Institution: University of Oxford

Unit of Assessment: 8 Chemistry

a. Overview

This Unit of Assessment equates to the Department of Chemistry ('Oxford Chemistry'). Our research emphasis is on basic science that will make major long-term impacts on society. We continue to attract internationally outstanding researchers and aim to provide an environment that will nurture and enable the highest quality science. Research is based in 4 buildings, including the Chemistry Research Lab (CRL, opened 2004), which houses ~600 researchers. We are one of the largest and most productive chemistry departments in the world, with >900 researchers comprising >70 permanent academic staff, >400 graduate students, 150 PDRAs, 170-180 4th-year under-graduates doing full-time research projects, and >100 visiting researchers (from postgraduates to senior academics in residence for more than a month). We are ranked as one of the top chemistry departments worldwide (6th in 2011/12,5th in 2013 QS Chemistry rankings). Academic leadership is provided by the Chemistry Management Board (CMB) comprising the Chairman of Chemistry and the 3 Heads of Sections, who are line managers for academic staff and research-facility heads.

Highlights for this UOA in the REF period include:

- The establishment of 8 priority research themes across Chemistry (see Section b) to actively promote interaction and collaboration between PIs and externally.
- Strong diversification and growth of research income.
- A series of strategic recruitments to permanent academic positions (19 since RAE 2008) to enable expansion into new research areas especially in interdisciplinary themes, such as Chemistry at the Interface with Biology and Medicine.
- Making the case for, and establishing, ground-breaking new joint academic appointments with Biochemistry, Oncology, Pharmacology and STFC to strategically develop areas of targeted interdisciplinary science.
- Investment of £ 3M leading to design and planning permission for a new Interdisciplinary Chemistry Research building with major fundraising efforts in progress.
- Investment of more than £ 4M in new core instrumentation supported by strategic departmental investment and grants (EPSRC, Wellcome).
- Election of 5 new FRS (H. Anderson, Armstrong, Bayley, Manolopoulos, Schofield) and a DBE to Robinson. Many Royal Society and other awards including 32 RSC prizes.
- >3400 peer-reviewed papers since 2008 - more than any other UK or US chemistry department.

b. Research strategy

Progress since 2008 and evidence of vitality of the research environment

Our vision is to advance, through research, the fundamental understanding of Chemistry, and to use that knowledge to address major challenges for society. We aim to maintain world-class core strengths in basic research, including the training of outstanding young researchers to acquire deep chemical knowledge, whilst being an outward-looking department engaging with other disciplines, industry, public services, government and the general public.

An important strategy since the last RAE has been to establish 8 priority research themes to focus future development of Oxford Chemistry. Some (e.g. Synthesis; or Kinetics, Dynamics and Mechanism) will sustain important traditional strengths, whilst others reflect a strategic aim to grow interdisciplinary research (e.g. Chemistry at the Interface with Biology and Medicine, Sustainable Energy, Catalysis). Since 2008 research in all 8 themes has been highly productive, with the greatest growth in Chemistry at the Interface with Biology and Medicine, owing to strategic new appointments and major collaborations (see Section c). Substantial improvements in our core instrumentation facilities have given greater research capacity and support, while significant increases in graduate student numbers have underpinned increasing strength in e.g. Catalysis and Synthesis. In our last RAE submission, priority was given to initiatives in Nanoscale Science and Catalysis, Biomedicine, Energy, and Measurement, and significant progress in these areas is described below under the relevant priority themes (T1/T4, T3, T6, T8 respectively) along with a range of other initiatives. New or expanding research areas since 2008 include, femtochemistry, ionic liquids and their interfaces, epigenetics, protein radiolabelling, lanthanide chemistry,

computational organic and inorganic mechanisms, new generation proteomics, and main group chemistry. A description of each theme and progress since 2008 is highlighted below with statistics (at Oct 31 2013) indicating activity levels. [Note that although PIs contribute to multiple themes, all other data (student/PDRA numbers, grant income) are attributed to specific themes.]

(T1) Catalysis (37 PIs contributing to theme). Current PDRAs: 20; Current graduate students: 75; Publications in REF period: 406 (Citations 6477); Patent applications in REF period: 21; Total value of new grants awarded (08-13) £14M. Catalysis crosses traditional boundaries of homogeneous and heterogeneous research and encompasses Inorganic, Organic and Biological areas. The EPSRC Research Areas website lists Oxford Chemistry as a major centre for catalysis investment. The Wolfson Catalysis Centre, led by Tsang, has grown its international reputation for innovative research in heterogeneous catalysis with a particular emphasis on nanocatalysts; it is well funded (> £ 2M in new grants, £ 0.5M from industry) with strong links to the spin-out Oxford Catalysts (AIM listed, see Impact Case Study 1). The Saudi - Oxford collaboration, KACST - Oxford Petrochemical Research Centre (KOPRC), established in 2012 by Edwards and allied with Cardiff, Cambridge and Imperial, focuses on heterogeneous catalysis applied to sustainability challenges in the petrochemical industry (see also T6). **Selected Published Highlights (2008-13) in T1 Catalysis include**: Rational design of nanocatalysts via chemisorption evaluation in liquid phase (*Science*, 2011); Mechanistic studies on glycosyltransferases (*Nat. Chem. Biol.*, 2011); Fundamental studies on chemical and enzymatic electrocatalytic energy conversion (*PNAS*, 2011).

(T2) Synthesis (36 PIs contributing). Current PDRAs: 38; Current graduate students: 113; Publications in REF period: 728 (Citations 10330); Patent applications in REF period: 22; New Grants £23M. Synthesis is a central pursuit of our activities, and includes studies on organic and inorganic reaction invention, efficient asymmetric synthesis, biological-probe synthesis and medicinal chemistry, supra-molecular synthesis, synthetic biology, imaging agents, CO_2 capture, fuel-production, and natural product chemistry. In many cases, we apply our leading expertise in academic and industrial collaborations in which synthesis is limiting, including in medicine /pharmaceutical development, basic biology, molecular electronics, and polymer science. We produce the largest cohort of highly-trained researchers in synthesis in the UK (> 30 PhDs p.a. with >90% taking up science-related positions). We have built on already strong industrial links relating to synthesis; current collaborators include Amgen, AstraZeneca, GSK, Eisai, Eli Lilly, Johnson and Johnson, Johnson Matthey, Novartis, Pfizer, Syngenta, and UCB. We have established many new collaborations, e.g. with CRUK, MOD/DSTL, and biomedicinal groups worldwide. Exemplary evidence for interest in our work comes from the award of an EU Innovative Doctoral Training Programme (IDP, € 3.8M). **Highlights include:** Invention of a Vernier strategy for template directed synthesis (*Nature,* 2011); Reagents for chiral electrophilic fluorination (*ACIE*, 2013); Synthesis of a solid rhodium(I) sigma-alkene complex (*Science,* 2012); and multiple examples of complex natural product syntheses.

