Institution: University College London

Unit of Assessment: Chemistry

a. Overview

Chemistry at UCL is dynamic and interdisciplinary with more than 150 research collaborations with industry, UCL departments and international research centres. Our vision is to produce world leading chemistry that is characterised by **innovation**, **insight** and **rigour.** The department has joint academic appointments with Medicine (**Selwood, Arstad**) and the London Centre of Nanotechnology (LCN, **Wills, Thornton, Michaelides, Hirjibehedin**). The department has appointed 15 academic staff since 2008 (as of 31/10/13) – a net increase of 6 HEFCE-funded staff over RAE08 - an indication of the continuing faculty and institutional support for the discipline. The department's research, as in RAE08, is divided into four sections for administrative purposes: Organic Chemistry and Chemical Biology (OCCB); Physical Chemistry and Chemical Physics (PCCP); Inorganic and Materials Chemistry (IM); and Computational Chemistry (CC). **All** academic staff in the chemistry department are returned in this submission.

b. Research strategy

The department's research strategy originates from its full management group, chaired by the Head of Department (HOD) **Parkin** and includes all 24 professors, in consultation with the Dean of MAPS (Mathematical and Physical Sciences). This strategy is further informed by an external international board (now led by Chisholm FRS) of 8 academics including 4 FRS and representatives from industry as well as by internal reviews by the UCL MAPS faculty. Each section meets on a regular basis to discuss objectives and provide input to the department's management working group (MWG) to determine strategic priorities. A yearly strategic review of research is conducted by the MWG (6 academics) who report to the full professorial committee. Much of the current strategy has evolved from recommendations by the previous RAE, the external board (2009) and internal MAPS review (2011). A full external review will be implemented in 2015.

2.1 Achievement of Strategic aims set out in RAE2008

All of the key strategies defined during the previous 2008 RAE exercise have been advanced, particularly to develop chemical biology by enhancing links with life and medical sciences; to develop links with the astrochemical and spin ice communities; to grow interactions in the field of "energy materials", particularly with AWE and Diamond/Harwell; and to become leaders in crystal polymorph prediction, computational biological chemistry and in developing computational methods for following catalytic processes.

The department has developed a strong funding base in OCCB especially in biological chemistry and sustainable chemistry. This has led to our playing key roles in the establishment of the Crick Institute (UKCMRI, **Caddick, Hailes**) and the UCL-based drug discovery initiative. The latter has led to a CDT in drug discovery (8 students, and an allied research masters course - started in 2012) and substantial new grant funding (>£9M EPSRC). Development, planning and appointments linked to the Crick institute have expanded our chemical biology initiative. The OCCB team have developed new glycoproteins, lantibiotics and peptide linking strategies – based on maleimide coupling. New mass spectrometry laboratories have been created especially for protein work. The success of OCCB in building on RAE2008 is exemplified in part by two medals to **Hailes** – the RSC Cornforth Award and the IChemE Innovation and Excellence Award in Bioprocessing.

During the REF period the PCCP section has made seminal contributions to developing and applying advanced instrumentation for fundamental and applied molecular science including: methodology for delivering macromolecules into live cells to probe cell dynamics (**Battaglia**); the first measurement of ultrafast non-radiative decay dynamics in green fluorescent protein (**Fielding**); and the discovery of a new phase of water-ice and fundamental insights into the crystallisation properties of supercooled water (**Salzmann**). **Wills'** spin-ice team was awarded the Times Higher Research award in 2010 for their work on frustrated magnetism. A new shock physics institute was set up with AWE (**McMillan**). **SL Price** has been at the forefront of polymorph prediction including substantial new funding from EPSRC and Eli Lilly (>£1.5M).

