Institution: University of York
Unit of Assessment: 8 - Chemistry

a. Overview

The Department of Chemistry at York distinguishes itself by its approach to research in identifying strong, core research areas, complemented by dynamic, multidisciplinary groupings (below – heads italicised). This is facilitated by the Department's and University's flat and flexible organisational structure, so that Chemistry is a lead or significant partner in the following multidepartment centres: *BioArCh, Biological Physical Sciences Institute (BPSI), Biorenewables Development Centre (BDC), Centre for Chronic Diseases and Disorders, Centre of Excellence in Mass Spectrometry (CoEMS)*, *Centre for Hyperpolarisation in Magnetic Resonance (CHyM)*, *York Centre for Complex Systems Analysis*, *York Environmental Sustainability Institute*, *York Institute for Materials Research and the York JEOL Nanocentre*.

Analytical Chemistry	**Keely, Lucquin (ECR), Penkman, *Thomas-Oates*, J. Wilson.**
Chemical and Structural Biology (York Structural Biology Laboratory – YSBL)	**Antson, Brzozowski, Cowtan, Davies, Fascione, Grogan, Hubbard, Shimizu, Wilkinson, *K. Wilson.***
Green Chemistry	***Clark*, Gai, Macquarrie, Matharu, North.**
Inorganic Chemistry	**Douthwaite, Duckett, Duhme-Klair, Lynam, Parkin (ECR), *Perutz*, Slattery, Walton.**
Materials Chemistry	**Bates, *Bruce*, Cowling, Goodby, Saez.**
Organic Chemistry	**Chechik, Clarke, Fairlamb, O'Brien, Parsons, Routledge, Smith, *Taylor.***
Physical & Atmospheric Chemistry	**Bernath, *Carpenter*, Cockett, Dessent, Dillon (ECR), Evans, Hamilton, Karadakov, Lee, Lewis, Moore, Rickard, Sebald, Wann (ECR).**

As part of our on-going strategy, Atmospheric and Physical Chemistry were recently merged, new staff were recruited, and **Carpenter** appointed as professorial head.

b. Research Strategy

Progress since 2007

Developments articulated through the document represent substantial progress during the period, among which we would identify the following highlights:

- Election of three staff (**Davies, Goodby** and **Perutz**) as Fellows of the Royal Society and **Gai's** naming as 2013 L'Oréal-UNESCO Woman in Science Laureate;
- New research grant wins for 2011-13 at an all-time high (**£25M**);
- **£17.9M** investment in buildings (4540 m^2 of new space) so that 95% of the Department's researchers are accommodated in laboratories eleven years old or less;
- Renewal of Athena SWAN Gold Award (2010) for our commitment to women in science;
- Establishment of the multidisciplinary BDC and CoEMS, and construction and equipping of purpose-built accommodation for the CHyM and Atmospheric Chemistry.

Vision

The department's vision is to undertake research that has global impact, fully embraces multidisciplinary science and communicates widely the transformative role that chemistry plays in everyday life. To realise this vision, a rolling programme of major investments in buildings and equipment is maintained, and leading researchers and talented support staff are appointed and supported. The approach sustains excellence in the core areas of Chemistry and engenders multidisciplinary and collaborative approaches to target grand challenges in, for example, global climate change, applied and sustainable materials, feedstocks and fuels, and health and disease. This strategy led to the now well-established groups in YSBL and Green Chemistry, and has continued with the growth of newer groupings in Analytical Chemistry (embracing archaeological science), Atmospheric Chemistry and Materials Chemistry. This multidisciplinarity extends outside the Department as it participates in the multidepartment centres mentioned in **Section a**.

Departmental Research Committee (DRC) identifies multidisciplinary themes where chemistry can bring major influence to bear; a recent example concerns Synthetic Biology where chemistry

has a central role. While many existing areas of strength would contribute to this development, key appointments in nucleic acid and medicinal chemistry (the latter building on funding success from the IMI initiative – below) will create a seamless link from synthetic chemistry through chemical and structural biology. Likewise, the newly created Biological Physical Sciences Institute will articulate major long-term challenges such as the human-electronics interface. This will require an integrated approach through which chemistry will develop further expertise in soft matter/membrane self assembly and in analytical methods, with major underpinning from expertise in handling large data sets. These examples show how both core and multidisciplinary chemistry are developed through larger visions. Our proven commitment to, and development of, multidisciplinary areas combined with our demonstrable agility in responding to opportunities (*e.g.* timescale for the establishment of CHyM described below) give confidence in this strategic approach.

In developing these initiatives, DRC works with the existing Joint Planning Groups with Biology and Physics while soliciting advice from our External Advisory Group of senior industrial and academic figures. The Department already has academic posts in its forward plans that can be allocated with additional positions becoming available through Departmental- and University-level initiatives. Some of these posts may be joint with other departments and/or at senior level, attracting substantial set-up funding from the University.

Meeting the Strategic Aims 2008-2013 (from RA5 in 2007)

Strategic aims from RAE2008 are given below. In all cases they have been met or exceeded, showing the vitality of our core chemistry and success in our multidisciplinary research and giving confidence in the quality of our planning and our ability to deliver.

- *Atmospheric Chemistry: in stage 1 of a cross-departmental initiative, an environmental chamber is being installed (**Lewis/Carpenter** with Environment and Biology); **and***
- *Development of high-resolution spectroscopy of the atmosphere through laboratory and remote studies (**Bernath**);*

York is now world-renowned for research on atmospheric trace gas and aerosol detection (**Lewis** was appointed Director of the NERC National Centre for Atmospheric Science in 2008, which is underpinned by an annual, five-year rolling research contract from NERC of **£0.9M**). Capability in high-resolution spectroscopy has been extended, for example, to measure trends in key atmospheric molecules including upper atmosphere carbon dioxide (**Bernath**: Canadian ACE satellite - www.ace.uwaterloo.ca). The grouping has built on these strengths in measurement science with the appointments of **Evans** (Chair) and **Rickard**, with expertise in global chemical transport modelling and atmospheric mechanisms, respectively, and of **Hamilton**, an expert in aerosol analysis. The recent appointment of **Dillon** (ECR) and a 2010 University investment in an interdisciplinary environmental chamber, strengthened further research capabilities in laboratory kinetics, physicochemical properties, aerosol processes and biosphere-atmosphere exchange.

