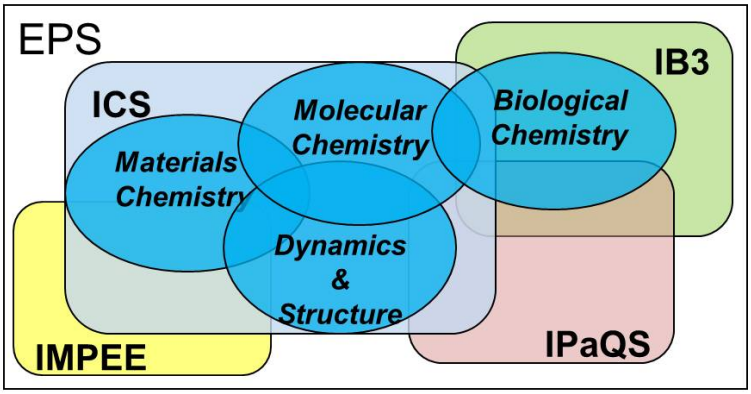
Institution: Heriot-Watt University

Unit of Assessment: 8 Chemistry

a. Overview

Chemistry at Heriot-Watt University (HWU) extends from mainstream chemistry into the boundaries with the life sciences, materials science, chemical engineering and physics. A total of 30 staff are returned here. The majority are in the Institute of Chemical Sciences (**ICS**), complemented by a significant proportion (7) from other Research Institutes, reflecting an increasingly multidisciplinary dimension to our research. The submission spans four research groupings, these being (with group leaders in bold):

- ***Dynamics & Structure*** (Bock, Costen, Greaves, Gutowski, McCoustra, **McKendrick**, Nahler, Paterson, Townsend, Westacott) - fundamental chemical and physical processes.
- ***Materials Chemistry*** (Arrighi, Bos, John, **Keane**, Ni, Vilela, Yiu) - the relationship between composition, structure, properties and application of advanced materials.
- ***Molecular Chemistry*** (Adams, Bebbington, **Dalgarno**, Lee, Lloyd, Macgregor, Mansell, McIntosh, Welch) - synthesis, structure and chemistry of molecules and supramolecular assemblies.
- ***Biological Chemistry*** (**Duncan**, Howarth, Leslie, Rickman) – the application of advances in the chemical and physical sciences to enhance life-science research.



ICS group leaders are members of the ICS Management Group, along with Paterson as PGR Coordinator. There are five Institutes within the School of Engineering and Physical Sciences (**EPS**). They are research-driven management units designed to achieve research excellence within core areas and to promote innovative joint research; as such staff have primary membership of one Institute and may have additional secondary memberships. **Macgregor** is Head of Institute, ICS, and **Duncan** is Head of the Institute of Biological Chemistry, Biophysics and Bioengineering (**IB3**). Both sit on the EPS School management group. Other Institutes that overlap this submission are the Institute of Manufacturing, Process and Energy Engineering (**IMPEE**) and the Institute of Photonics and Quantum Sciences (**IPaQS**). Beyond EPS, Chemistry has active interfaces with other Schools, including Life Sciences and Petroleum Engineering, two of the eight units that constitute Heriot-Watt University's high-level, research-intensive structure.

The REF2014 period has been one of development of existing strengths and the blossoming of staff appointed during the RAE2008 period. There has been significant further recruitment, particularly at an early-career stage and into new areas, enabled by sizable recent investment.

b. Research strategy

The strategy for Chemistry at HWU is founded on a strong performance in the Chemistry UoA (UoA18) at RAE2008. We have improved our position successively at every RAE since its inception. A particular strength at RAE2008 was the quality of our outputs, with 50% of the submission either 3* or 4*. We returned 19.0 FTE staff at RAE2008. The increase of over 50% in the current submission is evidence of the strong promotion of Chemistry within HWU's declared vision to be "world-leading within all its specialist areas of science, technology, engineering and business".

These high-level aims are being achieved in practice through investment in new research leadership posts (target of 20 p. a. across HWU, supported by earmarked funds of 2% of total Institutional income) and facilities under the 'Global Platform' Initiative and identified priority themes. The impact on Chemistry has been substantial, with 11 new appointments returned here and £2.4M from institutional funds invested in new infrastructure.

The strategy of EPS and those of its constituent Research Institutes align with the institutional

ambitions. The School was formed prior to RAE2008 by combining chemistry and physics, and chemical, electrical and mechanical engineering. The philosophy of removing barriers to collaborative research has been strengthened during the current REF period. Lines of management in EPS have been made more explicitly research-focussed through the creation of the Research Institutes, integrating staff from several different conventional disciplines.