One important feature of the department is the close synergy between theory and experiment. There is significant overlap between the research activity of the CC staff with that of the PCCP and IM sections (> 20 projects, including two on CO_2 utilisation which have >£3M EPSRC funding). The department's research on computational theory as applied to solid-state chemistry and catalysis remains internationally leading (Gordon lectures, 5 international advisory boards, >£5M in EU funding). **Catlow** obtained substantial funding (EPSRC >£5M) to lead the establishment of a

catalysis hub at the Harwell campus and to set up a UK catalysis initiative –both linked to Diamond and the facilities on the Harwell campus. This initiative involves extensive collaboration between CC (modelling), IM (synthesis) and PCCP (measurement) and over 20 chemistry academics.

In 2007 the Energy Research Centre (**Sankar**, **Darr**) was established and **de Leeuw** relocated from Birkbeck. An aim for IM during REF was to exploit their expertise to develop new interdisciplinary projects. This has led to initiatives in energy research: extending collaborations with LCN and developing a new hydrodynamics institute studying science under extreme conditions. This fostered growth of transparent conducting oxide programmes, new initiatives in battery, hydrogen storage, fuel cell and solar energy materials, and adoption of combinatorial CVD and hydrothermal approaches for energy nanomaterial synthesis (>£10M in funding; 75 papers). It also stimulated a new PGT one-year research masters course on energy materials that has attracted over 15 new students in both 2011/12 and 2012/13.

Overall, the department has published >1600 research papers during the assessment period (6 yrs) [compared with *ca*. 1200 over RAE08 (7 yrs)], with the number of papers published per year increasing almost linearly to 320. We expect this number to grow substantially in future through the recent expansion of staff numbers and via the establishment of early career researchers. Increased effort has been made in the past two years to publish in more general chemistry journals rather than specialist journals (a departmental REF total as of 31/07/13 of 33 papers in JACS and 23 in Science/Nature type). The visibility of **Cora, Bell, Slater, Beale** and **Michaelides** work led to the direct funding of four PDRAs by BP. Further we have annual departmental prizes for the best published research papers from both PDRA and PhD researchers for all the research sections.

During REF, research outputs have been published on the departmental and college websites, video and podcast, and through television, radio and newspapers. **Sella**, the department's publicity coordinator who has made over 150 TV/radio appearances during the REF period, champions UCL Chemistry's media exposure. Examples of work covered in the media include **Parkin's** work on antimicrobial catheters, **de Leeuw's** work on the origins of terrestrial water, **Powner's** work on the origins of life and **Evans'** work on nanocomposites ("the clay aeroplane").

2.2 Strategic aims and Vision

The department's continuing goal is to be internationally leading across major branches of chemistry: computational chemistry, especially for solid-state materials and catalysis; inorganic and materials synthesis and functional characterisation; development of new techniques for measurement in physical chemistry; and synthesis/mechanism in organic chemistry and chemical biology. We are determined to continue to play an internationally leading role in research in these areas, and to transfer it's results to industry, policy makers and the general public, especially for UK benefit. To achieve these goals the department's core research strategy that is now rolled into its forward vision is to:

- Maintain core strength through targeted appointments, rewarding excellence.
- Maximise success in grant applications- through internal review and incentivising success with internal resource (student match scheme, lab space, adjusted teaching/administration load).
- Maximise the number and quality of PDRAs and students through DTCs and grant success (51% increase in PhD student FTEs since 2007; vigorous multi-stage interview processes).
- Develop a balanced portfolio of grant funding from multiple funding sources and reduce our reliance on EPSRC funding by growing support from industry (open days, network and KT events), EU (through lectures and best practice in applications) and other RCUK funders.
- Maximise interdisciplinary research, especially with Diamond/Harwell and the Crick Institute.
- Provide state of the art computer resources, locally and through access to extensive UCL and national facilities, and be the leading Chemistry department in high performance computing.
- Act as an equipment hub for neighbouring universities and provide cutting-edge characterisation equipment.
- Develop closer links and joint funding with other research centres (UK /abroad -JAIST, A*).