- *Research into enhancement of magnetic resonance sensitivity* via *hyperpolarisation for imaging and spectroscopy will link Inorganic Chemistry (**Duckett**) to Biology and Psychology;*

Publication of results in *Science* (2009) quickly led to successive grants from Wellcome and Wolfson and support from the University and Bruker (**£13M** in total) for construction of a new building (completed 2012) to house CHyM, the acquisition of new equipment and recruitment of staff. Led by **Duckett** and Green (Psychology), CHyM also includes staff from the Hull-York Medical School and from Biology and has a strategic partnership with Bruker.

- *Investment in state-of-the-art, ion-trapping mass spectrometers to establish a Centre of Excellence (with Biology), enabling new research across all branches of chemistry and strengthening industrial links;*

Building on the appointment of **Thomas-Oates** (RSC-EPSRC Chair), the Centre of Excellence in Mass Spectrometry (CoEMS) was created with Biology using capital funding (**£1.6M**) from Science City York and Yorkshire Forward. The Centre is very well equipped (http://www.york.ac.uk/mass-spectrometry/), providing fee-for-service and research training, and supporting diverse research work across Chemistry, Biology and Archaeology, *e.g.* facilitating molecular studies of protein degradation in geological and archaeological contexts and underpinning industrial collaborations.

- *University initiatives will form an Institute in Nanoscience and Materials. Existing facilities for TEM at atomic resolution will be extended to allow environmental measurements;*

World-leading capability for environmental measurement (under reaction conditions) has been established by **Gai** and Boyes (Physics) and the York JEOL Nanocentre is supported by a **£1.4M** EPSRC Critical Mass Grant. The standard TEM/STEM instrument was re-engineered and the first sub-Å resolution environmental-scanning TEM (ESTEM) images of reacting single atoms at 500 °C in a gaseous reaction atmosphere were published (2013). Materials chemistry is also supported by a 2013 grant from EPSRC (Core Capability) providing a state-of-the-art, low-angle X-ray scattering instrument for soft matter science allowing in-house studies of complex mesophase architectures and a 400 MHz MAS-NMR instrument for characterisation of solid-state materials.

- *Biological Chemistry will tackle challenging structures (mammalian, multi-component or membrane proteins) and apply structure-based approaches to chemical biology of carbohydrate-binding proteins and fragment-based drug discovery (malaria) with Organic Chemistry and Biology;* ***Grogan****'s involvement with CoEBio3 will reinforce biocatalysis links with Biology and Manchester;*

Underpinning much of the work in YSBL is the strong crystallographic methods group led by **Wilson** and including **Cowtan** (funded by STFC to 2018 then employed by the Department). It facilitated important discoveries on challenging systems during the period *e.g.* in the molecular mechanism of viral DNA packaging (**Antson**), the molecular biology of *Bacillus subtilis* (**Wilkinson, Wilson**) and, of particular note, the long-sought-after structure of the complex between insulin and its cell surface receptor (**Brzozowski** and collaborators). **Hubbard's** work on structure-based drug discovery**, Wilkinson**'s on *N*-myristoyltransferases and **Shimizu's** insightful theoretical analysis of hydrophobicity all contributed to structural dissection of enzyme inhibition in the disease area. **Davies'** work on the human O-GlcNAc modification is having major impact in the Alzheimer's field (exploitation of O-GlcNAc inhibition by Merck and Alectos Therapeutics alliance http://www.merck.com/licensing/our-partnership/Alectos-partnership.html). Further depth in Chemical Biology comes with the strategic appointment of **Fascione**, whilst **Parkin** (inorganic) brings electrochemical insight to the growing metalloenzyme arena. Biocatalysis breakthroughs include **Grogan's** work on the enzymology and enantioselectivity of biotransformations (with *CoEBio3*), the long-standing collaboration with Novozymes A/S and in the structural and mechanistic bases of carbohydrate processing (**Davies**, **Wilson, Walton**).

- *Solar energy conversion will be emphasised in Inorganic and Materials Chemistry;*

A new White Rose Consortium enables research into use of photonic crystals (**Douthwaite**) with complementary projects in Hull, Leeds and Sheffield. Additional collaborations are developing with Krauss (Physics) on the use of photonics. Research into photochemical CO_2 reduction in solution revealed new photocatalysts that operate with long-wavelength visible light (**Perutz**). Research into macroporous photocatalysts has shown that unique microstructures can be obtained that increase catalytic rate (**Douthwaite**). Research into CO_2 chemistry will gain substantial additional momentum through the arrival of **North** who investigates chemical approaches to CO_2 fixation.

- *Metals in medicine is an emerging theme in Inorganic Chemistry;*

Walton and **Lynam** developed a range of water-soluble ruthenium complexes (patent pending) that show *in vitro* anti-tumour activity surpassing that of Ru complexes now in clinical trials. **Lynam** also collaborated with **Fairlamb** to apply metal-carbonyl complexes to the therapeutic, controlled release of CO. **Duhme-Klair** demonstrated (with **Routledge**) that siderophore mimics can be bound to antibiotic molecules creating new agents that overcome antibiotic-resistant bacteria, while with **Wilson** (YSBL) she revealed the structure of the Fe(III) complex of a tetradentate siderophore with an adaptor mechanism exploitable in new antimicrobials. **Duckett** (with Green, Psychology) discovered a new way to transfer the magnetic polarisation of *para*-hydrogen through a metal-based catalyst, revealing major new possibilities in MRI.