Following a major strategic review, with external input, that accompanied the formation of the Institutes, the number of themes within ICS was rationalised into the three current groupings, ***Dynamics & Structure***, ***Materials Chemistry*** and ***Molecular Chemistry***. This removal of increasingly artificial boundaries between, e.g., organic and inorganic synthesis or experiment and theory has promoted the achievement of aims identified at RAE2008. As we expand in (d) below, a substantial fraction of the >£16M in external grants that have been held at some point during the REF period involve multiple complementary co-investigators.

The forward-look at RAE2008 foresaw a number of new opportunities at the chemistry-chemical engineering and the chemistry-life sciences interfaces, which were seen to have potential for KT growth. Addressing the first of these areas, ICS was formed as an integrated interdisciplinary unit incorporating four staff returned here who were previously returned to Chemical Engineering (UoA 26) at RAE2008. Research at this boundary has now diversified significantly beyond the original opportunity in catalysis identified at RAE2008. New activity in the area of materials for energy was promoted through the strategic Centre for Advanced Energy Storage and Recovery (CAESAR) initiative. CAESAR fitted within the University's Energy Theme, combining staff in ICS, IMPEE and the Institute of Petroleum Engineering.

The development of the opportunities at the life-sciences interface has substantially exceeded expectations at RAE2008 by the creation of IB3, also supported under the broader HWU-wide Life Sciences Interface (LSI) theme through large-scale investments in personnel (see (c)) and infrastructure (see (d)). IB3 provides a focus for existing EPS staff and brings biological chemistry, biophysics and bio-engineering together in one research Institute. Existing staff have been supplemented by key external appointments, bringing new expertise and expanding the scope for collaborations with ICS and other units within and external to HWU. A group of four IB3 staff working in the broadly defined area of ***Biological Chemistry*** are returned here. Three are new appointments, whose activities have become established rapidly aided by £1.24M investment in new infrastructure.

ICS continues to be an active player within the ScotCHEM research-pooling initiative. ScotCHEM was a joint bid under which EaStCHEM (Edinburgh and St Andrews), WestCHEM (Glasgow and Strathclyde) and HWU received significant regeneration funds from SFC during the RAE2008 period. It continues as an umbrella organisation to enhance collaboration in chemical research in Scotland (incorporating Aberdeen and Dundee). It engages actively with research users through Chemical Sciences Scotland, an academic-industry partnership supported by Scottish Enterprise and through initiatives such as the SFC SPIRIT awards scheme (see (d) below). In addition, we engage fully via IB3 with the Scottish Universities Physics Alliance (SUPA) through the physics and life sciences (PALS) theme.

The further strengthening of targeted areas through new recruitment is described under (c) below. Specific examples of how **those staff in post at RAE2008** have worked together to deliver the strategy laid out in 2008 are:

Dynamics & Structure Experimental activities in the dynamics of fundamental processes at condensed-phase surfaces (Costen and McKendrick) have diversified as anticipated, extending to self-assembled monolayer surfaces through joint work with Bebbington. Experimental interpretation has been strengthened through molecular dynamics simulations in collaboration with Westacott, a co-investigator on successive large EPSRC grants in this area (see (d)). McCoustra has successfully expanded the experimental study of astrochemically relevant ice surfaces, in part with theoretical support from Paterson through the £5.5M LASSIE FP7 ITN led from HWU (see (e)). Theoretical activity overall has evolved and expanded substantially since RAE2008. Paterson, enabled by an ERC Starter Grant, has been active in the development of treatments of electronically excited states, including model biomolecular systems (with Townsend) and two-photon photodynamic therapy (with Bebbington). Townsend has established a successful independent activity in time-resolved photoelectron studies of model biochemical systems, also supported by synthesis (Bebbington). Paterson has other fruitful interactions with Dalgarno on supramolecular assembly and with Galbraith (IPaQS) on organic semiconductors. Gutowski's

condensed-phase work on electron-induced DNA damage, on potential hydrogen-storage materials and on heterogeneous reactivity complements *Materials Chemistry*. Further breadth is provided by Westacott's simulations of gas-liquid interfaces. Bock has pioneered the highly efficient simulation of the self-assembly of surfactants interacting with carbon-nanotubes and other nanofibres, and collaborated with Willoughby (IB3) on the elasticity of stem cells.

Materials Chemistry The core of the research emerging from RAE2008 was in solid-state chemistry and polymer chemistry, building on the work of Arrighi and (both in post until 2013) Powell and Vaqueiro. This activity has focused on correlating structure with property to facilitate rational design of new materials with controllable functionality. Chemistry was at the core of the CAESAR initiative and has led new research on materials for energy, particularly thermoelectrics. Independently, John and Wilson (IPaQS) have worked on diamond materials for fusion-reactor walls. Keane has continued to develop heterogeneous catalytic materials for sustainable chemical processing. Further opportunities for growth have been identified through the combination of this heterogeneous catalytic expertise with expanding activity in homogeneous catalysis underpinned by theoretical support (Macgregor, Gutowski). Ni's activities in the characterisation of continuous-flow mixing provide an important link to practical exploitation at the chemistry-chemical engineering interface, in part through an EPSRC Centre for Continuous Manufacturing and Crystallisation (£6.0M in total - see REF3a and REF3b).