A key departmental strategy has been to develop a wide range of collaborations between sections and to develop large-scale research collaborations with other universities and UCL departments. This strategy has led to a myriad of new collaborations with the fields of medicine, life sciences, materials and physics (>50 over the REF period) both internal and external to the university (section 5.1). This has also led to strategic talks with Kent and Imperial (IC) about further collective grant applications and bids. It is our intention to encourage the growth of our collaborations through linked studentships, joint grant applications and knowledge transfer activities. These links and

others have established UCL as a key hub in many large-scale UK collaborations during the REF period (Diamond, Harwell Campus, Supergen, Photocatalysis Network).

To enable successful grant applications in the evolving funding landscape, it is a continuing objective that all staff are encouraged to adapt as appropriate their research approach. For example, a number of PCCP staff have translated their technical expertise to problems of applied interest in medicine and biosciences (**Fielding, Holt**) and materials science (**SD Price**, £1M EPSRC, **Caruana**, new patented pollen detection). OCCB staff have arranged "speed-dating" events with LCN, Chemical Engineering and the School of Pharmacy, and invited industrial guests to PhD talks, generating new collaborations. These links will be fostered in the future.

The OCCB section will work to strengthen its funding base mapping forward by increasing interdisciplinary collaborations in biological chemistry with the Crick Institute; in sustainable chemistry with UCL Engineering and industry; and in organic materials and photovoltaics with the LCN. The group will push the boundaries of research in chemical biology/medicinal chemistry and simultaneously address real problems in clinical and preclinical research. Specifically, we will develop new chemical materials for applications in the health sciences to underpin therapeutic innovation – focussing on new multi-modal probes, anti-cancer and TB drug precursors. This initiative benefits from UCL's core strength and investments in biomedicine (No.1 in Europe).

Objectives for PCCP include continuing to design, build and exploit innovative instrumentation for measuring and understanding the structure, properties and reactivity of molecules and extended solids in a range of environments; and to use this to tackle problems in the priority areas of healthcare, quantum technologies, new materials and energy. We will also translate our advanced instrumentation into new technologies; for example **SD Price** will complete (2014) a new apparatus to dope surfaces with free radicals to enhance their functional properties.

A key future goal for IM and CC will be to strengthen our links with Diamond through the new catalytic research laboratory at the Harwell campus. Over 20 chemistry academics now work with the centre, including **Sankar** who has been seconded two days a week to strengthen the interaction, and 10 UCL research co-workers are currently based there. The number of UCL chemistry PhD and PDRAs at Harwell will grow to approximately 25 in the next two years. We have established a dedicated Harwell PG tutor and new appointments (**Scanlon** now holds a joint position -started 1/9/13, **Beale** is based at the catalysis hub).

Energy research will be further strengthened by a new appointment in PCCP, by a recently awarded EPSRC award to study energy storage (**Guo**) and by closer links with UCL Chemical Engineering. A recently awarded programme grant (2013) on nature-inspired engineering to Chemical Engineering (Coppens, £5M) has three investigators from the chemistry department.

Staff are regularly assisted by the research committee, Heads of Section (HOS) and HOD in developing grant applications and publications to improve both their quality and quantity- this will continue. There is a departmental expectation that every academic submits two grant applications a year as PI, one to a research council. The policy has helped enhance our total non-facilities grant portfolio to > £40M compared with *ca*. £22M at the start of the REF period. This has been achieved by fostering a culture of collaboration and support. Indeed we consider this culture a defining attribute of UCL in general, and UCL Chemistry in particular. This culture underpins our vitality and helps to ensure our sustainability in the future- where we aim to further enhance our funding.