- *Green Chemistry: applications of Starbon® technology for biorefining are under development;*

Starbons®, a patented class of mesoporous materials derived from polysaccharide wastes, are being exploited by spinout company, Starbon Technologies Ltd (http://www.starbon-technologies.com/), winner of a 2013 Rushlight Environment Award for water treatment and the 2012 ACHEMA Biochem business plan award. Further developing its translational agenda, Green Chemistry established the Biorenewables Development Centre (BDC) in a collaboration with

Biology. Supported initially by £2M from the ERDF to establish a microwave biorefinery and a bioethanol demonstrator (2009), the University established the BDC as a company, which was then (2012) awarded grants exceeding £7M from ERDF, BIS and ETDE Contracting Ltd. It now has *ca* £3M of equipment and employs some 22 staff, acting as a commercial demonstrator to work with interested companies to apply a range of proprietary technologies to the conversion of biomass into chemicals and materials. Starbons® are manufactured within the BDC.

The following major developments add, with the BDC, to aims indicated at RAE2008:

- *Chemspeed Investment in Robotics;*

Led by **Fairlamb**, a new partnership was created with Swiss-based company Chemspeed, enabling synthetic and catalytic chemists to modernise the way in which reactions are evaluated and optimised. The company established a 'demonstrator centre', placing two robotic platforms (**£750k**) in the Department and giving Chemistry 50% instrument time. A Robotics Centre will be developed facilitating study of complex synthetic/mechanistic systems, exploiting this opportunity.

- *Innovative Medicines Initiative IV (CHEM21);*

CHEM21 (Chemical Manufacturing Methods for the 21st Century Pharmaceutical Industries) is Europe's largest public-private partnership (*ca* £20M) dedicated to the development of manufacturing pharmaceuticals sustainably, funded by the Innovative Medicines Initiative (IMI). At **£1.2M**, York has some 35% of the UK funding, which is led locally by **Clark**, with involvement from **Fairlamb, Macquarrie** and **Taylor** and collaboration with industry (most notably with GSK, Pfizer, Orion Pharmaceuticals, Bayer and others) and academia (Manchester, Leeds and Durham).

Statement of Goals for 2013-2018 for Research Groupings

Analytical: Central to the group's approach and organisation are long-term collaborations with a wide range of subjects (Biology, Archaeology, Environment and Complex Systems) where the desire to address significant problems drives development of analytical methods and approaches. This is based primarily on excellence in mass spectrometry, chromatography, amino acid analysis (**Penkman** directs the NERC-recognised North East Amino Acid Racemization Laboratory) and mathematical approaches to data treatment. Methods for handling large data sets underpin much of this work. The group will nurture the active links with external partners (*e.g.* FERA, the Natural History and British Museums and international equivalents). In the coming period, the goal is to discover and analyse archaeological and geochemical biomarkers and their survival over palaeontological/geological timescales.

Chemical and Structural Biology will extend the scope and challenge of its structural work to embrace larger macromolecular assemblies including viral molecular motors, mammalian proteins (*e.g.* glycosidases) involved in human disease, proteins involved in human life-span regulation and membrane proteins involved in signal transduction in cancer and diabetes. Methods developments will continue to extend the boundaries of structural investigation, supported by the permanent appointment of **Cowtan**. These endeavours will be underpinned by a new robotics-equipped crystallisation suite (**£0.5M** Wellcome) and by expansion of mammalian gene-expression facilities supported by **Brzozowski**'s MRC programme grant (**£1.5M**, 2013-2017 to work on the insulin receptor), **Davies'** ERC award (**£2M**; 2013-2018 to work on carbohydrates in viral infection, cancer and lysosomal storage disease) and **Antson's** WT Senior Fellowship (**£1.3M** 2012-2017, renewal). Collaborations with inorganic and organic chemists, and with cell biologists will be strengthened to exploit structural insights in (i) disease and drug discovery and (ii) biocatalysis and biomass conversion, both benefitting from continuing industrial collaboration and extensive BBSRC funding.

Green Chemistry will integrate its new research laboratories and the BDC, providing a seamless progression for new green technologies through to demonstrator-level scale, and taking the most successful through to joint ventures, licensing and spin-outs. The group will integrate the skills of **North** on waste CO_2 chemistry and exploit new research on metal capture (EPSRC/G8, TSB) alongside growing research on biomass and food waste valorisation (EPSRC, EU, TSB, ERDF, industry, new York-led COST Action). Specific targets include development of novel Starbon®-based filtration systems to refine metallic waste streams, base metal and mixed-metal catalysts derived therefrom, and their use in making platform molecules and monomers from biomass and CO_2, as well as downstream products including bio-solvents and bio-polymers. Building on their proprietary microwave technology, they will develop further novel processes

including combined microwave-heterogeneous catalytic transformations (EPSRC) with the aim of creating a worldwide network of microwave bio-refinery demonstrator units (ERDF, EU, industry).

Inorganic Chemistry: In *fundamental studies*, the group will develop time-resolved NMR on ms and μs time-scales utilising hyperpolarisation and automated computational routines for surveying potential energy landscapes and Fourier-transform voltammetry as a probe of biocatalytic mechanisms in natural and artificial metalloenzymes. In work directed to *healthcare*, hyperpolarised NMR methods will develop towards use as an imaging tool in clinical diagnosis, while therapeutic agents will derive from: antimicrobial metal-siderophore complexes, therapeutic CO-releasing molecules, Ru anticancer drugs, and hydrogenases for pathogenesis. *Energy-related research* will integrate photonic materials and electrodes into a functioning solar fuel device, develop bioinspired photo-redox catalysts and new CO_2 reduction catalysts. Advances in biofuel processing will accrue from study of Cu-metalloenzymes, biomimetic chemistry and ionic liquids. Many aspects of this work will link to Chemical and Structural Biology.