Molecular Chemistry: The expansion of catalysis research anticipated at RAE2008 has proceeded, with prominent contributions in gold-catalysed reactions and organocatalysis from Lee and new ligand systems and bond activation in heteroboranes from Welch. Much of this is synergistic with the flourishing computational work in mechanistic organometallic chemistry by Macgregor, heavily supported by EPSRC (8 grants in total – see (d)). These activities in homogeneous catalysis are complemented by the expertise in heterogeneous catalysis and reaction engineering in *Materials Chemistry* (Keane & Yiu). With Dalgarno, HWU has a strong presence in co-ordination chemistry, particularly of calixarenes. As anticipated at RAE2008, Adams' work has been successfully extended into the stem-cell field. *Molecular Chemistry*'s core synthetic expertise is exploited in extensive collaborations within ICS and with others in EPS (*e.g.* Bebbington/Paterson, Bebbington /Townsend(IPaQS), Adams/Willoughby(IB3)) and external collaborations (see (e), including a £9.5M ITI Scotland multicentre programme) that have been funded or led to published work.

The future strategic vision for Chemistry at HWU, as broadly defined here, is further expansion into our areas of strength. We expect this to continue into the next REF period, with an agreed plan with the University for further growth of 10 FTE academic staff through high-calibre 'research leadership' appointments. This will be supported through increased external grant winning and HWU investments in infrastructure, including anticipated new build (see (d)).

c. People

i. Staffing strategy and staff development

Recruitment to this UoA during the current REF period has primarily been of relatively early-career staff. The healthy state of our current demographic profile (ages at the census date of 31/10/13) is shown opposite.

Age	≤35	36-45	46-55	≥56
No.	6	13	8	3

The total number of new appointments in the REF period being returned here is 11. Although departures have been limited, we also regard it as positive that our staff are attractive to other institutions and organisations beyond the university sector. Unplanned departures have impacted most on *Materials Chemistry* (van der Laak, Tao, Powell, Vaqueiro). We have reacted quickly to these events by further recruitment (see below). We now summarise our strategy to strengthen each of the groupings through **targeted new appointments** and their anticipated, and some already realised, synergistic interactions with existing staff:

Dynamics & Structure This area has been substantially strengthened through the linked appointments in 2012 of Greaves (an EPSRC CAF), developing independent methods to study reactions at liquid surfaces, and Nahler (Royal Society URF), investigating photochemistry at atmospherically relevant ice surfaces. Nahler's interests overlap and diversify McCoustra's work on ices in a different temperature and pressure regime. The backgrounds of Greaves and Nahler in gas-phase and interfacial dynamics (see REF2 for outputs in *Science* (x2), *Nature* and *Nature*

Chem.) complement the established experimental activity of Costen, McKendrick and Townsend, all underpinned by Paterson's computational expertise.

Materials Chemistry Targeted recruitment in this area has been very active, although, as noted, this has been amplified by staff turnover. Work in materials for energy under the CAESAR umbrella on thermoelectric power generation was initiated by Powell and Vaqueiro, and this area has been strengthened and carried forward by Bos, recruited in 2009. He is building on his established expertise in superconducting materials and already winning independent funding from EPSRC and the Leverhulme Trust (see (d)). Further diversity is brought by the appointment of Vilela in 2013, whose interests are in nanostructured materials for energy storage, conversion and photocatalysis. The emphasis in fuel-cell and hydrogen-storage materials has shifted away from experimental work with the departure of Tao, but continues in the theoretical modelling and predictions of Gutowski. Yiu's recruitment (2010) brings expertise in porous nanomaterials with potential applications in carbon-capture, biomedicine and catalysis, with funding now being won from EPSRC and Scottish Carbon Capture and Storage (see (d)). This complements Keane's established work in heterogeneous catalysis and the new capabilities brought by Vilela (already an experienced lead author in *Angew. Chem. Int. Ed.* and *Chem. Commun.* - see REF2). We are committed to seeking to recruit at Chair level to further strengthen *Materials Chemistry* early in the post-REF period.

Molecular Chemistry The very successful development of supramolecular chemistry during the REF period has been further strengthened through the recent appointments of McIntosh (2013) and Lloyd (2012). Lloyd's activities extend to low-molecular-weight gelators and crystal engineering, and have attracted support as part of the EPSRC Directed Assembly Network. They link to practical application via Ni, and have scope to exploit an established experiment-theory interaction with Paterson. Mansell (2013) has also been very recently appointed and will bring expertise (see REF2, including *Nature Chemistry*) in main group ligand synthesis leading to new transition metal complexes with potential in homogeneous catalysis, thereby affording potential future collaborations with Lee, Bebbington, Welch and Macgregor.