(T3) Chemistry at the Interface of Biology and Medicine (46 PIs contributing). Current PDRAs: 51; Current graduate students: 70; Publications in REF period: 687 (Citations 13880); Patent applications in REF period: 104: New grants £27M. Our activities in this area have increased very substantially since 2008, and involve overlapping sub-themes including Chemical Biology, Bio-inorganic and Enzyme Chemistry, Medicinal Chemistry/Probe Synthesis and Analysis, Biophysical Chemistry and Biotechnology. We have developed particular strengths in biological mass spectrometry (both studies on large complexes and proteomics); novel ultra-rapid sequencing; post-translational modifications; epigenetics, signalling and synthetic biology; single molecule science; supernatural biosynthesis, biocatalysis /enzymology; enzyme crystallography; and biological NMR. Links between Chemistry and Biochemistry/Biology/Medicine (both in Oxford and beyond) were already strong and we have further enhanced these via major new collaborative initiatives/grants, e.g. establishing the Target Discovery Institute (with Clinical Medicine), a 5-year CRUK drug discovery grant (£ 2.5M) 'Oxford Chemistry for Cancer' (Davies), a Wellcome grant to develop epigenetic probes (with the Structural Genomics Consortium). **Highlights include**: 3D Printing of tissue-like materials (*Science*, 2013); Hydrogenase-modified nanoparticles for producing H_2 using light (*JACS*, 2009); MS anaylses of membrane proteins (*Science*, 2011); Palladium catalysed labelling of cells (*JACS*, 2013); Use of porphyrins to measure potentials across lipid membranes (*ACIE*, 2013); Discovery, structural, functional and mechanistic studies of the

ribosomal oxygenases (*Nat. Chem. Biol*., 2012); Use of nanopores for analyses of multiple biomolecules (*Nat. Nanotechnol*, 2009).

(T4) Advanced Functional Materials and Interfaces (32 PIs contributing). Current PDRAs: 17; Current graduate students: 42; Publications in REF period: 431 (Citations 5635); Patent applications in REF period: 20; New grants £9M. We continue to advance diverse and multidisciplinary work in this area, e.g. on superconducting metal pnictides, reduced metal oxides and nitrides, framework and zeolitic materials, nanoparticles and supported catalysts, layered materials, nanocomposites, thin films/surface chemistry, solid catalysis, drug delivery and vaccine adjuvants, magnetic, conducting, optical & multiferroic materials, nanowires and nanorings, soft matter and organic photovoltaics, underpinned by substantial theory and computational work. Since 2008, we have built strong interactions with other disciplines (Physics, Materials, Engineering, Biochemistry) making extensive use of major facilities such as the Diamond Light Source and the ISIS Neutron Facility including via joint studentships and residency at the Research Complex at Harwell (Clarke, O'Hare). SCG Thailand has established (in Oxford Chemistry) the SCG-University of Oxford Centre of Excellence, with O'Hare as Director. With SCG funding committed to 2017, it is focusing initially on applications of layered double hydroxide compounds. Moloney has invented new methods for the modification of polymer surfaces under mild conditions, permitting introduction of useful functionality onto inert materials, leading to commercial developments at the spinout Oxford Advanced Surfaces. The Oxford Centre for Biological and Soft Matter (Dullens, Aarts, Perkin, Doye) collaborates with Physics to develop new techniques enabling exquisite control over the size, shape and interaction of particles and new measurement techniques, e.g. confocal microscopy and laser tweezers, allowing the study of interfaces with unprecedented accuracy and control. A new research area is the study of ionic liquids at interfaces, which brings opportunities to interact with industry (lubricants and additives) and links up the recent appointment of Perkin with expertise of Compton in this area. **Highlights include**: Discovery of a material (zinc dicyanoaurate) that expands under pressure (*Nat. Mater*., 2013); Nature of the band gap and origin of conductivity of PbO_2 (lead acid batteries) (*PRL*, 2011); New methods for evaluating adsorption of substrates onto metal nanoparticles by NMR (*Science*, 2011); Synthesis of porphyrins fused to anthracenes to generate large planar π-systems with strong electronic infrared absorption (*JACS,* 2011); Use of multiwall WS_2 nanotube templates to prepare defect-free inorganic nanotubular structures (*ACIE*, 2009); photocatalysis by zinc oxide nanoparticles; size and shape effects on activity (*JACS*, 2009).

(T5) Theory and Modelling of Complex Systems (20 PIs contributing). Current PDRAs: 6; Current graduate students: 25; Publications in REF period: 307 (Citations 3517); New grants £4M. We have one of the largest theoretical/computational chemistry groups in Europe. Research has an emphasis on condensed phases, including the quantum theory of strongly correlated materials and nanoscale devices; quantum and chemical dynamics of condensed phases; optical excitations in conjugated and polymeric materials; atomistic simulations of complex inorganic solids; soft matter, colloids and biomaterials; biological self-assembly, structure and function; fluid flow and diffusion kinetics. New appointments (e.g., McGrady, Paton) since 2008 have brought additional emphasis on computational chemistry in catalysis and inorganic/organic reaction mechanisms. Strong external partnerships have been developed with Cambridge (EPSRC Programme Grant on Simulation of Self-Assembly), with Birmingham (EPSRC Critical Mass Grant on catalysis in nanoalloys), with Bristol (EPSRC Programme Grant on chemical and photochemical dynamics), and with Oxford Physics (EPSRC, Quantum Condensed Matter Theory). **Highlights include:** New methods for including quantum effects in molecular dynamics simulations: from liquid water to gas phase H-atom transfer (*PNAS, 2013*); New many-body methods for nanoscale devices; first consistent theoretical understanding of zero-bias conductance in carbon nanotube quantum dots (*PRL*, 2008); Determination of the influence of low-symmetry distortions on electron transport through metal-atom chains: When is a molecular wire really "broken"? (*JACS,* 2011); Computational research revealing the structure and function of an antibiotic synthesis enzyme (*Nature,* 2012); Development of oxDNA, the most successful coarse-grained model of DNA at the nucleotide level; applications in DNA biophysics and nanotechnology (*ACS Nano,* 2013).