Materials: The multidisciplinary nature of the Materials group allows identification of a range of challenging goals. Thus, through synthetic and computational approaches, and deploying strengths in materials design and property measurement, it will develop new display materials (*e.g.* blue phases, dyes, bistable smectics, LC-OLEDs), address issues relating to surfaces and alignment (functionalisation of natural fibres and nanoparticles, development of command surfaces, liquid-crystalline graphenes and alignment materials for smectic devices). Amphi- and poly-philic systems will be designed to control order, generate broken-symmetry materials, direct self-organisation and provide ordered media for chemical transformations. Biomaterials will also feature strongly with continued development of gel phantoms, carbohydrate LCs and their membrane properties, and materials for cell imaging and drug delivery.

Organic will build on strengths in fundamental research *via* interdisciplinary projects in two areas: (i) **synthesis** focusing on sustainable/green catalytic methodology (augmented by **North**, Green Chemistry), high-throughput synthesis *via* the Chemspeed robotic platforms and *de novo* screening libraries; (ii) **complex systems**, to include self-assembly processes to form nanoscale materials and medicines and pre-biotic complex systems. Multidisciplinary interrogation of complex mechanistic pathways will be supported by assimilation of **Fairlamb** to academic staff bridging organic and inorganic chemistry, and using, for example, EPR, NMR and *in situ* IR spectroscopy. A key strategic vision is to achieve **translation** of the fundamental research, particularly into pharmaceutical/medicinal applications (antibiotics, post-surgical recovery and fragment-based drug discovery) *via* multidisciplinary approaches with key industrial and international collaborators, as well as end-users. The group also forms key interdisciplinary links with Green and Materials Chemistry and Chemical Biology through its methodologies.

Physical & Atmospheric will exploit cutting-edge analytical and spectroscopic techniques, combined with theoretical/computational chemistry, to study physicochemical properties of a range of molecular systems in the laboratory and the atmosphere, and develop theoretical frameworks using classical and unconventional computation to understand such systems better. New appointments in laser spectroscopy (**Dillon**), gas-phase electron diffraction (**Wann**), chemical mechanisms (**Rickard**) and atmospheric composition (**Hamilton**) and modelling (**Evans**), strengthen and broaden group coherence, offering opportunities for collaboration and increased ability to study chemical change over a wide range of temporal and spatial scales. For example, development of time-resolved gas-phase electron diffraction will allow observation of atomic movement during reactions. The highly instrumented experimental and modelling infrastructure of the new Wolfson Atmospheric Chemistry Laboratory (below) will advance globally important atmospheric and climate science. Its research will enhance the interface between modelling and world-leading measurement science, providing the scientific basis for informed predictions of future atmospheric impacts and new ways to mitigate negative pollution and climate effects.

c. People, including:
I. Staffing strategy and staff development

Twelve appointments were made in period with at least one into each research group, each with a clear strategic dimension. In Physical & Atmospheric Chemistry, **Hamilton** and **Rickard** provide complementary expertise (aerosols and mechanisms, respectively) in atmospheric chemistry, while additional strength and leadership is provided by **Evans** (Chair) whose appointment allows global modelling to be incorporated seamlessly into the group's work. ECRs **Wann** (electron diffraction)

and **Dillon** (laser spectroscopy applied to atmospheric problems) add vitality to the section and provide the laser group with critical mass. With substantial new grant income and development of the BDC, the leadership of Green Chemistry was augmented and its focus broadened with the appointment of **North** to a Chair, while in Materials Chemistry, **Bates** and **Saez** moved from RS-URF and independent researcher, respectively, to academic staff, and **Cowling** was promoted from EO to independent researcher. The future of catalysis and mechanism in Organic Chemistry was secured by **Fairlamb**'s move from RS-URF to academic staff, while Chemical Biology was strengthened by appointment of ECRs **Fascione** (Marie Curie Fellow: joins YSBL staff 2014) and **Parkin** (Inorganic). In Analytical Chemistry, **Lucquin** (ECR) develops further the link to Archaeology.

The strength of the Department is also reflected by rather few departures. Murshudov was recruited to the prestigious MRC Laboratory in Cambridge, Lee and K. Wilson went to promotions (Chair, Reader – Cardiff) and E. Taylor and Görtz secured lectureships.

An important development has been strategic appointment of teaching-only staff to run the teaching laboratory and contribute more widely to UG teaching. This has released a significant amount of time to research, most notably in substantial reduction in demonstrating loads.

Support staff were appointed to reflect the research strategy and investment. The post of Research Facilitator was created (2013) to interface effectively with external agencies and to support the construction of large bids for funding. EOs were appointed in mass spectrometry (2010), NMR spectroscopy (2013 – replacement), Atmospheric Chemistry (2013) and CHyM (two positions - 2012) and a research technician was appointed (2010) to support organic chemistry. The quality of our EOs is exemplified by their co-authorship of more than 150 papers in the period.

Career development support

Procedures are informed and guided by the University's Learning and Development Team, which won the THES awards for 'Outstanding Leadership Development' in 2009 and 'Outstanding Support for Early Career Researchers' in 2012.

Research and academic staff belong to one of the academic groups and each Group Leader is pro-active in reviewing the career progress of all group members and encouraging applications for promotion. There are currently more than 60 PDRAs in the department. All staff benefit from an annual performance review, which includes a discussion of the strategy for research publications and grant applications, a review of administrative roles and (for academics) a discussion of research leave. All of these areas are reviewed and followed up by the Personnel Advisory Group, HoD and Academic Group Leaders. Staff are encouraged actively to take research leave and an effective, managed policy operates in the Department allowing staff at all levels to have regular 'research terms'. Year-long research leave is possible through the University's Anniversary Lectureship scheme, open to more junior staff. **Lynam**, **Matharu** benefitted in this way, *e.g.* catalysing the latter's successful move to Green Chemistry.