To increase the number of PGT and PGR students and ensure that the best quality candidates are selected, a departmental matching scheme that generates a studentship for every £500k of RCUK income has been established (2011) as an incentive to staff. In addition, the UCL impact scheme provides matching funding for studentships to staff (*ca*. 10 PhD students supported in chemistry in each of the last three years). Further, our EPSRC funded ITC and two internal DTCs established during the REF period have allowed good access to students across all of the sections. The department recognises the key role that a large PhD cohort has on research outputs, and so will continue its support of part-funded studentships. In addition we will maintain our current CDTs and develop new centres in, for example, Therapeutics, Sustainable Chemistry and PCCP.

c. People, including:

i. Staffing strategy and staff development

As with the research strategy, the department's staffing strategy is decided by the MWG in consultation with the Dean of Faculty and informed by the decisions taken by the full professorial group. Following recommendations from the external board and faculty review we have increased PhD student numbers (113.6 FTE in 2007, now 171.26 (2012/13) – fractions of students due to

start dates occurring at different times throughout the year); expanded numbers on research masters courses (from 2 to 28 students over 4 courses); enhanced our interactions with the LCN (4 joint appointments); and expanded staff numbers in soft materials/polymers (3 new appointments).

Our primary staffing strategy has been to maintain core staff numbers in each of the four research sections (13-15 staff per section) while expanding in key areas relating to the department's research vision and national initiatives. Expansion has involved an increase in staff numbers in catalytic science to align with UCL Chemistry's major role in the EPSRC UK catalysis hub (2 staff appointed – **Beale, Scanlon**); appointments that will strengthen upcoming interactions with the Crick Institute (**Gervasio, Battaglia, Bucar, Christie**); and developing new research areas in soft materials chemistry, energy materials research and in the origins of life (**Powner**). In addition, **Bronstein** and **Blunt** joined to strengthen links with the LCN and UCL Physics through their work on organic polymers and nano-patterned surfaces. Professor Choi will join UCL in Feb 2014 as head of a new materials discovery institute. This stand-alone institute will be closely linked with chemistry and we plan two joint lecturer appointments between the institute and chemistry in 2014 and 2015. We plan for a further new appointment in 2014 in PCCP.

Nineteen technician and research officers and nine administrative support staff support the department's work. An additional four laboratory managers have been appointed during REF to ensure smooth running of labs, develop best safety practice and to provide expert training on instruments and in experimental technique.

All staff that have left (**Brown, Perkin, Lewis, McKay, Wilitsch, Bramwell**) or retired from research (**Motherwell, Ewing, Day**) during REF have been replaced. All departing staff fill in a questionnaire and all have spoken very positively about UCL Chemistry, leaving for promotions or a change in career direction. All academics (51 as of 31/10/13, 49 as of 31/07/13) have open-ended contracts, while 4 of the 11 fellows are on proleptic appointments and 7 are on fixed funding from fellowships (10 fellows as of 31/07/13). Research fellows will continue to be strongly encouraged and supported in the application process to apply for future permanent positions.

The Chemistry department at UCL has actively sought to reward and support all staff, and has a particularly strong record in the promotion of women in science. The department is currently applying for a bronze Athena Swan award, submitting its documentation in November 2013, and notably, has been regularly used as a base by the RSC for its promotion of "women in science" events. Professors **Fielding** and **Price** have been very active nationally in supporting such events through the RSC and IOP. The department has more female professors (6) than any other chemistry department in the UK.

The department has deliberately grown from 49 to 55 HEFCE supported academic staff (55 to 62 category A staff) over the REF period. This growth has focused on areas of interaction with life science, catalysis, energy materials and origins of life/synthesis. New appointments in each area have been coordinated at the faculty level and have occurred in response to the national agenda, especially to priority areas set by EPSRC. During the REF period 15 new academic staff have been appointed (as of 31/10/13, 13 appointments as of 31/07/13) and 9 have retired/ left UCL.