(T6) Sustainable Energy Chemistry (16 PIs contributing). Current PDRAs: 3; Current graduate students: 14; Publications in REF period: 130 (Citations 2239); Patent applications in REF period: 10; New grants £3M. Since 2008 our energy research, which has clear synergies

with the Catalysis theme (T1), has grown and diversified to encompass: Hydrogen storage in solids, chemical hydrogen storage; new solid-state (inorganic or polymer) materials for batteries; solar cells materials; CO_2 conversion and reduction; catalysis and biocatalysis for fuel cells and solar hydrogen production/artificial photosynthesis; methanol and formic acid fuels; nanocatalysts for future energy provision; radiochemistry for nuclear fuel cycles; sugar processing enzymes for biomass. The KACST-Oxford Petrochemical Research Centre (KOPRC) led by Edwards tackles frontier challenges in obtaining clean energy from fossil fuels, including fuel economy materials and tri-reforming techniques for CO_2 conversion (see also T1). Collaboration with the Rutherford Lab (David) addresses hydrogen storage research, and Edwards co-founded the UK Sustainable Hydrogen Energy Consortium. Armstrong leads the EPSRC Supergen Biological Fuel Cells Consortium 2010-14 and has elucidated mechanisms by which enzymes responsible for bacterial hydrogen production can avoid being inactivated by oxygen, opening the way for continuous photosynthetic algal biohydrogen production (hydrogen farms). The work was highlighted at our RS Summer Exhibit in 2013. **Highlights include**: Demonstration of high capacity hydrogen storage in lithium and sodium amidoboranes (*Nat Mat,* 2008); Very fast production of hydrogen using sunlight as energy source: special role for enzymes as efficient electrocatalysts (*JACS, 2009*); First report of completely selective reduction of CO_2 to methanol in homogeneous solution (*ACIE*, 2009).

(T7) Kinetics, Dynamics and Mechanism (24 PIs contributing). Current PDRAs: 9; Current graduate students: 34; Publications in REF period: 286 (Citations 3596); Patent applications in REF period: 4; New grants £7M. Studies under this theme impact on almost all our research. Areas that have grown since 2008 include interfacial and (bio)electrochemical kinetics and mechanism; reaction dynamics; photochemical and radical processes and spin chemistry; femtosecond spectroscopy; computation of reaction pathways. Funding in the REF period includes one of the first EPSRC programme grants in the UK involving a new collaboration between 6 Oxford and 4 Bristol groups, which extends methods of gas-phase dynamics towards more complex molecular systems and condensed phases. Foord, J. Davis, Compton, Armstrong and Vincent have made powerful use of voltammetry and other electrochemical techniques for studies of heterogeneous, homogeneous, and enzyme kinetics. New areas include the measurement of electron transfer kinetics at the single nanoparticle level (Compton), development of diamond-based electrode materials (Foord), and the use of protein film voltammetry for enzyme mechanisms (Armstrong). Kukura has developed femtosecond-dynamics experiments; Mackenzie pioneered work on reactions on metal clusters and cavity-enhanced spectroscopy for condensed-phase dynamics. Hore leads a major £ 3.4M Defense Advanced Projects Agency (DARPA) funded international collaboration studying spin dynamics in biological systems, and has performed ground-breaking studies on the magnetic field effects on bird navigation. **Highlights include**: Demonstration that a chemical reaction can respond to magnetic fields as weak as the Earth's and to the direction of a magnetic field (*Nature*, 2008); Kinetics of ultracold ion-molecule reactions using laser cooled ions and a velocity selector for neutral molecules (*PRL,* 2008); new quantum mechanical mechanism for collision-induced orientation (*PRL,* 2013); Experimental and theoretical elucidation of the mechanism of the avian magnetic compass (*PNAS*, 2012); Dynamics of the primary photo-isomerisation event in vision: ultrafast spectroscopy reveals the role played by a "conical intersection" (*Nature*, 2010); Electron transfer kinetics at single nanoparticles (*NanoToday*, 2012).

(T8) Innovative Measurement, Imaging and Photon Science (41 PIs contributing). Current PDRAs: 26; Current graduate students: 49; Publications in REF period: 493 (Citations 6646); Patent applications in REF period: 53; New grants £16M. This theme is interdisciplinary and collaborative, and includes: labelling and imaging; genome sequencing technologies (nanopores); microscopy and single-molecule optics; laser applications and photonics; electrochemical sensors and biosensors (diagnostics); spectroscopic techniques; magnetic resonance (NMR and ESR); mass spectrometry; diffraction and structure (X-ray, neutron); microfluidics; soft matter techniques; laser scanning confocal microscopy. The work is underpinned by investment in outstanding mechanical and electronic workshops and core instrumentation (Section d). Kukura has brought new expertise in nanoscale imaging; Softley has developed novel instrumentation for studying ultracold reactions. We have secured the long term future of the Centre for Advanced Electron Spin Resonance (CAESR) via Departmental and new EPSRC funding. CAESR is used by 30 groups from across the sciences, and has driven important technological and methodological

advances in EPR with wide-ranging applications from biology to quantum computation. In imaging, there have been new developments in lanthanide chemistry (Faulkner) and radio-labelling (B. Davis, Gouverneur) and we have made significant contributions to the advancement of PET imaging at the CRUK/EPSRC funded Oxford Cancer Imaging Centre through the chemistry of ^{18}F labelling (Gouverneur). J. Davis has pioneered the development of new MRI imaging probes (Wellcome-supported) and the generation of biomarker tools based on capacitance and impedance, including development of a Parkinsons diagnostic tool. Improvements in novel measurement techniques using electrochemical and laser sensing have led to, and sustained, 3 spin-out companies with applications in medicine and environmental monitoring: Oxford Medical Diagnostics (Hancock/Ritchie), Oxtox and Senova (both Compton). Strong links with the ISIS neutron scattering facility have continued (Penfold and David have been Visiting Professors in the Department – David is now a joint appointment with STFC). Brouard/ Vallance established a major collaboration in fast imaging using a pixel-imaging mass spectrometry camera (£2M STFC/EU/EPSRC funding). **Highlights include**: Use of dual-mode contrast media based on *d-f* hybrids for imaging applications (*JACS*, 2011); Invention of Parkinsons and cardiovascular diagnostic devices (*Chem Sci.,* 2012); First fluorescence-free optical detection of single molecules (*JPC Lett*., 2010); Pixel imaging mass spectrometry-fast imaging sensor for time-of-flight particle imaging applications (*Physics Today*, 2013); Electrochemical sizing of nanoparticles in solution; observing the state of aggregation and concentration (*ACIE*, 2011).

Future Strategy for Oxford Chemistry:

Our vision for the next 6 years for Oxford Chemistry research and its environment is summarised in the objectives below, with mechanisms for their achievement then described:

1. To further advance our world-class fundamental-research profile by appointing, training, supporting and retaining the best people – faculty, students, research and technical staff – to carry out world-leading fundamental research.
2. To develop strengths in, and take advantage of, critical mass in our 8 research themes.
3. To further develop our strong relationships with other Physical and Mathematical Science departments, and with Biological & Medical Sciences.
4. To build and sustain long term strategic and effective engagement with industry and other external partners (e.g., Diamond Light Source, Rutherford Appleton Laboratory and Harwell Science and Innovation Campus) capitalising on the success of existing collaborations.
5. To ensure that our research facilities and shared core instrumentation match our ambition to remain a world-leading centre for innovative Chemistry.
6. To continue to attract world-class postgraduates and PDRAs from around the globe by providing a leading research environment, high quality training and scholarships.
7. To advance translation of our work through spin-outs, licencing, patents, consultancy and multi-company industrial collaboration taking full advantage of our strong track record.