Biological Chemistry Duncan was recruited as Life-Sciences Interface Theme co-Director in 2010. He has been joined by Rickman and Leslie as part of an on-going sequence of appointments in electrophysiology, cancer biology, ultrasound imaging, super-resolution fluorescent imaging and diagnostics. This area has expanded rapidly and already has had substantial tangible success in terms of major grants, some from funding sources not previously accessed by Chemistry staff (inc. £2.6M funding held in the REF period – see (d)) and publications (inc. *Nature Communications* and *Nature Cell Biology* – see REF 2). The new appointments are complemented by Howarth, an established staff member working on synthetic chemistry with potential medicinal applications. As noted, there are also close links with the medicinal chemistry work of Adams.

A particularly satisfying aspect of our strategy for existing staff has been the progress of a group (including Bebbington, Bock, Costen, Dalgarno, Lee, Paterson, Townsend) who were new, relatively early-career appointments during the RAE2008 period. (Tao and Vaqueiro were similarly successful and have been recruited to positions elsewhere, in one case to a Chair.) Their sustained ability to win external funds (including major EPSRC, Leverhulme, and ERC Starter grants - see (d)) and establish significant research groups has resulted in them being much of the powerhouse of the current submission. This has been recognised appropriately through the promotions process (Costen, Dalgarno and Lee to Reader; Paterson to Professor), and externally (inc. e.g. Dalgarno's *RSC Harrison Meldola Award* – see (e)) providing direct evidence of the positive environment we provide for new appointments. All were supported by our mentoring system that matches new appointees with suitable experienced staff during the probation cycle (typically 3 years). Time dedicated to research is optimised through careful management of teaching loads that ramp up only slowly during the probation period.

More formal training of academic staff is provided by the Centre for Academic Leadership and Development (CALD), including modules specifically targeted at research, which may be combined into a full Post Graduate Certificate in Academic Practice qualification. The broad-ranging support provided to research staff at all levels, including PGR students, is formalised by adoption of the Concordat to Support the Career Development of Researchers. HWU has created a Research Futures Programme to increase research capability and success across the University. It has

invested in 6 full-time specialist posts for its delivery. In addition, HWU leads the award-winning Scottish Crucible programme for early career researchers (see REF3a for further details).
For all staff, HWU has an active Performance and Development Review (PDR) policy, brought in since RAE2008, within which staff prepare forward job plans and are formally reviewed annually. This ensures that researchers are contributing actively and have the necessary support from colleagues and funding, via specific budgets held by the EPS Research Institutes, for e.g. pump-priming research ideas, items of communal equipment and other generic infrastructure. We have dedicated travel budgets for academic, postdoctoral and PGR (see below) workers, supplemented by SFC career-development funds that have supported two extended exchanges at postdoctoral level (to Sandia Livermore and Rutgers, USA).
HWU has a robust framework to support equality and diversity. The University has recently been awarded Athena SWAN Institutional Bronze Status for all STEM departments (covering this UoA). The submission included an Action Plan, championed by the Head of School of EPS, to further embed the principles and effect continued culture change, including an improvement in the gender balance of academic staff. Of the 30 staff returned here, 3 existing (and 2 recent departures) are female. A University-wide Equality and Diversity Advisory Group oversees and advises on operational and legal compliance and ensures effective linkages across the University's governance structures. The positive actions that HWU has taken to support the career development of all researchers and the measures in place to implement its declared principles have been recognized externally. In 2010, it was amongst the first 10 HEIs in the UK to receive the "HR Excellence in Research" award from the European Commission. This was re-awarded against a renewed action plan in January 2013.

ii. Research students

The vital role that research students play in our research strategy is reflected in our recent investment in scholarships to sustain student numbers. Data for FTE-equivalent research students enrolled on doctoral programmes in each academic year are shown below:

