators or small-group tutors with appropriate training from our University Teachers. Many of our PhD students are part-funded by industry through CASE-type studentships, and this provides them with an opportunity to work in an industrial setting, develop employability skills and apply their research to solving practical problems.

Each PhD student's independent advisor is responsible for supporting the student's professional development. The University's 'Research Student Proposition', published in 2012, outlines what research students can expect from Sheffield and what Sheffield expects in return, and QA is embedded in procedures for supervising and training PhD students. A recent QAA report commended many aspects of the University's approach to this: areas specifically praised by the QAA include the induction events, the doctoral development programme, mechanisms for monitoring progress, and representation of PhD students on committees within the UoA.

The quality of the research training programme is reflected in the success of our students. Particular highlights include the Syngenta Scholarship Award in 2008 (Browne), Gold Medal at PhD level in the European Young Chemist Awards in 2008 (Mínguez Espallargas), RSC Dalton Young Researchers Award in 2009 (Mínguez Espallargas) and the Macro Group UK prize for the best PhD thesis in polymer science in 2012 (Thompson). PhD students in the UoA have been particularly successful in securing one-year EPSRC doctoral prize fellowships. Seventy-five per cent of our submitted REF outputs have PhD students as co-authors, further testifying to the

quality of our training.

d. Income, infrastructure and facilities

Research Funding. Support for research in the UoA comes from many sources, including EPSRC, BBSRC, ERC, EU and industry, reflecting our successful staffing strategy, which maintains expertise across the breadth of chemistry. This continues to be important for the long-term sustainability of our research because we are not heavily reliant on one income stream. Senior staff have led many successful major grant applications, which are particularly important for the vitality of a UoA of our size: Leggett led a programme grant (£4M) and a basic technology grant (£3M), Armes led a platform grant (£1M), Hunter led a critical mass grant (£2M), and Hunter and Armes were each awarded ERC advanced investigator grants (2 x £2M).

Plans for income capture are discussed and agreed in annual meetings of individual staff with the HoD and research cluster head; efforts at grant winning are rewarded in the allocation of resources. Grant applications are reviewed internally by two academic colleagues before submission, ensuring high standards (our EPSRC grant success rate was 70% last year). In addition, ECRs receive mentoring in grant writing and are assisted to develop collaborations. The research committee identifies funding opportunities and matches these to staff expertise, and the HoD targets teaching relief to allow staff to take advantage of appropriate opportunities. Following a coordinated effort to improve EU income initiated at an Away-Day in 2008, with support from University Research Office staff, the UoA secured two ERC advanced investigator grants and three Sheffield-led Marie Curie ITNs.

Knowledge-transfer activities in the UoA have been supported by 50 grants from the EPSRC Knowledge Transfer Account, and from HEIF, totalling £1.1M (the largest share within the Faculty of Science). The Molecular Engineering Translational Research Centre (METRC), established with a £2.2M grant from the Northern Way, is a Sheffield-led regional consortium fostering the academic-industrial interface for the N8 Universities. METRC has supported 14 projects in the UoA through funding RAs, PhD students, vacation studentships and industrial secondments.

Future funding plans are dictated by the skills of our research staff and therefore shaped by our recruitment strategy. This is, in turn, based around the four clusters, which combine core chemistry with our interdisciplinary strengths. In the short to medium term, much research is aligned with current RCUK priorities, including energy generation and storage *via* photovoltaics (Weinstein and Ryan); catalysis (appointment of Conte in heterogeneous catalysis to complement the expertise of Haynes, N Williams and Grasby in homogeneous and biocatalysis); healthcare technologies (Harrity, Armes, Rimmer); imaging (Thomas, Weinstein, Ward); surface chemistry (Leggett); and synthetic supramolecular chemistry (Ward, Armes, Hunter, Thomas, Brammer). Our balanced portfolio of staff expertise, and tradition of collaboration both within and between departments, gives us the flexibility to respond well to new opportunities as and when they arise. This is demonstrated by the successes in establishing CDTs, most recently in Polymers, Soft Matter and Colloids, and representation in EPSRC 'Grand Challenge' networks.

Research Infrastructure and Facilities. Research groups work in state-of-the-art laboratories resulting from a 10-year programme of refurbishment. All PG students are accommodated in dedicated writing-up areas with PCs, adjacent to their laboratory space. The University provides electronic access to a comprehensive range of chemistry and general scientific periodicals supported by state-of-the-art data searching software.