The CMB will monitor progress against these objectives and define strategies to achieve them. A key element of our forward-looking strategy is the construction of a new research building, as a focus for areas of interdisciplinary science where Chemistry makes a major contribution. It will facilitate progress towards co-location of researchers under the 8 research themes described above. It will also offer an exciting opportunity to make new top-class appointments as well as to retain key existing staff (objective 1). The provision of state-of-the-art research equipment and instrumentation to underpin research quality is another feature of our enabling strategy (Section d.)

As we move towards the transformative step of a new building, initiatives have already been planned, or are ongoing, to improve networking and collaboration to strengthen the 8 themes, as well as to develop greater interdisciplinarity. These are supported by the Research Facilitators in Chemistry and Chemical Biology. Broadly, our strategy is to develop the themes through (a) collaborative grant applications, (b) thematic graduate training programmes, (c) periodic mini-conferences under each theme, (d) a joined-up approach to industry, (e) websites and publicity, (f) co-location of researchers where possible, (g) leadership appointments.

In T1 Catalysis the Oxford Catalysis Network, (led by Willis and Weller) was facilitated by University pump-priming and was established to promote collaboration, and encourage outward-facing activities and industrial engagement. The strong link with the recently established EPSRC

Harwell Catalysis Hub will be sustained in terms of both the collaborative projects (17 Oxford PIs involved) and the management of the Hub (Weller, B. Davis sit on the Steering Panel). Building on this ongoing momentum, we are also devising a new graduate training programme, for which industrial support is being negotiated, across the full breadth of our catalysis research areas.

In T2 Synthesis we will increase the breadth of synthetic activities, in particular with respect to sustainable synthesis, functional materials, miniaturised/flow synthesis, catalyst design, and synthesis for energy. To achieve this we will strengthen links with Oxford Materials, Engineering and Medical Sciences, including by promoting collaboration via Oxford Synthesis Connections (OxSynC), which has already enabled collaborations between synthetic chemists and >20 research teams in 10 departments, and by making further joint appointments. To strengthen our outstanding expertise in supramolecular synthesis (e.g. H. Anderson, Beer, Hamilton), we plan to make a new appointment in this field within 18 months. A key strategy is to build long-term relationships with multiple companies in pre-competitive areas of basic research; this will be developed via a new graduate training programme in Synthesis for Medicine and Biology (EPSRC CDT funding secured), which has attracted a combined industrial commitment of £ 5.1M cash.

In T3 Interface with Biology and Medicine we will promote strategic large-scale collaborations in the University and worldwide, rooted in our strengths in basic chemical science. This will be delivered in part by our Research Facilitator for Chemical Biology (MacCoss, ex-Merck), who has been extremely successful in working with PIs to forge links between the chemical and medical sciences at Oxford. Since research in this area cuts across traditional chemical boundaries, there will be a centre for Chemical Biology within the planned new building. This will enable us to bring synergy of chemical and biological expertise (in departments including Biochemistry, Computing, Physiology and Genetics, Mathematics, Plant Sciences and Clinical Medicine), to focus on 'big' biological problems such as real-time quantitative analyses of molecules in whole organisms, the chemistry of genetics, combating resistance (e.g. antibiotic, herbicide, pesticide) and engineering organisms to change the Earth's atmosphere.

In T4 Advanced Materials we recognise the need to support new materials research by developing new characterisation techniques. To facilitate this we will continue to grow existing strong connections with the Diamond Light Source and ISIS Neutron Facility, taking advantage of the proximity of these world-leading facilities and expertise; Goodwin now leads the team to build a new X-ray pair distribution function beamline. The appointment of David to a joint STFC–Oxford professorial position illustrates our strengthening links with ISIS/Harwell and we will look to make more joint appointments with the national facilities in the future (e.g. Diamond).

In T5 Theory and Modelling a future emphasis is to develop the underpinning of experimental work by computational studies, building on recent appointments (e.g., Paton, McGrady, Goodwin). Oxford Chemistry is leading a graduate training programme in Theory and Modelling in the Chemical Sciences, in partnership with Bristol and Southampton, and EPSRC CDT funding is secured from 2014. The EPSRC-funded National Training Schools in Theoretical Chemistry will continue biannually for (*ca* 40 UK $1^{st}/2^{nd}$ year graduate students) to train in key concepts and techniques that underpin research in the field. The location of a Theory and Modelling Centre in the proposed new interdisciplinary building will enable us to improve linkages in computational sciences across the physical and life sciences, aimed at applying theory to major challenges, such as the understanding of assembly of multi-component protein complexes.

In T6 Energy our goal is to provide greater cross-disciplinary coherence to the existing high-quality work and to develop Oxford Chemistry as a world-class centre for sustainable energy chemistry, taking advantage of our strengths in numerous areas such as catalysis, synthesis, electrochemistry, and functional materials. We see energy research as a major component of the proposed new research building and will make at least 2 new appointments in this area over the next REF period. Solar energy to liquid hydrocarbon fuel conversion has been identified as one of the major multifaceted challenges to address. The appointment of Peter Bruce to the Wolfson Chair of Materials from 2014 indicates an intention by Oxford to build strength in the energy-storage field. We also need to build new links with the energy industry and will take advantage of the University's new post of Business Development Manager in Energy to pursue longer-larger industrial collaborations. A new website on sustainable energy chemistry has been established to capture and promote ongoing work in this area, linked to the broader Oxford initiative connecting Energy research across all departments and led by Llewellyn-Smith. We will expand work in

spectroscopic probing of nuclear fuel cycles (led by Faulkner) to support the anticipated growth in importance of the nuclear component of national energy provision.

In T7 Kinetics, Dynamics and Mechanism major funding has been secured to establish the future growth of new areas including two ERC Advanced grants to Hore (development of organic spintronic magnetic sensors/magnetometers) and Compton (mechanistic electron transfer studies to underpin applications of energy storage and conversion devices). A new EPSRC Programme grant 2014-19 in imaging methods for chemical dynamics and imaging mass spectrometry (Mackenzie, Brouard, Vallance joint with Bristol) has been awarded, underpinning strong collaborations.

In T8 Innovative Measurement we will target support towards the development of new methods such as ultrafast detectors, novel light sources, MS-based imaging of biological samples, single molecule reaction studies, novel NMR techniques for biomolecular systems. We will develop a major co-ordinated departmental initiative in imaging, recognising its widespread importance as an enabling technology, encompassing developments in bio-imaging, surface imaging, and imaging mass spectrometry, and the use of new imaging agents. Sharing of facilities provides a core mechanism to deliver interdisciplinary collaboration with cutting edge technology. The Centre for Advanced Electron Spin Resonance (CAESR) is a collaboration of the Oxford Departments of Physics, Chemistry, Materials, Biochemistry, and Pathology. With new EPSRC funding (£ 1.2M for X/Q-band pulsed ESR spectrometer) this is being expanded to broaden the frequency range of the existing spectrometers and to interrogate shorter timescales of reactions and dynamic processes.