08-09	09-10	10-11	11-12	12-13
53.0	48.0	45.0	40.0	48.0

Numbers enrolled, and corresponding graduations (see REF 4a), have been relatively constant across the REF period, in a climate in which they have been under pressure as a result of the decline in studentship funding from traditional sources. HWU has responded actively by creating its own James Watt Scholarship scheme in 2012. Across HWU, this offers up to 80 three-year fully funded studentships annually. Of these, 11 studentships have been allocated to staff in this UoA (6 in 2012 and 5 in 2013) at a total value of £643k. In addition, we participated actively in the SFC-supported SPIRIT award scheme through the ScotCHEM pooling initiative, providing a further 4 studentships, supported by £90k from SFC, £60k from industry and a matching HWU investment of £115k. We anticipate future growth in PGR numbers as a result of the recent strong upswing in grant winning (see (d) below) and expansion of academic staff numbers.
The mutual obligations on staff and students to ensure a high-quality student experience are formalised in the PGR Student Code of Practice, which is fully aligned to the Concordat (see (c)(i)). All PGR students have 1st and 2nd supervisors, for whom training is mandatory. Student progress is monitored annually, with a report and oral examination at 1st-year level and further formal reporting at higher levels. This process is managed by Paterson as PGR Coordinator in ICS and by counterparts in other Institutes, and overseen by the EPS Graduate School (Welch is overall Director of PGR). In addition to relevant technical skills training, which can include HWU Masters-level taught courses, there is a minimum requirement for 10 days pa transferable-skills training. This is provided either internally, e.g. Research Futures courses offered by CALD or information skills by the University Library, or externally, e.g. a joint course with EaStCHEM on thesis and paper-writing skills. Students are given ample opportunity to present their work, including: regular meetings of the research groupings; an annual EPS PGR conference at which all 2nd-year students display posters (broadening their exposure to other disciplines); and an annual ICS PGR student symposium at which all final-year students speak. The Institutes have dedicated travel budgets to assist all PhD students to attend at least one major international meeting during their degree. Many of the in-house meetings take advantage of the dedicated facilities for PGR students, not least the £9M invested in a new postgraduate centre providing high-quality lecture, seminar and social space.

d. Income, infrastructure and facilities

We have enhanced the already well-founded core chemistry analytical facilities, including NMR, X-ray and mass spectrometry; mechanical and electronic workshops, glassblowing, etc, that were in place at the start of the REF period. Specific upgradings of these core facilities are indicated below in the context of the groupings that are their principal users. In addition, substantial infrastructure spend and other direct support from HWU funds has been more specifically targeted at the new appointments. All are provided with, as a minimum, a fully funded PGR studentship and fit-for-purpose laboratory space. As detailed below, tailored additional facilities have been put in place to enable the new staff to begin rapidly winning external funding to sustain their research efforts.
The total research spend (see REF 4b) during the period across all funding sources and the corresponding income in kind (REF4c) is:

	08-09	09-10	10-11	11-12	12-13
Total spend	£1,827k	£1,781k	£1,269k	£1,610k	£3,231k
Income in kind	-	£369k	£123k	£171k	£59k

The investments are now demonstrably bearing fruit in the level of activity, with a strong upswing in spend in the final year of the period reflecting recent grant winning. The figure for 2012-13 is almost three times the average of £1.13M pa at RAE2008, with current holdings indicating that this is likely to be sustained. Principal HWU infrastructure investments (£2.4M in total) and major sources of external funding, broken down by research group, are summarised below. Headline figures represent:
*(**infra.** = internal infrastructure investment, excluding personnel, in the REF period)*
*[**total grants** = value to HWU of all grants held for some part of the REF period]*
*{**current grants** = value to HWU of all grants current at the end of the REF period on 31/07/13}*

Dynamics & Structure (infra. £339k); [total grants £5,199k]; {current grants £3,519k}
An existing laser laboratory has been upgraded for Greaves, in addition to a contribution of £112k towards a laser system and vacuum and data-acquisition equipment. A further £155k was paid to transfer a crossed-molecular-beam apparatus from Bristol and for other equipment costs associated with his EPSRC CAF. A separate space was refurbished (£50k) to create a purpose-built laboratory for Nahler and £22k spent to upgrade a laser system.
The major external funding streams for this grouping include five separate EPSRC grants (£1.77M in total), with contributions from Leverhulme Trust (equipment grant, £109k, and Royal Society Leverhulme Trust Senior Research Fellowship, £45k) and EOARD (European Office of US Air Force, £22k), to Costen and McKendrick for gas-liquid and gas-phase dynamical scattering, in part jointly with Westacott and Townsend. Townsend's work on ultrafast, angle-resolved photoelectron spectroscopy has been funded by two successive EPSRC grants (£391k & £453k), in part joint with Bebbington and Paterson, and a Leverhulme Trust research grant (joint with Belfast, of which £140k to HWU). Greaves is supported by an EPSRC Career Acceleration Fellowship, including major project funding (£896k to HWU). Nahler is funded by a Royal Society URF (£263k to HWU). McCoustra's astrochemical research has also been supported by EPSRC grants (£510k in total), with the funding base being broadened by a major FP7 ITN network grant (LASSIE, £685k to HWU), on which Paterson is a co-I. Other strands of Paterson's computational work have attracted major EU funding (ERC Starter Grant, £1.10M) in addition to EPSRC grants (£724k as PI), in part joint with Bebbington and with Galbraith (IPaQS), and a grant from the Leverhulme Trust (£139k).