All new academic staff participate in formal induction and mentoring schemes and receive cash support and a studentship to start their research; most are also supported by the University's research priming fund. Teaching/administrative loads are typically set at 25%, 50%, and 75% in the first three years. The mentor's role is, *inter alia*, to provide advice in establishing research programmes and in helping staff deal with the new challenges of teaching and administration.

HoD-run promotion seminars are held annually for academic, research and teaching staff and include members of the Department who sit on the University Promotion Panels. The effectiveness of this approach is demonstrated by an 88% success rate in promotions in the assessment period. Thus, there were five promotions to Personal Chairs; three to Readerships, five to Senior Lecturer and one each to Grade 7 & 8 research. A third of the promotions were of female members of staff.

Attending and presenting work at conferences is an important aspect of CPD for all research staff, which is funded both out of research grants and with Departmental support.

Established staff are presented with development opportunities through involvement in more senior University and Departmental committees, often as Chair, and by taking the opportunities presented by courses offered by the POD team, such as 'Leadership in Action' and 'Strategic Leadership'. Such courses supported *e.g.* the incoming HoD and the Chair of the Graduate School.

Evidence that these support and development mechanisms enable effective contributions to research is provided by the external recognition of staff at all stages of their careers (**Section e**).

The success of the training and mentoring offered is represented by the observation that of *ca* 190 PhD students who graduated in the period, some 50% remained in academia (9 with lectureships) while a further 29% hold positions in industry. Similarly from 90 PDRAs who left during the period, 66% remained in academia (12 with lectureships) with 16% holding industrial positions; none is recorded as being unemployed.

Implementation of the Concordat

Transition from researcher to academic. The University engaged enthusiastically with the 2008 re-launch of the Concordat as a means of extending its commitment to staff development and the Department has two staff members on the University Implementation Group (http://www.york.ac.uk/admin/hr/researcher-development/staff/concordat.htm). The University achieved the European Commission 'HR Excellence in Research' Badge very early with its Concordat action plan (2010-12) and renewal followed in 2012 when a new action plan and report were submitted detailing the progress, achievements and actions, and KPIs for 2012-14.

To help researchers develop independent ideas with a view to enabling an academic career, University and Departmental pump-priming funding is targeted in their direction. For example, an award to Görtz led to a patent being filed, a successful application for a Dorothy Hodgkin Fellowship and recent appointment to a lectureship at Lancaster.

The Department continues to develop its Concordat Action Plan which, in addition to career development support (above), includes i) review of contract status during the annual performance review and each time a contract is extended, ii) mentors and induction organised for all research staff, iii) inclusion of research staff on Departmental Committees, iv) regularly held Researcher Forums and v) moving to the redeployment register all staff within six months of redundancy (including those on fixed-term contracts) giving them priority access to job vacancies at the University. Since 2008, eight research staff have been redeployed successfully.

Staff with Personal Research Fellowships

The Department actively encourages personal research fellowship applications from internal and external applicants. During the assessment period: **Bates** and **Fairlamb** were RS-URF holders (now both academic staff); **Antson** had his Wellcome Trust Senior Fellowship renewed; **Wann** has an EPSRC Career Acceleration Fellowship; **Cowtan** secured an STFC independent fellowship; **Lee** and **Rickard** are supported by NERC National Centre for Atmospheric Science Fellowships, while **Lucquin** and **Fascione** hold EU Marie Curie Fellowships. **Davies** and **Dessent** hold ERC Advanced and Starter Grants, respectively.

International Staff Appointments and Visitors

The Department regards scientific quality as the prime criterion in academic appointments and as such has attracted staff from around the world. Currently, more than 20% of academic staff were born outside of the UK. Similarly, the quality of staff in the Department attracts international academic visitors, including postdoctoral fellows bringing their own funds. During the period, the Department welcomed 25 such visitors from 18 different countries for >400 months of research.

Support for Diversity and Equality

The Department of Chemistry strives to provide the facilities and the working environment that allow staff and students to contribute fully, to flourish and to excel. It is well recognised for its work on equality and was the **first academic department in the UK** to hold the Athena SWAN Gold award for its commitment to women in science (awarded 2007; re-awarded 2010). Support for women at all stages of their career is recognised as important and the Department's Athena SWAN Working Group continues to address gender inequalities and ensure a culture that supports equality and encourages full representation throughout the department. This work informs policies and working practices and, in particular, attention is drawn to: formal and informal flexible working (in 2012-13, 4 research staff (3 female, 1 male) and 6 academic staff (4 female, 2 male) were formally working part-time including 3 members of Professorial staff); active invitation of female seminar speakers (31% in 2012-13) and external examiners (40% since 2009); enhanced Departmental Maternity and Paternity Leave policy; meetings and seminars at family-friendly times and diversity training during induction. York is also influential (inter)nationally as **Perutz** was a member (to 2011) of the Athena SWAN Steering Committee, while **Walton** makes numerous presentations at home and abroad on diversity as an Athena SWAN and INTEGER ambassador.

The Department has made strong efforts to improve the diversity of its staff and students, and in this context has used the Wild fund (**£1M**) created by an alumnus to help support overseas

students in the department's Graduate School. This fund has succeeded in its aims of increasing the number of overseas students, and increasing the ethnic diversity of the graduate school. Thus, in 2004, at the start of the fund, the percentage of non-white students in the graduate school was 11%, while in 2013 this figure is 29.5%. Integration of all staff, PG students and researchers is promoted by Chemical *Inter*Actions, which runs a busy social programme with events that reflect the Department's diversity. The Department also provides a quiet/prayer room.