Core facilities include NMR (5 spectrometers) and X-ray crystallography (3 diffractometers) and a computer cluster. The most recent investment has been the centre for mass spectrometry, which combines facilities for chemical and biological mass spectrometry (5 spectrometers) in a single facility serving the Faculty of Science and located in the Chemistry department. We have agreed a long-term plan with the University for maintenance and replacement of all major analytical equipment on a 10-year cycle, starting with a £1M upgrade of core NMR, X-ray and mass spectrometry facilities. This will ensure the sustainability of our key infrastructure. The first investment of £200k in an upgrade to our NMR facilities has just been made.

Each major facility is run by a Senior Experimental Officer with dedicated technical support. We have an extremely capable technical staff team, which combines experience with planned

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progression of junior technicians to develop skills and expertise with core equipment facilities. In addition, training is provided to our PhD students and RAs so that they can become expert users of all instrumentation required for their research projects. The UoA benefits from a dedicated glassblower and a microanalyst. We have just established a combined mechanical/ electrical workshop with two dedicated technicians providing support for all research groups. Computer support across the UoA is provided by two specialist technicians, who will also support our substantially expanded theory group.

The UoA supports and maintains many smaller items of equipment, which are available to all researchers and underpin our broad portfolio of research programmes: steady-state and time-resolved UV/vis absorption and emission spectroscopy, IR and UV/vis spectroelectrochemistry, fluorescence anisotropy, analytical and preparative HPLC, GPC, GC-MS, LC-MS, ICP-MS, AAS, IR, FTIR, TGA, DSC, elemental analysis, Grubbs dry solvent system, H-cube and React-IR. The total spend on new equipment was £1.1M over the REF period, including investments in a new laser facility, a major upgrade of the computer cluster within Chemistry, a new cell-culture laboratory and a new suite of particle size analysis instruments. We are extensive users of the imaging facilities in the Kroto Research Institute, including TEM and SEM, confocal microscopy and multi-photon microscopy, XPS and SIMS. We also have access to state-of-the-art optical techniques in Physics, and structural biology infrastructure in Biology.

The University has established an institutional equipment register to publicise equipment available for sharing both within the University and with other HEIs. There is a formalised capital equipment pipeline so departments can plan and manage new capital investment, and structured working groups have been established to enable new collaborative equipment developments with our N8 partners (Durham, Lancaster, Leeds, Liverpool, Manchester, Newcastle, York). Members of the UoA (Fairclough, Brammer, Weinstein, Armes, Mykhaylyk, Hippler, Ryan) also make substantial use of national and international specialist facilities: neutron and X-ray at Diamond/ISIS, ESRF/ILL, Brookhaven; ultrafast spectroscopy, laser loan pool and cell imaging at RAL.

Specialist Facilities. The Polymer Centre provides state-of-the-art facilities for the complete characterisation of polymeric materials: 7 GPC, 3 DLS, 2 laser diffraction instruments, 2 aqueous electrophoresis instruments, 2 helium pycnometers, TGA, BET surface area analysis, stress rheometer, ellipsometer, 2 preparative centrifuges, 2 surface tensiometers, FT-IR, MALDI-MS, AC, 2 disc centrifuge photosedimentometers, hot-stage optical microscope, SAXS. Much of this equipment was purchased during the 2008–13 REF period and a £90k upgrade of our NanoStar SAXS instrument is scheduled to take place late in 2013.

The Sheffield Surface Analysis Centre houses an IonToF SIMS, a Kratos Axis Ultra X-ray photoelectron spectrometer, an ellipsometer, fluorescence correlation spectroscopy and facilities for surface energy measurements. We have extensive facilities for scanning probe microscopy (3 AFM and 3 SNOM, one of which is a shear-force near-field microscope built in Sheffield). The Sheffield "Snomipede" is a unique parallel near-field optical microscope, which provides 100 nm resolution nanolithography over areas in excess of 1 cm². Additional near-field microscopes are used for nanofabrication, and to support this area of work, we have a range of lasers, including three argon ion lasers (two are frequency-doubled UV lasers), a HeCd laser and a Ti-sapphire femtosecond pulsed system. A Lloyds mirror interferometer is also used for nanofabrication.