Materials Chemistry (infra. £337k); [total grants £2,771k], {current grants £1,032k}
The *CAESAR* initiative was resourced with two new academic positions (Bos, van der Laak). Both were provided with start-up funds (£30k for equipment) and £149k was spent on laboratory refurbishment. Yiu was provided with a separate refurbished space (£38k) and received additional start-up support from the EPSRC Science & Innovation Award that funded his position. A key infrastructure development just prior to the formal assessment period for income (Feb 2008) was the establishment of a new powder X-ray characterisation laboratory through SRIF funds and EPSRC support, providing two new instruments.
Interdisciplinary projects in thermoelectrics have received significant external funding (EPSRC, £549k in total; ETP & FP7, £353k). Thermoelectrics research is also supported by an EPSRC First Grant (£80k) and a Leverhulme Trust Research Grant (£146k) to Bos. Yiu's work on materials for

carbon capture and utilisation is funded by EPSRC (AMPGas consortium, £19k) and enzyme application (with Keane) for carbon dioxide utilisation by Scottish Carbon Capture and Storage (SCCS, £63k). This follows on from Keane's EPSRC funded work (£129k) on enzyme/synthetic catalyst applications in reductive amination. *Materials Chemistry* research has involved particularly close collaboration with industry. This has encompassed SFC SPIRIT awards (to Arrighi, Keane, Ni and Tao – see(c)) and joint funding of a PhD through the ETP (with European Thermodynamics Ltd). Industrial collaboration through a KTP grant (with Helia Photonics) to Arrighi is directed at polyurethanes for ink formulations. Ni receives further industry-linked funding (£412k) through the CMaC IMRC with Strathclyde.

Molecular Chemistry (infra. £484k); [total grants £5,722k], {current grants £2,501k}

Lloyd has been provided with £33k laboratory start-up and travel funds. Broader-based internal investment of principal benefit to *Molecular Chemistry* has included a major spend, anticipated in RAE2008, of £357k on enhanced NMR facilities including an attachment for solid-state NMR (also valuable to *Materials Chemistry)* plus additional refurbishment of associated office space for the manager of the NMR suite; enhanced database provision (full-site licenses for Scifinder (£17k p.a.) and Cambridge Structural database (£2k p.a.)); a new solvent purification system and titrator (£25k) plus refurbishment of a laboratory (£23k) to house it alongside additional analytical equipment; and a new compressor for piped-N_2 generator (£10k).

Heteroborane research by Welch has been supported by two major grants from EPSRC (£1.00M in total) as well as support from the Royal Society (£12k). The development of new catalysts and catalysis reactions has been funded by the Royal Society (£27k) and two EPSRC grants (£279k & £571k) to Lee (in part with Macgregor), with additional support in related areas from the Leverhulme Trust to Lee (£97k) and separately to Bebbington (£99k). Computational modelling of transition-metal catalysis by Macgregor has been heavily supported (8 grants, £1.60M in total) by EPSRC, who have also provided substantial grants (£311k & £355k) to Dalgarno for supramolecular chemistry. The portfolio is diversified by major medicinal-chemistry grants to Adams from ITI Life Sciences (£989k); NHS CSO (£285k) and Scottish Enterprise (£116k).

Biological Chemistry (infra. £1,240k); [total grants £2,579k], {current grants £2,394k}

HWU has invested heavily to establish the 'Life Science Interface Laboratory' which contains £3M of high-end microscopes, electrophysiology, ultrasound and associated equipment funded for Duncan, Leslie and Rickman. This was established with £1.08M of HWU funds, a £100k Robertson Trust donation and £200k from MRC and Wellcome Trust grants to Duncan and Rickman. A further £163k HWU investment created adjacent state-of-the-art molecular-biology, cell-culture and biochemistry laboratories.

Duncan's biophysical and biological chemistry research has been funded through successive Wellcome Trust personal fellowships and project grants (current, £311k) as well as awards from MRC, EPSRC, STFC and the Royal Society. Leslie is funded by an MRC Programme grant. Rickman is a co-I with Duncan on Wellcome Trust and MRC grants and PI on an MRC 'New investigator research grant' (£405k). IB3 was recognised recently (Dec 2012) with the award of £1.95M (Duncan, PI) from the MRC/BBSRC/EPSRC/STFC 'Next generation in optical imaging' initiative, bolstered by £110k from the BBSRC and £175k from EU FP7 (all in 2013), in the area of nano-scale live cell imaging. These awards include £1.1M of equipment (£550k based at HWU). They extend the already exceptional infrastructure within the LSI Laboratory, now under the Edinburgh super-resolution imaging consortium (ESRIC) umbrella. Recognising this unique capability, Duncan and others at HWU, jointly with Edinburgh and Bath, have been awarded £9.3M in total to establish an Interdisciplinary Research Centre developing in vivo imaging and molecular sensing (SERS) technologies for use in acute medicine.