In all areas we will accelerate our research collaborations with external organisations with a particular emphasis on building industrial collaborations in the UK and beyond. We will expand the major funded initiative with KACST to promote frontier scientific and technological challenges associated with clean energy from fossil fuels. The SCG (Thailand)-Oxford Centre of Excellence in Chemistry will expand into other areas such as olefin isomerisation, metathesis and polymerisation; Foord and Moloney have a £1M grant from IRPC in Thailand for the fabrication of polymer nanocomposites and this relationship will be expanded.

c. People, including:

i. Staffing strategy and staff development

Link to research strategy and infrastructure

Recruiting *and* retaining the best staff (academic and support) is crucial to our future research strategy. Excellence in research at an international level (or promise of such excellence) remains the overriding criterion for academic recruitment. Since 2008, new appointments have actively supported, and enabled us to build on, our strategic research strengths, including multidisciplinary collaborative research and/or translational opportunities and promoting new/difficult fields (e.g. proteomics). We also strongly believe that individuals must have the freedom to follow 'bottom-up' blue-skies research. A mark of the attractiveness of our research environment is that only one permanent member of academic staff (Klein) has left since 2008 for reasons other than retirement. 19 new appointments at Lecturer or Professorial level in the REF period now give the Department a young age profile for its PIs with 34 (40%) under the age of 40, compared to 29 in 2008.

In the Synthesis and Catalysis areas we have augmented our renowned senior scientists with outstanding younger/mid-career appointments (Aldridge, E. Anderson, Burton, Dixon, Fletcher, M. Smith, Weller, Willis), who take advantage of the first-rate synthetic chemistry facilities of the CRL building. We have appointed T. Brown (joint with Oncology), to promote the field of nucleic acid synthesis/chemistry of genetics and Paton/McGrady to build expertise in reaction modelling as well as to extend the links between theory/computation and experiment.

The election of Robinson to the Dr Lees Professorship, a core physical chemistry appointment, signals a move towards greater interdisciplinarity and supports the development of the interface with Biology as well as enhancing innovative measurement capabilities. It exemplifies how we are working to ensure that traditional branches of chemistry (Physical, Inorganic, Organic) do not create barriers to research and collaboration. The appointments of Benesch, Conway, Vincent, and the arrival of Hamilton, further enhance research strengths at the chemistry-biology-medicine interface. We have made significant efforts to enhance links between basic physical and applied biomedical science, through building expertise in method invention and development (Baldwin, Benesch, Kukura, Mohammed, and Robinson). To enable even stronger collaboration with

Oxford's Medical Sciences Division we have pioneered 2 new joint appointments (50:50) with Biochemistry (Mohammed - Proteomics), and Oncology (Brown - Nucleic Acid Chemistry) adding to the existing joint post with Pharmacology (Russell - Medicinal Chemistry). Likewise the joint appointment (25 (Oxford):75 (STFC)) of David (ISIS/Harwell) shows our desire for stronger collaborations with the Harwell campus and a deeper awareness of the capabilities of the world-leading facilities there.

We currently expect that at least 6 new permanent academic appointments will be made (through retirement) up until 2020. We will use these appointments to strengthen and provide leadership in areas identified in Section b (e.g. organic and supramolecular materials, energy chemistry) as well as to enhance interdisciplinarity (biophysics, chemical scale-up engineering) and our external links (e.g., joint with Diamond). We will continue to use 5-year research fellowships as a means to strengthen such key areas with younger PIs, aiming for 1-2 new fellows per year.

Career development support in research careers

For many years, we have made the overwhelming majority of academic appointments at the University Lecturer (UL) level at a relatively early career stage, and created the environment that allows talented individuals to flourish in their research. Heads of Section (Inorganic, Physical and Theoretical, Organic) play important roles in mentoring and advising new academic staff members, and each individual has an additional advisor appointed in their 5-year probationary period. The 2 Research Facilitators in Chemistry and Chemical Biology give special attention to supporting and guiding younger academic staff in grant applications.

New Lecturers have reduced lecturing and demonstrating loads in their initial 5-year period to facilitate the setting up of independent research operations (e.g. < 2 hours demonstrating a week, 8-12 lectures a year). The University has a generous sabbatical-leave scheme, in which ULs take leave from teaching and administrative duties 1 term in every 7. Start-up funds of at least £ 100k are granted to new ULs to facilitate rapid set-up of their research. 13 ECRs also received a total of £ 246k in small-equipment grants from an EPSRC block grant to the University in 2012. Many ECRs, and all those appointed to ULs, benefit from additional research support provided by Oxford colleges, typically including the appointment of a college mentor and access to additional research funding to support conference travel. Moreover, the colleges provide a truly interdisciplinary environment in which meeting with faculty members or students from other departments is an everyday occurrence, often opening doors to collaborations either directly or indirectly.

Early-career researchers take advantage of the extensive range of career development support provided by the wider University through the Oxford Learning Institute, the Careers Service and the Mathematical, Physical and Life Sciences (MPLS) Skills Training programme. We encourage ECRs to participate, providing details of the available support (including courses, IT resources and coaching schemes) at the half-day departmental induction session for all new researchers held 3 times p.a.. The National Research Concordat is implemented via the University's Code of Practice for the Employment and Career Development of Research Staff. In Chemistry, we have introduced a Personal Development Review (appraisal/mentoring-type) process for all research staff in 2013, comprising a one-on-one review (supervisor and researcher) at which progress against objectives, career development, and support are discussed. We initiated an annual Careers Day for research staff in 2013, introduced by the President of the RSC and featuring alumni in a number of professions ranging from academia to patent law. Feedback from 50 participants highlighted the valuable networking opportunities and the breadth of career options presented. The University's systems and practices to support researchers' career and professional development were acknowledged by a European Commission HR Excellence in Research Award (2012).

Personal (ad hominem) Research Fellowships

There have been 16 holders of 5-Year Fellowships in the period (EPSRC/BBSRC/RS): Benesch, Kukura, Willis, Flashman, Fletcher, Sartbaeva, Goodwin, Domene, Peverall, Snoek, Titmuss, Mackenzie, Kawamura, E. Anderson, Vincent , Smith and Baldwin, 9 of whom were appointed to Lectureships in Oxford and 3 to Lectureships/Readerships elsewhere (3 others are still Fellowship holders). We hosted over 70 researchers appointed to 2-3 Year Fellowships (Newton (3), Leverhulme (1), Ramsay (2),1851 Fellow(1), Marie-Curie (53) and fully-funded college Junior Research Fellowships (~10). We advertise the opportunities for researchers to apply for independent research fellowships hosted by the Department on our website. The Chemistry

Management Board (CMB) reviews and ranks (for quality, subject area and "fit") all expressions of interest and interviews promising candidates. Selected applicants are given advice and support in preparing their applications. We attract young scientists of outstanding quality, who bring expertise and vision to the Department in areas that complement and/or strengthen existing areas. One example is Andrew Baldwin, a BBSRC David Phillips Fellow who is an expert in the use of NMR for study of very large biological macro-molecular complexes and collaborates with experts in MS (Robinson/Benesch). Another is the hosting of Kukura, an EPSRC Fellow, to develop femtosecond spectroscopies and dynamics to complement existing strength in the chemical dynamics field. In appropriate cases we also put forward permanent academic staff for higher-level EPSRC Leadership or Established Career Fellowships. Willis and Dixon have held such awards in the REF period and have been supported by reduced teaching and administrative loads.