The Centre for Chemical Biology provides laboratory space and facilities for cell culture work (level 2 containment), protein production and purification (incubators, French press, sonicator, centrifuges, cold room, hplc, mplc, fplc), biomolecular synthesis (oligonucleotide and peptide synthesisers), and a biophysical instrumentation suite (DSC, ITC, CD, Biacore, stop flow, quench flow, UV/vis absorption and emission spectrometers, WAVE machines, photodoc transilluminator, phosphor imager). The biological NMR facility has 3 Bruker Avance spectrometers: 800 MHz, 600 MHz with cryoprobe and 500 MHz. During the REF period, a high-pressure (2.5 kbar) rig was installed (unique in the UK). There is an adjacent wet lab for sample preparation and extensive data processing facilities, including two multicore hubs purchased in 2013.

Consultancies and professional services. Farapack Polymers and Sheffield Synthesis Solutions have each played important roles in identifying consultancy opportunities for individual academics. This activity has involved engagement with various companies in the pharmaceutical, polymer and

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speciality chemical sectors. Several members of staff have acted (and continue to act) as expert witnesses in legal cases. The chemical analysis facilities provide an extensive service throughout the university, and also for industry, offering surface science analysis, polymer analysis, NMR, mass spectrometry, and X-ray crystallography.

e. Collaboration or contribution to the discipline or research base

Wider Influence. Members of staff in the UoA make major contributions to Chemistry as a whole through engagement with external bodies (e.g. funding agencies, learned societies and research networks).

- *Research networks:* Leggett is director of the EPSRC Grand Challenge network on *Understanding the Physics of Life*. Ward and Brammer are champions of the EPSRC Grand Challenge on *Directed Assembly*. Both networks have provided important contributions to establishing a new agenda for national research priorities and initiatives.

- *National body committees:* Members of staff in the UoA serve on RSC's Dalton Council, Astrophysics Group, Physical Organic Chemistry Group, Nucleic Acids Group, NMR Discussion Group, advisory committee on Chemistry and Healthcare, and the UK Macro Group. They also contribute to management of national infrastructure and resources: Ryan served as the chair of the STFC Science Board and a non-executive director of Diamond Light Source plc; Jackson served on the HCUK standing committee; Leggett served on both the Chemistry and the Nanotechnology Strategic Advisory Teams; Brammer serves on the Diamond Light Source peer review panel; Weinstein is on Rutherford Appleton Laboratory laser loan pool steering committee; Ward chairs the EPSRC National Crystallography Service management panel; Meijer is on the HECToR UK National Supercomputing Service resource allocation panel; Waltho is a member of the Wellcome Trust Capital Awards Panel and the Scientific Advisory Committee of the Lister Institute of Preventive Medicine; Weinstein was on the international steering committee of STFC's Free Radical Research Facility and is a member of the working group for the New Light Source project. Hunter, Fowler and Waltho each serve on Royal Society Committees.

- *Activities with wider international impact:* Ward chaired EU-COST Action D31 '*Organising Non-Covalent Chemical Systems with Selected Functions*' to promote EU-wide research networks; Leggett was a member of the Board of Directors of the American Vacuum Society; Ward was an international assessor for the Italian Ministry of Education Evaluation of Research Quality exercise; Rimmer was a member of the Finnish Academy of Science International Review panel and is on the executive board of the UK-China Advanced Materials Institute; Weinstein is on the advisory board of the Training Centre for High Energy Chemistry in Moscow. Ryan has been invited to join the AkzoNobel scientific advisory board.

- *Grant Review Boards.* In addition to membership of peer review EPSRC colleges, most members of the UoA have served on grant-awarding panels both nationally (RCUK, Royal Society, Cancer Research UK, Leverhulme Trust) and internationally (ERC, Academy of Finland, Danish National Research Foundation, Oak Ridge National Lab, Science Foundation Ireland, Institut Universitaire de France, Hong Kong Grants Council, National Science Foundation, Petroleum Fund).

- *Journals.* Members of the UoA have served on the Editorial Boards and the Editorial Advisory Boards of 23 journals including *Chemical Science*, *ACS Nano*, *Biomacromolecules*, *Langmuir*, *J. Mater. Chem.*, *Macromolecules*, *CrystEngComm*, *Nanoscale*, and *RSC Advances*.

- *Conference organisation.* Members of the UoA have been on the organising committees of 28 major conferences. Sheffield hosts two regular chemistry conferences, the Nucleic Acids Conference 'NACON' and Sheffield Stereochemistry, both of which are very well attended. Dalton Discussion 13 (2012, on 'Inorganic Photophysics and Photochemistry') – organised by Ward and Weinstein – led to a dedicated issue of Dalton Transactions.