Recognition of those with disabilities, which includes academic, technical and support staff, is built into the inclusive ethos of the Department and we have had successful graduate students during the REF period with long-term health issues and with dyslexia. Support is provided by our Departmental Disability Officer, **Perutz**, who also brings influence to bear nationally as a member of the STEM Disability Committee (http://www.stemdisability.org.uk/).

c. II. Research students

Numbers of FTE postgraduate students registered per year (numbers in parentheses is the total student head count – the difference is students registered jointly with other Departments).

2008/09	2009/10	2010/11	2011/12	2012/13
112 (112)	110 (118)	93 (109)	92 (100)	99 (100)

Postgraduate Recruitment

Postgraduate places are in demand from high-quality, in-house, UK and international students, many coming from our highly successful, high-profile MSc in Green Chemistry and Sustainable Industrial Technology. Recruitment information is provided *via* the Department's website and PG Open Days, and potential applicants are strongly encouraged to visit (travel costs are paid). In addition to the various sources of external funding (RC-UK, EU, industry, charities *etc.*), Chemistry offers its own scholarships. For EU and Overseas students, our Wild Fund (see above) provides support towards fees/maintenance, while all applicants can apply for four-year departmental studentships where a proportion of the student's time is dedicated to technical support or teaching. Individuals benefit from a unique opportunity to develop specific additional expertise, enhancing their career prospects, while the Department receives support in these vital areas of its provision.

In 2012, the Department began a pilot, in-house Centre for Doctoral Training in Catalysis, currently involving 14 PhD students and 11 academic supervisors; it is proposed to move all new PG students to a CDT structure from 2014. The Department collaborates internally in the four-year Wellcome Trust CIDCATS PhD programme, which includes a foundation year of laboratory rotations and skills development. Other four-year studentships are offered as part of the White Rose BBSRC Doctoral Training Partnership, joint with Biology and with Leeds and Sheffield.

PG Training, Support and Monitoring

Students whose first degree was not obtained in York are assigned a first-year mentor. Research students undertake a training programme tailored to their needs and throughout their degree, they develop research skills through techniques training, taught courses, literature seminars and training on report/paper writing and preparing posters. They take part in the third-year Poster Competition and can be nominated for the KMS PhD prize, which is based on scientific excellence and communication skills. Employability skills sessions and language courses are available for those who require them.

Student progress is monitored by day-to-day meetings with supervisors and at six-monthly intervals by a Thesis Advisory Panel (TAP), consisting of the student, the supervisor(s) and an Independent Panel Member (IPM, another member of staff). Interim reports are produced for mid-year meetings, while formal, end-of-year reports are produced for the others, being considered in a *viva voce* examination, culminating in a mock viva. The IPM/TAP arrangement provides an important support mechanism and encourages a critical approach. Presenting the results of research at national and international conferences is an important aspect of postgraduate development and the Department provides students with an annual conference grant.

d. Income, infrastructure and facilities

Provision and Operation of Specialist Infrastructure

The Department is housed in modern laboratories with significant upgrades as described below. By the time that the new laboratories for Green Chemistry are occupied in Q1 2014, >95% of the Department's researchers will be housed in facilities completed within the last eleven years.

Evidence of Investments in Infrastructure and Facilities

Investment in new buildings has totalled **£17.9M** in the period:

- The second phase of the Dorothy Hodgkin Building (first phase 2004) was completed in 2012 (**£9.5M**), providing high-quality, three-storey accommodation (1750 m^2) for research groups in inorganic, organic and materials chemistry, and housing the Chemspeed facility.
- Competitively awarded funds (**£2.8M**) from The Wolfson Foundation and the Wellcome Trust to Duckett and Green (Psychology) provided a new two-storey building (840 m^2) to house the Centre for Hyperpolarisability in Magnetic Resonance, also occupied in 2012.
- **£3.5M** of a total build project of **£9M** will provide new accommodation (1150 m^2) for Green Chemistry and will include an Industrial Engagement facility (£1.5M: ERDF) with labs purpose-built for industry-academic collaboration. The remainder of the project will provide new Chemistry teaching space, including new teaching laboratories (to be completed Q1 2014).
- The Atmospheric Chemistry group will be housed in a new two-storey building (800 m^2) costing **£2.1M** (**£1.2M** from the Wolfson Foundation) opened in Q4 2013 supported by a five-year rolling investment of **£0.9M** pa from NERC in research staff and **£2M** of new equipment from DEFRA and NERC, including a high-resolution TOF-MS.

Equipment spend in the period has totalled **£13.4M**. Major items include:

- **£2.8M** of equipment for the Biorenewables Development Centre
- **£4M** for the purchase of NMR spectrometers, including a 400 MHz MAS-NMR machine.
- **£1.8M** to equip and develop a Centre of Excellence in Mass Spectrometry.
- **£0.53M** for X-ray diffraction equipment (single crystal and low-angle).

Of particular note:

The Department is exceptionally well equipped for **NMR spectroscopy**. There are 13 instruments from 700 to 300 MHz (including three wide-bore) and a 7T-30 BioSpec imaging instrument, overseen by two dedicated EOs and a senior technician. This strength supported capital investment from Wellcome Trust (above) and over **£2M** in research grants in the period.

In **mass spectrometry**, existing equipment was augmented significantly (**£1.6M** from the former RDA and later **£0.2M** from EPSRC) to form CoEMS, equipped with a wide range of instrumentation including a 9.4T FT-ICR-MS instrument and managed/operated by a dedicated EO and a senior technician. As well as providing enhanced facilities for Chemistry, CoEMS established a fee-for-service facility, research training and user access, and has generated £576k of direct income through contract research services involving 71 external organisations including 22 companies.