International staff appointments, recruitment and visiting scholars

We seek to recruit the best staff from around the world and advertise academic positions internationally (e.g. Nature Jobs) resulting in many international applications - approximately 50% for recent lecturer appointments. Permanent academic staff appointed from overseas in the REF period are: Kukura (Germany), Goodwin, Vincent (Australia) and Mohammed (Netherlands), reinforcing the list of earlier overseas appointments (Aarts and Dullens (Holland), Timmel (Germany) Wong and Tsang (Hong Kong), Vallance (NZ), Moloney (Australia), Bayley (US), Gouverneur (Belgium) and Goicoechea (Spain)). Research Fellows recruited from outside UK include Sartbaeva, Kukura, Snoek, Heazlewood, Christensen, Ceriotti and Baldwin. Typically ~1/3 of the 150 PDRAs are of non-UK origin.

We host 100-150 visitors at any one time (postgraduates, postdoctoral researchers and senior academics), and the majority are international. We also act as host for a number of prestigious named visiting professorships and lectureships, including the Hinshelwood Lectureship, the Newton Abraham Professorship, the Robert Robinson, the RJP Williams, Malcolm Green and the Derome Lectureships, and college-hosted visiting fellowships. Appointees in the REF period include the Nobel Prize winners Ketterle, Schrock, Suzuki and Hoffmann. Joint publications (e.g., Schrock/Dixon and Edwards/Hoffmann) have emerged from these visits as well as numerous scientific interactions which promote new ideas and opportunities.

Chemistry has had 5 formal University Visiting Professorships in the REF period (David and Penfold both from STFC (ISIS/Harwell), Pepper (Penner Chair in Electronic Engineering, UCL), Fenske (Karslruhe), and Jinghai Li (VP of the Chinese Academy of Sciences)) who are senior external researchers spending significant proportions of their research time in the department and are actively involved in collaborations. There have been 70 joint publications since 2008 between Oxford researchers and these Visiting Professors.

Equality and Diversity

Since 2008, the gender balance of our PIs has improved; REF entries include 9 female permanent staff compared to 6 at the time of the last RAE, and a further 6 females with fixed term research fellowships/posts (*cf* 5 at RAE). In 2011, we reviewed our culture, work and study practices, and researcher development activities. In part, this was undertaken in response to the Athena SWAN initiative. The review was informed by a survey of undergraduates, postgraduates and employees, which highlighted areas of success/ good practice and concern, leading to an action plan. The Athena Panel awarded Oxford Chemistry a Bronze Award (2012) noting our awareness of the key issues, forward-thinking commitment, and commended our women's discussion forum ('WICKED' – Women in Chemistry Knowledge Exchanged). Subsequent actions included appointing more women onto decision-making bodies, introduction of annual PDRA appraisal, changing regular seminar times, and a careers day with mainly female speakers. 4 Female academic staff returning from maternity leave have been supported by distribution of 'Returners Grants' (£ 54.6k EPSRC funding) and the Personnel team have worked energetically to find nursery places in several 'difficult' cases. In the future we will take advantage of the new £ 1M Vice-Chancellor's Diversity Fund to support work towards addressing under-representation of women in senior posts, and providing additional research support for those in leadership roles. We have publicised and celebrated vigorously the achievements of female PIs, e.g. the DBE for Robinson, and the Woman of the Future Prize to Vincent. CMB devotes significant time to strategic human resource management and will be developing a new Chemistry HR strategy in 2014. Overall, our objective is

to improve communication and decision–making, enhance career development processes, and provide support to researchers for whom family commitments restrict available working hours. We aim to ensure improvements in work conditions are of benefit and attractive to all researchers.

ii. Research students

Graduate students are at the heart of our research activities with an intake of ~100 graduate students p.a., probably one of the largest such intakes worldwide. Numbers of graduate students registered in years 1-4 grew systematically over the REF period (see table).

2008-09	2009-10	2010-11	2011-12	2012-13
282	303	324	340	352

Recruitment: We receive ~300 applications a year for PhD Studies; our policy is to admit the best students available worldwide. We use Oxford Clarendon Scholarships, college fully-funded studentships, and other international studentships to fund overseas graduate students (in the intake years 2011-13, 26% RCUK studentship funding, 10% partial or full industry, 9% university scholarships, 11% EU, 18% external or other scholarships, 26% private funding.) The award of an EU-funded IDP programme brought in 13 new international graduate students in the area of synthesis for cancer research (2013). Oxford Chemistry is also a first-choice target for overseas students with independent scholarships (Rhodes, NSF, Fulbright, Marshall, Commonwealth). We hold open days each year for graduate students and have a dedicated website to target and assist graduate applicants (alongside the central University's website).

Training and Support: PhD students are members of the MPLS graduate school and can select a suite of courses, tailored for their needs, from the MPLS Graduate Academic Programme (established in 2010 by a working group led by Softley). Over 400 training courses are available, including 37 contributed by Chemistry (2012-13). Many students have entered the Department via the EPSRC-funded Life Sciences Interface DTC, Systems Biology DTC and Systems Approaches to Biomedicine IDC. We contribute substantially to the training, management and supervision of these programmes. From 2014, two new EPSRC-funded Oxford-Chemistry-led CDTs (Theory and Modelling in the Chemical Sciences, and Synthesis for Biology and Medicine) will form the heart of an expanded training programme for all Chemistry PhD students.

Progress Monitoring: All PhD students have an academic advisor in addition to 1 or more supervisors; there are 3 departmental Directors of Graduate Studies (DGS) with responsibility for oversight of progress, admissions and academic standards. Supervisors are required to provide 3 written reports p.a. via an online reporting system, which also enables students to comment on their progress. Reports are reviewed by the appropriate DGS and academic advisor and action taken if needed. At the end of their 1st year, each student is assessed *via* a report and examination in order to progress to their 2nd year. At the end of the 2nd year, students participate in a poster session. In the 3rd year all students have to present another formal progress report and typically also a departmental research presentation. Each student is a member of a college and has regular meetings with a college advisor, an academic providing support and advice independent of the Department. For PhD students the average submission time is 3.6 years. A very high proportion of completed PhD students continue in research; a recent snapshot showed 61% progressing to an academic PDRA, 29% to industry/government R&D. The quality of support provided to PDRAs and PhD students in the REF period is illustrated by the hiring of > 75 of these into full academic positions and >20 into 5-year fellowships at universities from Stanford to Beijing.

d. Income, infrastructure and facilities

65% of researchers are based in the world-class Chemistry Research Laboratory (CRL, est. 2004). The CRL is a focus for Synthesis, Catalysis, Chemical Biology, and Advanced Measurement and Instrumentation research. Other researchers are located in the Inorganic Chemistry Laboratory – upgraded and refurbished in all areas since 2004 – and the Physical and Theoretical Chemistry Laboratory, currently undergoing similar upgrades to laboratory and office facilities. We have planning permission to construct a new laboratory (20000 m^2) focused on interdisciplinary research (Centres for Chemical Biology, Sustainable Energy, and Theory and Modelling of Complex Systems) following University investment of >£ 3M for design and planning. The building is a key element of the research strategy (Section b) and will house ~500 researchers; fundraising for its construction is currently underway, led by Softley and an external board, from diverse sources

(philanthropy, industry, IP agreement, university and government).