Looking forward, we anticipate a continued upward growth in research income generated by staff now in post. We aim to exploit, in particular, our proven track record of developing the careers of new appointments (see (c)). As an increasing proportion of staff achieve higher prominence in their fields they will win more large individual-investigator grants. Having built critical mass in a number of selected areas, we have also enhanced our competitiveness for major, multi-investigator projects. Our position will be strengthened by further recruitment into both ICS and IB3. HWU has already committed a further £400k in infrastructure investment in 2013 to build new tissue culture and molecular biology laboratories adjacent to the ESRIC facilities, to accommodate new staff

recruits as well as numerous collaborative users. The University is committed to a new 5,800m^2 shared-use building associated with attracting the British Geological Survey (BGS) to the HWU campus at a cost of £17M (with contributions from NERC £8.5M, HWU £5M, and SFC £3.5M). Co-location with BGS of existing activities in the environmental sciences will liberate space for more general expansion, including of this UoA.

e. Collaboration or contribution to the discipline or research base

Support for and exemplars of research collaborations

As described in sections (a) and (b), a design feature of our structure is the removal of barriers to interdisciplinary research. This has borne substantial fruit through the healthy levels of internal collaboration within HWU. This philosophy extends to our wide range of collaborations with other research groups and research users in the UK and internationally. We actively encourage staff to develop collaborations through PDR and other processes such as mentoring. We support this through targeted budgets at Institute level for travel by staff and postdocs/postgrads and to provide pump-priming funds to initiate new collaborations.

We have worked with over 150 identified **international collaborators** and a larger number in the UK. Of those with an international dimension, a number have included out-going funded visits, notable examples including Costen (and co-workers) to Chandler (Sandia National Laboratory, Livermore, USA) resulting in joint publications (including a special-issue cover article in *J. Phys. Chem. A*) and a substantial (£541k) follow-up EPSRC grant; Dalgarno to Teat and Beavers (ALS, Berkeley, USA) leading to joint publications; Duncan to Lang (Bonn), Merrifield (Paris), Gaisano (Toronto), Yang (Phillips Research Asia, China) and Chow (LA), each of which has involved funded visits and/or joint publications; Gutowski (and co-workers) on a visiting research fellowship at the Pacific Northwest National Laboratory, USA, resulting in 5 joint publications, including one in *Science*; Keane and co-workers to Université Pierre et Marie Curie (Paris) leading to joint publications in *J. Catal.*; Leslie to Eickholt (Charite University, Berlin) leading to 3 co-authored papers, including *Nature Cell Biology,* and Barata (IMM, Lisbon) resulting in a heavily cited co-authored article in *J Clinical Investigation*; Lee on a Royal Society-funded visit to Crowley (Otago, New Zealand), linked to a joint paper in an *Emerging Investigators Themed Issue* of *Chem. Commun.* and an invited review; Macgregor as Visiting Professorial Fellow (University of NSW, Australia), leading to 3 joint publications; McKendrick to Minton (Montana, USA), resulting in 2 joint publications, including one in *Nature Chemistry*, and a recently announced jointly funded NSF/EPSRC ($427k & £619k) project with additional UK collaborators (York); Paterson (and co-workers) to University College Cork (Tyndall Research Institute) leading to the joint release of an electronic structure code; Rickman and Leslie, as part of the strategic alliance with the Institute of Genetics and Molecular Medicine (IGMM) that led to ESRIC, have had separate invited perspectives in *Science* and Rickman has a paper in *Nature Communications*; and Welch's visit to Zanello (Siena) has led to further joint publications.

As noted in (d), we hold a wide range of grants for collaborative projects within and beyond the UK. As explained in more detail in REF3a, many of these involve **interaction with research users**, including industrial partners, and are also often **interdisciplinary**. Notable examples include: Adams - with Glasgow and Strathclyde on drug discovery through ITI Scotland (£9.5M multicentre programme) and Scottish Enterprise (£495k), and with Willoughby(IB3) on the SFC Horizon Red Blood Cell programme (£2.5M) with St Andrews, Edinburgh and Glasgow; Bos (and formerly Powell and Vaqueiro) joint EPSRC and EU-funding for thermoelectric research with engineers at Cardiff, Loughborough, Glasgow and QMUL, chemists at Caen, France, and industrial involvement from SMEs (European Thermodynamics, Diamorph, Kakagu Analysis) and a multinational (Tata Steel); Duncan and Rickman – £12.1M for in vivo imaging with collaborators at Edinburgh (Edinburgh Super-Resolution Imaging Consortium) and Bath and international industrial partners including Leica Microsystems, Zeiss, Olympus, Hamamatsu, Scientific Volume Imaging and Edinburgh Instruments; McCoustra through the LASSIE FP7 ITN on laboratory astrochemistry (total £5.5M, coordinated from HWU) with 13 academic and 7 industrial partners across Europe; Ni – with Strathclyde and an array of industrial users including Astra Zeneca, Fujifim, Genzyme, GlaxoSmithKline, Pfizer, and others through an EPSRC IMR Centre for Continuous Manufacturing and Crystallisation (£6.0M in total).