Research Funding Portfolio

The Department finished the assessment period by recording more than £25M in new grants won during 2011-13, its most successful period to date. Its income from NERC and BBSRC places it third for each among chemistry departments nationally and it is unusual in enjoying substantial support from Wellcome and MRC as well as from European agencies (EC, ERC, ERA, ERDF, ESA, IMI/EFPIA). Thus, Research Councils, UK-based Charities and the EU represent its major income streams and these remain healthy and fast-growing at the end of the period, having dropped slightly in the intervening years. Success in diversity in funding reflects the multidisciplinary approach to research and further growth will be predicated on extensive engagement with EPSRC's research landscape and Grand Challenges.

Consultancies and Professional Services: Consultancies are detailed in Section **d**, while external organisations make use of the Department's first-rate equipment either *via* fee-for-service (*e.g.* CoEMS) or longer-term contracts (*e.g.* in YSBL).

e. Collaboration and contribution to the discipline or research base

Staff make substantial contributions and the following list is illustrative rather than exhaustive.

Collaboration: The Department promotes an ethos of collaboration and requests for resource that involve collaboration within/between Departments are prioritised. Regional collaboration is fostered through the N8 (*e.g.* successful EPSRC Core Capability bid) and the White Rose Consortium (York, Leeds and Sheffield) that allocates studentships to projects involving staff from at least two institutions. The academic reputation of staff in the Department naturally leads to extensive collaboration at national and international level with both academic and user groups. Such collaborations are funded through schemes such as EU Networks, various exchange programmes and, with industry, through direct funding, CASE schemes and KTN/KTPs. Evidence

that this is a strong and productive feature comes from the fact that of our returned outputs, which represent some of our best science, 34% have ≥2 York authors, 40% involve UK collaborations and 48% represent international collaborations; many fall into more than one of these categories. Only 15% have a single York author. Particularly effective collaborations are represented by **Brzozowski**'s work with groups in Australia (x3), USA (x2) and the Czech Republic on insulin binding (*Nature* and subsequent £1.5M MRC programme grant), **Perutz**'s work with Eisenstein (six papers in period, 160 citations), **Wilkinson**'s work within an EU consortium (16 groups) on *Bacillus subtilis* (*Science* x 2) and extensive collaboration between our atmospheric chemists and those in Leeds and Cape Verde (plus others and through NCAS) (*Nat. Geosci.* (x2), *Nature* (x2), *PNAS* (x2)). Collaborations with users are exemplified by the Materials grouping's significant collaborative projects with DTI, QINETIQ, DSTL, Merck, Smith & Nephew, Baker Hughes, Kingston Chemicals, Halation and Dymatic (both China) and TTP (patent + >£725k in period) and YSBL's on-going collaborations with Novozymes (patent + >£800k in period).

Interdisciplinary Research: With a strong, supportive culture of collaboration, inter- and multi-disciplinarity feature strongly in the Department's work and is exemplified by internal collaborations through the many multidisciplinary centres of which Chemistry is a part (Section **a**) and the fact that three members of staff are joint appointees (**Gai** – Physics; **J. Wilson** – Maths; **Hubbard** – Vernalis Ltd.). For example, CHyM (above, **Duckett**) represents an interdisciplinary approach to the application of hyperpolarised NMR (*Science*, *JACS* (x2)) in neuroscience (Psychology) and medicine (Medical School), while BioArCh is a powerful grouping in which rigorous scientific methods are applied by our analytical chemists to archaeological study and has spin-outs into food security with FERA (*Nature* (x2), *Nat. Chem.*, Impact Case Study). Similarly, within the York Centre for Complex Systems Analysis, work between **Sebald** and Clark (Computer Science) has applied genetic/evolutionary algorithms to the development of NMR pulse sequences (Humie Competitive Bronze Award, http://www.genetic-programming.org/combined.php).

Influence of Collaborations with Research Users on Activity and Strategy: Research users are important partners in our work and so our interactions with them are planned carefully. For example, in relation to staffing we actively encourage flexibility that strengthens links to users, *e.g.* **Hubbard's** 40% contract with Vernalis that continues through the period, secondment (20%) of Bergström (EO) to spin-out Paraytec and release of **Lewis**'s time as a Director of NCAS, which brings the atmospheric group's science closer to users such as government and the Met Office. These links also underpinned decisions surrounding the appointment of a Chair and three new staff in Atmospheric Chemistry. Similarly, creation of the Biorenewables Development Centre by the University with **Clark** provided a vehicle to allow focus of external funding (£10M) to provide a microwave biorefinery and bioethanol plant and to act as a commercial demonstrator for interested companies. Similarly, the breadth of Green Chemistry's activity with users led to the inclusion of an Industrial Engagement Facility in the plans for the new accommodation that they will soon occupy. This expansion in the activity in Green Chemistry was also influential in the creation of a new Chair position (**North**) to diversify in this area.

Leadership in the Academic Community – Prizes and Awards: Some 18 staff won 38 prizes or awards both nationally and internationally, demonstrating the extent of their esteem among their peers and their leadership of their academic disciplines. We highlight (i) election of **Davies**, **Goodby** and **Perutz** as Fellows of the Royal Society (ii) **Gai** as 2013 L'Oréal-UNESCO Woman in Science Laureate and as 2010 Gabor Medallist of the IoP (iii) award of the Sacconi Medal of the Italian Chemical Society and the Franco-British Award of the French Chemical Society to **Perutz** (iv) award of the RS Gabor Medal and Membership of EMBO to **Davies** (v) award of an Honorary Degree to **Clark** (Ghent, Belgium) (vi) RSC Prizes to **Bruce** (Tilden), **Clark** (Environment) and **Smith** (Corday-Morgan) and Awards to **Davies** (x2), **Duckett**, **Goodby**, **Lewis**, **O'Brien** and **Taylor** (x2) (vii) Bronze Medal: Malaysian Association of Research Scientists to team including **Matharu** (2013) and (viii) awards to younger staff: **Hamilton** (Desty Memorial Award), **Parkin** (Biochemical Society Early Career Award) and **Penkman** (Philip Leverhulme Prize, Lyell Fund Award of the Geological Society, Lewis Penny Medal of the Quarternary Research Association).