Provision of specialist Infrastructure and Facilities

We will continue to equip our Department with world-class, state-of-the-art core instrumentation so as to support all areas of our current and emerging research portfolio. We have strategically enhanced, developed and enlarged these facilities across the board in the REF period, and will continue to target resources to provision of advanced new equipment in the next period. In addition to instrumentation, we maintain a full range of glassblowing, electronic and mechanical workshops (total 12 technicians) and have an IT support team of 7 staff. The main instrumentation facilities are grouped as described below. Each facility has an academic or senior manager, who reports to a CMB member to ensure clear communication lines and strategic leadership. Much instrumentation is open-access, free at the point of use, and is supported by technical support and user training. Technical service measurements augment the open-access services, allowing maximum research use of the instrumentation and of bespoke experiments/measurements as required.

The **NMR facility**, operated and supported by 5 staff members, is one of the largest and best equipped in academia. It comprises 14 solution and solid-state FT NMR instruments with ^{1}H operating frequencies ranging between 200 and 700 MHz. **Mass Spectrometry** has a further 3 full-time research technicians and comprises 15 MS machines making use of a wide range of ionisation techniques and inlet systems. Oxford's **Centre for Advanced ESR (CAESR)** is a collaboration of researchers from across the Departments of Physics, Chemistry, Materials, Biochemistry, and Pathology. It provides state-of-the-art equipment (e.g. Bruker X-band, CW EMX and X-band/W-band (9.7GHz /95GHz) pulse Elex680 spectrometers) and an academic focus for Oxford's multi-disciplinary research in ESR. Oxford's single crystal and powder **X-ray diffraction facilities** are supported by 3 full-time staff. The equipment includes 2 dual-source and 2 single-source single crystal X-ray diffractometers, a protein diffractometer and 8 powder diffractometers. **SQUID magnetometry** comprises 2 instruments with full-time technical support. The **Surface Analysis Facility** contains a broad suite of equipment including: AFM, STM, XPES, SEM. We have strong links with the nearby ISIS Neutron Facility, and the Diamond Light Source, where we are responsible for developing one end station (Goodwin) and also have a block allocation of beam time (1-2 days a month) for small-molecule and (in collaboration) bio-macromolecule analyses.

Investment in infrastructure and facilities: Since 2010, we have carried out, through strategic actions of the Chemistry Management Board, an ongoing and wholesale programme of upgrade and/or replacement of our core instrumentation arsenal (total investment of *ca* £ 4.85M in new equipment, see below). A HEIF-funded post is used to generate more external usage and income for these facilities, which is then re-invested in upgrading them. In **NMR**, a combination of University pump priming (£ 290k), EPSRC (£ 780k) and Wellcome Trust (£ 620k) funding for 5 new/upgraded solution and solid-state instruments has been secured since 2011, and further bids are in preparation. In **ESR** we have secured £ 1.3M Strategic Equipment funding (£ 200k university/department pump priming) from the EPSRC to acquire a UK-unique, state-of-the-art spectrometer to augment CAESR's fleet of instruments. In the **X-ray facility**, 2 dual-source single crystal diffractometers and a powder instrument (total £ 670k) have been installed since 2010, while in **MS,** Departmental (£ 120k), Wellcome Trust (£ 420k) and EPSRC (£ 550k) funding has been won to install 5 new types of instrumentation. In the **Surface Analysis Facility**, *ca* £ 100k of departmental or EPSRC funding has been invested to keep/bring this instrumentation up to date.

CMB has established a detailed rolling timetable for investment, maintenance and upgrading of the other instrumentation that is between 5-10 years old and this will continue to be proactively pursued through direct investment, pump-priming and RCUK and charity sources. The Chemistry Department accounts show expenditure (non-grant) of £ 4.05 M in equipment purchase and maintenance in the financial years 2008-2013 including the pump-priming listed above.

Research Funding Portfolio

The total value of grants held by Oxford Chemistry (including only Oxford parts of collaborative grants) has increased from £ 63 M in 2008-09 to £ 90M in 2012-13. The balance of funding diversified in that period, with significantly greater industrial and EU funding, as illustrated below.

	Charity	EU	Govt	Industry	BBSRC	EPSRC	Other RC	Royal Soc.
08-09	£9.4M	£7.2M	£1.5M	£4.7M	£6.6M	£27.2M	£2.6M	£4.2M
12-13	£10.9M	£28.7M	£3.2M	£10.6M	£4.3M	£25.0M	£3.4M	£4.1M

A mark of our success in EU funding is 7 ERC Advanced Investigator grants and 6 ERC Young Investigator awards held in the REF period. Major new industrial collaborations have been established including > £ 2M of contracts with SEC (Thailand). The University's internal and highly competitive 'John Fell Fund' is a source of pump-priming funds for grant applications and we give priority to younger researchers – Oxford Chemistry has received over £ 1.7M of John Fell grants in the REF period. In the future we will seek to retain a strong core of RCUK funding while continuing to diversify and grow our funding sources; we aim to increase the proportion from medical research organisations/charities including MRC, CRUK, Wellcome, BHF, and to establish longer-term larger funding with industrial partners with the support of the 2 research facilitators and the MPLS Business Team. We will use the enhanced leadership, communication and collaboration within the 8 priority research themes as a springboard for larger funding applications.

Library Provision: The Radcliffe Science Library holds >1 million items and provides electronic access to >26000 journals, as well as databases such as SciFinder and Reaxys/Beilstein.