Exemplars of leadership in the academic community

We strive to increase our visibility by being actively involved in the **organisation of major international scientific meetings**, some of which have been hosted locally making use of the excellent conference facilities on the HWU campus. Representative examples of higher profile meetings include: Costen chaired the *22nd International Symposium on Gas Kinetics*, Boulder, CO, USA (2012), and was secretary for the *21st and 20th Symposia* in Leuven, Belgium (2010) and Manchester (2008); Dalgarno chaired the *14th International Seminar on Inclusion Compounds* at HWU (2013); Keane was a member of the international scientific committee for the *International Symposium on the Feedstock Recycling of Plastics and Other Innovative Plastic Recycling Techniques* meetings in Chengu, China (2009) and Delhi, India (2013); Macgregor was co-chair of the *IUPAC Symposium (Impact of New Physical and Computational Methods)*, Glasgow (2009); McCoustra chaired *Faraday Discussion No. 141* at HWU (2008) and the *29th European Conference on Surface Science*, Edinburgh (2012); Welch chaired *EuroBoron5* at HWU (2010) and was a member of the international committee of *IMEBORON-XIII*, Platja d'Aro, Spain (2008) and *XIV*, Hamilton, Canada (2011).

Our staff are also recognised through numerous (>115 known in the period) **invited/plenary lectures** at international meetings, with notable examples including repeated invitations to *ACS National Meetings* (Gutowski 237th-240th & 242nd, Macgregor 239th & 244th, McCoustra 238th, McKendrick 241st); *Gordon Research Conferences* (Adams, 2010, Macgregor, 2008); *Pacifichem* (Gutowski and Macgregor, 2010); and *RSC International Symposium on Advancing the Chemical Sciences* (Dalgarno - Award Lecture, 2011, Lee, 2012). Duncan delivered the invited Keynes Lecture at the EMBL Summer School in 'Advanced Imaging' (2012).

We hold **senior editorial positions** with a range of international journals, including: Duncan - *Guest Editor of RSC Advances (*2013*)*; John - *Editorial Board of Advanced Materials/CVD*; Keane - *Executive Editor, Journal of Chemical Technology and Biotechnology(*since 2012*)* and *Editorial Board* of *Recent Patents in Materials Science (*since 2008*); Editorial Board, Environmental Technology (since 2010);* Macgregor – Advisory Board, *Dalton Transactions* (since 2011) and *Guest Editor Special Issue* (2012); McCoustra - *Guest Editor for PCCP Themed Issue* (2008); Ni – Advisory Boards of *Journal of Chemical Technology and Biotechnology* and *Journal of Chemical Engineering and Processing* (throughout REF period), and *Guest Editor of Journal of Chemical Engineering Research and Design* (2011–2012).

The **quality of our own publications** has been widely recognised, e.g. by featuring as *Chemical Communications Emerging Investigators* (Lee (with Crowley, as above, 2011); Dalgarno, Paterson (2012); Bos, Lee and Lloyd (all 2013) - Lee was also selected for the *Gold 100 Article Collection* by the RSC and World Gold Council); through numerous journal cover articles, including notably *Science* (Greaves, Gutowski), *Nature Chemistry* (Greaves, McKendrick), *Angew. Chem. Int .Ed.* (Dalgarno), *J Biol Chem* (Duncan, Rickman), and *JACS* (Dalgarno), and a wide array of 'hot', most-downloaded or otherwise highlighted articles (>75 identified). Our status as authorities in various fields is confirmed by widespread invitations to write reviews or book chapters (>40 identified).

We have played **leadership roles** in the Research Councils, learned societies and other professional bodies, with notable examples including: Costen - Secretary and then Chairman of *RSC Gas Kinetics Discussion Group*; Duncan - member of the *Canadian Foundation for Innovation International Funding Committee* and reviewer panel for the *Wellcome Trust Strategic Fund*; Gutowski – Chair of the Chemistry panel of the *INCITE* program for US DOE; Lee - *SCI Young Chemist Panel*; Macgregor - Chair of funding panel for *National Service for Computing Chemistry Software*; McCoustra - *Chair of British Vacuum Council*; McKendrick – member of *RSC Faraday Council* and *STFC Physical and Life Sciences Committee*.

Our staff have been awarded a number of prestigious **fellowships and prizes**, including: Dalgarno - *RSC Harrison Meldola Award* (2010) and *Inaugural RSC Chemical Communications Emerging Investigator Lectureship*; Duncan – *Wellcome Trust Research Career Development Fellowship (2004-8);* Greaves – *EPSRC Career Acceleration Fellowship*; Lloyd - *Herchel Smith Fellowship* (2010-2012) and *CCDC Chemical Crystallography Prize for Younger Scientists*; McKendrick - *Royal Society Leverhulme Trust Senior Research Fellowship* (2008-09) and election to *Fellowship of the Royal Society of Edinburgh* (2011); Nahler – *Royal Society University Research Fellowship*.