Among appointments to *Advisory Boards*: **Taylor** - Senior Advisor, Singapore A-Star ICES Institute; **Davies** - External Assessor, Dutch Review of Chemistry; **North** - member of FROPTOP (From Renewable Platform Chemicals to Added-Value Products) White Paper working group and **Lewis** - Technology Strategy Adviser to NERC (2008-2013) and a Director of NCAS (2008-). **Evans** chairs the Operations Committee of the Facility for Airborne Atmospheric Measurements

(FAAM) which runs the UK's large research aircraft, and the Chemistry Group for the GEOS-Chem Chemistry Transport Model (part of the NASA and Beijing Climate Center's Earth System Models), brokering decisions on data to be incorporated into the GEOS-Chem Chemistry Transport Model. **Bernath** and **Carpenter** were primary reviewers for Chapter 1 of the United Nations Environment Programme (UNEP) assessment report *Scientific Assessment of Ozone Depletion 2010* and members of the Scientific Assessment Panel. **Carpenter** is lead author for Chapter 1 of the 2014 report. *Consultancies* are held by eight members of staff across more than fifteen companies.

York Chemists makes significant contributions to *Learned Societies*. **Davies** Chairs Section Committee 6 and **Perutz** was a member of Section Committee 3 of the Royal Society. **Walton** was Chair of HCUK at the time it initiated discussions with EPSRC about research equipment, which led to the announcement of EPSRC's Core Capability funding. As **Chair** of the RSC's Diversity Working Group, he enabled the Society to re-gain lost momentum in this crucial area. He is also an Athena SWAN and INTEGER ambassador. **Bruce** is a member of RSC Council and Chair of its Audit Committee, influencing decisions concerning RSC's recent move to substantial funding of many new projects. In addition, York provided three RSC Division Presidents, namely **Bruce** (Materials to 2009), **Perutz** (Dalton to 2011) and **Keely** (Environment – President Elect) and **Taylor** was President of the International Society of Heterocyclic Chemistry (2009-11).

During the assessment period, staff in Chemistry delivered 124 Plenary Lectures, 374 Keynote/Invited Lectures and have given >370 seminars worldwide. In particular, these staff have given the following numbers of plenary and keynote/invited lectures, respectively: **Clark** 23 and 45; **Davies** 9 and 20; **Hubbard** 12 and 37; **Perutz** 9 and 17 and **Taylor** 16 and 2.

Consistent with the standing of a department such as that in York, all staff act as journal reviewers and the majority are part of the Research Council Peer Review College. Journals have recruited many staff to serve on their Advisory Boards and, in particular, the following serve in an editorial capacity: **Keely:** Associate Editor Organic Geochemistry (2008-09). **Brzozowski:** Co-Editor *Acta Cryst. D*, *Acta Cryst. F* and *Frontiers in Endocrinology*. **Carpenter:** *Atmos. Chem. Phys.* (to 2011). **Chechik:** Co-editor RSC SPR on EPR spectroscopy. **Gai**: *Curr. Opin. Solid St. M.*; *Microsc. Microanal; Microsc. Res. Techniq.*. **Lewis**: *Analytical Methods*. **Thomas-Oates:** Associate Editor, *J. Int. OMIC*. **Smith:** Volume Editor: *Supramolecular Chemistry: From Molecules to Nanomaterials*, Volume 7, *Soft Matter*, Wiley-VCH; Associate Editor (*Tetrahedron*, throughout period). **Taylor:** UK Editor of Tetrahedron from 1997 - continues; Joint Editor-in-Chief, Comprehensive Heterocyclic Chemistry III (15 Volumes), Elsevier, 2008; **Bruce:** co-editor (with O'Hare, Oxford and Walton, Warwick) of the Wiley Inorganic Materials Chemistry Series (six volumes in period and two in press); **Walton** (Chair, *Dalton* Editorial Board to 2008).

Departmental members have positions of influence within the Research Councils, guiding policy and allocation of resources: **Carpenter:** Programme Advisory Group of NERC Arctic Programme (2010-2015); Steering Committee - NERC SOLAS (Surface Ocean, Lower Atmosphere Study) Programme to 2010; **Cowtan:** CCP4 executive committee; **Lewis**: EPSRC Cross-disciplinary Interfaces Programme (2009-2011) and STFC Futures (2011-) Advisory Panels; **Hubbard:** Chair BBSRC Committee D (to 2009), BBSRC Appointments Board (2011-), BBSRC Bioscience for Industry Strategy panel (2013-), Chair Management Advisory Panel, Chemical Database Service (to 2012); **Karadakov:** Independent Technical Steering Committee of EPSRC National Service for Computational Chemistry Software; **North**: Deputy Director EPSRC CO_2Chem Grand Challenge; **Thomas-Oates:** BBSRC Strategy Advisory Panel/ENWW Portfolio Group; EPSRC Mass Spectrometry Facility Tender Advisory Group; NERC NEOMICS expert working group; NERC Mathematics & Informatics for Environmental Omic Data Synthesis Advisory and Implementation Group member; **Wilkinson:** BBSRC Studentships and Fellowships Panel.

Again consistent with the standing of the Department, the following held visiting positions during the assessment period: **Bernath:** National Center for Atmospheric Research (NCAR), Boulder, CO; University of Florida (2010); **Bruce:** Universidad de Concepción (2013), University of Buenos Aires (2012) National Sun Yat-Sen University (2010); **Clarke:** Universidad Complutense, Madrid (2010 & 2011); **Cockett:** Tokyo Institute of Technology (2010); **Goodby:** Université d'Artois (2009-11); **Keely:** Curtin University (March 2011 to present); **Macquarrie:** ESCOM / Université de Compiegne (2010 to present).