Consultancies and Professional Services

Our research facilities (NMR, MS, Crystallography) are available as a service to an increasingly wide range of users including industrial contracts (e.g. BP, Infineum, Oxford Nanopore). We recently ran a 'Services open day' for external users and provide a dedicated website to advertise what is on offer, in addition to the university's online database of equipment (shared with 4 other universities). The CRYSTALS structure-refinement software suite is upgraded and distributed by Oxford Chemistry to hundreds of users worldwide. Individuals also provide wide-ranging types of consultancy, with the support of Oxford University Consulting (see Impact Template).

e. Collaboration or contribution to the discipline or research base

Research Collaborations

We recognise that major impacts of Chemistry are increasingly rooted in interdisciplinary science, and make a concerted and conscious effort to enhance collaboration across subject boundaries, with hundreds of collaborators locally, nationally and internationally. Of > 3400 Oxford Chemistry papers published since 2008, 2062 have a non-Oxford author, and 1423 of these a non-UK based author. In the same period Oxford Chemistry has been involved with 3 EPSRC Programme grants, collaborating with other universities and other Oxford departments (New Horizons in Chemical and Photochemical Dynamics with 6 Oxford and 4 Bristol research groups; theory programme grant with Cambridge; condensed matter physics grant with Oxford Physics.) Cooper has a new EPSRC critical mass grant in the understanding and engineering function in switchable molecular crystals (with Leeds, Warwick and Bath, £ 2.2M total). We currently participate in 9 European networks (Marie Curie) and coordinate 2 of these. Funding for numerous international collaborations includes a DARPA grant with Oldenburg, and the KOPRC centre with Saudi organisation KACST.

Exemplars of interdisciplinary research

Oxford Chemistry has a strategic objective to stimulate and support interdisciplinary research exemplified by the establishing of joint appointments with Pharmacology (Russell), Biochemistry (Mohammed) and Oncology (Brown). Examples of interdisciplinary programmes in which we are major participants include: the CRUK-funded Cancer Imaging Centre (Oncology) – Gouverneur is a co-PI and develops fluorine chemistry for radioactive labelling in PET imaging; the British Heart Foundation programme with 15 medical/physical sciences departments; the Wellcome–industry joint programme on epigenetic probe development. The appointment of a Chemical Biology research facilitator has helped to build new relationships with Medical Sciences and NHS researchers across multiple sites, taking advantage of the critical mass of high quality medical and clinical research in Oxford (pre-clinical sciences rated no 1 in THES world rankings 2011-13). The Oxford Synthesis Connections network was established to link synthetic chemists with collaborators as described earlier, but also to develop and enhance links both with large pharmaceutical industries and with smaller companies located in the 3 local science parks. We have hosted a CRUK funded collaborative programme in Cancer Research (Davies, Russell), and an ongoing EPSRC funded programme in ESR research (CAESR) joint with Materials, Physics, Pathology and Biochemistry. Chemists are strong participants in the Oxford Centre for Soft and Biological Matter (with Physics), and Vallance was a founder member of the Oxford Photonics Network (40 PIs, 10 other departments). Chemistry (Tsang) and Materials (Bagot, Smith) collaborate in the atomic-level resolution microscopy of catalysts taking advantage of world-class

EM characterisation facilities in Materials. There are a range of other strong collaborations with Physical Sciences departments, both Oxford and elsewhere, e.g. Softley has a joint £ 1M grant with Sussex Physics (EPSRC, Ultracold chemistry), and Edwards an Armourers and Braziers Material Sciences Venture award on transparent oxides for fuel cells with Oxford Physics and Engineering. O'Hare is a co-PI of the multi-disciplinary Centre for In-situ Processing Studies (CIPS) at the Harwell Research Complex. The Brouard/ Vallance collaboration on fast-imaging detectors involves researchers in Particle Physics and the Rutherford Lab.

Impact of research collaboration with research users on our research strategy

Oxford Chemistry PIs have widespread interactions and dialogue with industry. We have held an average of 70 grants or research contracts with industry at any one time and > 50 PIs have had an industrial research agreement in the REF period. PIs are supported in discussions with industry by the 2 Research Facilitators and the MPLS Division Business Development Team, especially where high-level discussions spanning more than one department occur. PIs are also board members for 17 companies. On occasions, such as the Oxford Chemistry Annual Industries Symposium, or the 2012 visit of 8 BP research leaders, we offer the industrial partners the opportunity to speak about their needs and challenges to ensure their input to our research planning. Examples of new research initiatives undertaken in direct response to the needs of industry include the development by Compton of electrochemical devices for the food industry, petrochemicals and pharma (e.g., development of Chilli meter and a calibration-free pH Meter development – Impact Case Studies 4 & 6). At the same time, this substantial dialogue with industry has encouraged us to continue to focus on innovative fundamental research – this is what industry tells us we should be doing in a university environment. For example Schofield's leading fundamental work on determining the mechanism by which cells respond to oxygen has led to commercial sales of compounds, and clinical trials (see Impact Case Study 3).

Exemplars of leadership and esteem in the academic community

Since 2008, Oxford Chemists have been highly active in giving leadership in the community and received recognition of their esteem. Hamilton was on EPSRC Council and 31 Oxford Chemists were members of the EPSRC Peer-Review College. Schofield currently chairs BBSRC Responsive-Mode Committee D, and B. Davis is on the joint MRC/TSB Development Pathway Funding Scheme Committee. PIs serve on national facilities access panels including Diamond, ISIS, Laser Support Facility, NSCCC, and the National EPR service. Robinson and Edwards were members of the selection panels for ERC Synergy grants and Advanced Investigator Awards respectively. Oxford Chemists have also acted as reviewers and sat on committees for many major, global science research councils/charities, including NSF, ERC, DFG and the Swiss NSF.

Over 1000 invited lectures have been given by Oxford Chemists in the REF period and PIs have taken up >50 visiting professorships and lectureships since 2008 including at Berkeley, Paris, Beijing, Monash. PIs have taken up senior roles in divisional or subject groups of the RSC, including 2 Vice Presidents of the Organic Division (Donohoe, Gouverneur), President of the Faraday Division (Clary), 2 Presidents of the Chemical Biology Interface Division (B. Davis, Bayley) and membership of 20 RSC subject group committees including 6 as chairman/secretary. Cooper was elected Vice President of the British Crystallographic Association. Edwards, Armstrong, Robinson and Clary have sat on key Royal Society Committees (including Robinson on Council). Oxford Chemistry PIs acted as editors, board chairmen, or associate editors of 14 international journals and are represented on 62 editorial boards. Clary was Chief Scientific Advisor to the Foreign and Commonwealth Office and Robinson sat on the Blackett Review Panel for Biosecurity.

5 new Fellows of the Royal Society (H. Anderson, Armstrong, Bayley, Manolopoulos, Schofield) were elected and a DBE awarded to Robinson. Logan was elected Foreign Fellow of the National Academy of Sciences India, and Edwards a member of the American Philosophical Society. 32 RSC medals were awarded and 6 equivalent overseas awards (e.g. ACS, American Biophysical) to 27 PIs in the REF period. Royal Society awards included the Davy Medal twice (Robinson, Armstrong) and the Bakerian Lecture (Edwards). Other highlights include the Woman of the Future prize (Vincent), the FEBS/EMBO Woman of the Year award (Robinson) and RSC World Entrepreneur of the Year (Bayley). Goodwin was selected by the NY Academy of Sciences as one of ten 'future leaders' to attend the Science and Technology in Society Forum 2013. Armstrong, B. Davis, Manolopoulos, and Gouverneur won Royal Society-Wolfson Merit awards.