2008/9	2011	2012	2013
Anderson (1/4/09) Head of OCCB group, leads interaction with School of Pharmacy	**Powner** (1/10/11) Origins of life	**Palgrave** (1/3/12) Water splitting catalysts using solid-state epitaxial particles **Blunt** (1/11/12) STM to characterise new nanostructures	**Gervasio** (1/2/13) Chair in multiscale computer modelling (biomolecular science), with emphasis on NMR measurements **Battaglia** (1/3/13) Chemistry of biological polymers
Arstad (1/5/08) Radiotracers for in vivo imaging	**Salzmann** (1/10/11; RSURF) Development of new ice polymorphs		**Bronstein** (1/4/13) Organic polymer materials
Colour codes: Professor appointment Lecturer appointment Lecturer-previous fellow at UCL	**Blackman** Inorganic materials including ALD **Macmillan** (RSURF) Glycoprotein research	**Zwijnenburg** (EPSRC career acceleration fellow) Computational materials chemistry related to energy	**Wolthers** (NERC fellow, 1/11/12) Analytical chemist climate change through the fossil record **Scanlon** (Ramsay, 1/09/13) Computational studies of oxides **Woodley** (1/09/13) Computational nano-chemistry

Both **Gervasio** and **Battaglia** act as link points to the new Crick Institute research centre and to the life sciences at UCL, enabling us to combine computational and membrane structural studies with functional studies. **Bucar** (drug polymorphism, 1/10/13) and **Christie** (computation

bioinorganic chemistry- especially bone formation) have been awarded UCL funded Crick Fellowships (2013), strategic 4-year fellowships to develop interactions between chemistry and the new Crick research centre at the chemistry-biomedical sciences interface. A number of Staff hold research fellowships in the department: Ramsay (**Dunnill, Roldan**); RSURF (**Tilocca, Salzmann**); EPSRC career advancement fellowships (**Beale, Kerridge, Powner**, **Zwijnenburg**); NERC (**Wolthers**). The department has an excellent track record of appointing fellows to permanent academic positions through their participation in an open-to-all recruitment call (7 during REF). Fellows are given extensive mentoring and interview practice. The department's appointment process requires women to make up at least 25% of any appointment panels. Women and ethnic minorities are specifically encouraged to apply for posts.

3.3 *Staff Development*

All new academic staff, RSURF and EPSRC fellows have been provided with a minimum of £25k in cash support as start-up, and a fully funded PhD or EngD studentship. These new staff have also been given access to the extensive research equipment base within chemistry, and use of state of the art laboratory and computer resources at below FEC rates. New staff can also recruit up to 3 full year MSc students from the expanded one-year taught masters courses to work in their laboratory. Senior academics monitor the appointees.

UCL Chemistry has adopted the model pioneered by IC for PDRA, research fellow and early-career lecturer support. This involves each person being assigned an academic mentor, unconnected with their research, who assists with integrated careers support including CV development, grant applications and interview techniques. This development process has allowed a large number of fellows and PDRAs to progress to academic appointments either at UCL (**Beale**, **Blackman, Salzmann, Scanlon, Zwijnenburg, Macmillan**) or other universities (**Perkin** (Oxford); **Binions**, **Di Tommaso** (QMUL); **Mellot-Draznieks** (Paris); **Grau-Crespo** (Reading); **Walsh** (Bath)). This support also allows these new academics to have great success in expanding their research groups; for example – **Beale** and **Powner** each have 2 PDRAs (from the fellowships) and 4 PhD students (from industry and charity sources).

All new non-proleptic appointments supported by Royal Society, Ramsay or EPSRC fellowships are not obliged to carry a teaching load. However, most chose to deliver at least one lecture course to obtain teaching experience. Other new academic staff carry a maximum 1/3 teaching load in year one, ramping up to a full load by the end of year three (typically no more than 30 lectures and a maximum of 200 contact hours). All new lecturing staff take an accredited higher education teaching qualification. The priorities for individual staff training are set at annual appraisals. All staff are required to attend at least two training courses a year from an extensive college list. Popular courses include research group management, grant writing, PhD mentoring, appraisals and equalities training. External life coaching and mentoring is available for professorial staff and all non-professorial staff have a mentor. Internal departmental training is also organised for subject-specific grant writing, publication in high impact journals and best practice in safety.