Fellowships and Awards. The impact of our academic staff on the discipline has been recognised through several prestigious awards and fellowships, which were listed in part c. Other awards include the RSC Peter Day prize for Soft Matter (Armes), the RSC Tilden Prize (Hunter and Armes), the RSC Physical Organic Chemistry Award (Hunter), the Macro UK Medal (Ryan), and the IChemE award for innovative product of the year (Fairclough). Hunter was the Howard lecturer at Sydney and the Derome lecturer at Oxford. Ryan was the RSC Materials Chemistry lecturer.

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Armes is the 2014 RSC/SCI Thomas Graham lecturer.

Academic Collaboration. Promoting collaboration is at the heart of our research. This is facilitated by our cluster structure, and examples of our interactions with scientists in other departments and in university-wide research institutes and *via* CDTs, have been described earlier. Major collaborative research projects within the UoA, with other departments across the university and with other universities include: a £2.2M 'critical mass' grant on non-covalent chemistry; £3.1M Snomipede basic technology grant (with physics); £4.1M programme grant on low-dimensional chemistry (with physics); £1.0M platform grant on biocompatible polymer colloids (with biology); £3.4M LOLA grant on biological membranes (with physics and biology); £2.7M programme grant on organic supramolecular chemistry (with Manchester, Edinburgh); £1.1M and £1.2M polymer photovoltaics grants (with physics, chemical engineering, Diamond Light Source, Cardiff, Cambridge); a £1.5M nanotechnology grand challenge grant (with Sheffield physics, Durham, Imperial College, Manchester).

The strong ethos of collaborative research during the REF period is exemplified by Meijer's interactions with no less than 18 academic colleagues within the UoA. Fowler's outputs with international authors include mathematicians, computer scientists, physicists and engineers from 30 different universities/research institutes in 10 countries. Harrity has published 26 papers co-authored by industrial scientists from 7 different companies based in the UK and Europe. Armes has many interactions with both industry (14 industrial co-authors from 8 companies) and academia (40 international co-authors from 14 countries). The strongly interdisciplinary nature of much of our research results in a large number of joint grants, either within the UoA or with colleagues elsewhere in the University, or at other institutions. Our international collaborations are supported by small grants for travel and staff exchange (e.g. Royal Society, British Council, Leverhulme Trust, EU-COST): they are often small in value but of high strategic significance, as reflected in the high proportion of our REF outputs (> 40%) with international co-authors.

Industry Collaboration. Collaboration with industrial partners is an important part of our research activity and a large proportion of our PhD students are working on industrially-supported projects. We collaborate with over 40 different companies from the UK chemical sector: this activity provides us with insight into important technical challenges that also lead to opportunities for exploitation of our research. The importance of our expertise in organic synthesis to the fine chemicals, pharmaceuticals and agrochemicals sectors is reflected in the number of industrial collaborations over the assessment period (25 projects with 11 companies across Europe). Several members of staff consult for companies on topics within their specific area of expertise. Fairclough has been involved in 5 KTPs, and 9 members of staff have been involved in a total of 23 projects funded by the University Knowledge Transfer grant. In addition, Harrity is a scientific advisor for AF ChemPharm, and Hunter is on the Scientific Advisory Board of Cresset BMD. The UoA hosts three organisations that foster the academic-industrial interface: the Polymer Centre facilitates interactions between third parties and a network of polymer science academics across the University; Farapack Polymers is a spin-out company with five employees that undertakes contract research in polymer chemistry with a turnover of £1.4M in the REF period; and Sheffield Synthesis Solutions offers contract synthesis for industry and the wider academic community. Many of these collaborations have led to commercial exploitation (as shown by our four impact case studies with OpenEye, Cresset BMD, DSM and AkzoNobel). The new chemistry-led CDT in Polymers, Soft Matter and Colloids (50 CASE studentships) will further enhance our industrial links.

Public Understanding and Outreach. The UoA engages in a range of outreach activities to promote the long-term health of the subject as a whole: engagement with the media, national events and local schools. We have built a dedicated Sheffield Schools' Laboratory, providing pupils from across the region with access to facilities not available in school.

Outlook. The UoA has a strong research base in fundamental chemistry supporting long-term research programmes with applications in materials, energy and medicine. Members of the UoA play leading roles in the discipline nationally and internationally through their interactions with external bodies and their collaborations with industry and other universities. The on-going investment in new staff and infrastructure will ensure that Sheffield remains at the forefront of new developments in the discipline well into the future.