Staff performance is monitored annually via staff appraisal. Clear measurable objectives are set for all aspects of teaching, research, enabling and KT activity. In grant applications objectives are set in terms of number and quality of applications. HOS and HOD give extensive advice on improving applications that are unsuccessful. Academic staff are strongly supported by grant facilitators at faculty level. These highlight current calls for proposals, provide guidance in proposal structuring, provide mock interviews for larger scale grants and monitor success rates. This insight has helped successful awards during REF of platform grants (**Parkin, Caddick, de Leeuw**), programme grants (**Catlow, de Leeuw, Guo**) and the catalysis hub application (**Catlow**), as well as EPSRC fellowship applications (**Powner, Beale, Zwijnenburg, Kerridge**).

As part of the strong emphasis placed during the REF period on publishing in the highest impact journals, colleagues have been given guidance, from senior academics within the department, in writing high-impact research papers. It is common for staff to circulate draft manuscripts to others for comment prior to submission. A series of seminars and workshops have been organised in the department with the Nature Group, Wiley, Elsevier and RSC publishing. These measures have resulted in an increase in the number of publications in journals with an impact factor >10 from *ca*. 30 publications in 2008 to over 70 in 2012. This increase in "high-impact" publications has resulted in an increase in citations, and indeed an increase in the overall total number of publications from 2008 to 2012. This publication rate is expected to grow significantly as the new junior staff develop their careers.

Staff are encouraged to attend conferences. Most staff fund conferences and invited lectures from their grant funding, but support in covering travel funds is provided both from the graduate school at UCL and the department. An active seminar series in each section as well as joint seminars with the LCN supports over 120 invited lecturers a year.

The department makes use of a workload model for allocating teaching and administrative duties. HOS are able, if the staff member desires, to reward staff for success in research applications through a reduction in teaching duties. Each staff member is able to have a sabbatical leave to develop new research ideas and to help foster the impact from their work (KT sabbatical); a scheme managed by the HOS and HOD. Staff on sabbatical leave (3-5 staff at any one time) get a full year's remission from all teaching and administration duties, and their workload is shared between other staff and trained PDRAs, the latter hired to provide tutorial and demonstration cover. Goals are set prior to the sabbatical with the HOD who interviews each person and helps set objectives. A further interview is held at the completion of the sabbatical to assess achievement against the goals. Successes from such sabbaticals include **Hailes** work on imaging that led to a £6M imaging grant and **Howorka's** publication of 4 papers in high impact journals (IF>16). The sabbatical programme is set to continue through the next REF period.

Departmental meetings are held within core hours of 10am - 4pm to facilitate childcare and carer responsibilities. Established policies are in place to support career breaks, and the department provides additional support to staff returning from maternity leave including a centrally funded 6-month reduction in teaching duties. All staff are able to work flexible hours as best suits their research needs, and around half of staff work offsite at least one day per week. They are able to work away from UCL for extended periods. This is particularly valuable for staff involved in experiments that require central facilities, of which the department is a significant user. Cover for supervision of students and safety whilst staff are offsite is coordinated within each section.

The department has a well-developed promotion process, which promotes on merit and achievement and has no caps for promotion numbers. Candidates are encouraged after consultation to submit their CV to a meeting of professors, who consider applications, give advice and appoint a mentor to develop the case. The case is submitted to a Dean's committee and then to a Provost committee for ratification. The department has promoted 15 academics since 2008, including 4 women who have been promoted to professor (**Carmalt, de Leeuw, Tabor, Hailes**).

ii. Research students

It was noted in both the previous RAE and in our 2009 external review that the number of PhD students in UCL Chemistry was lower than the sector average for top chemistry departments in the UK. This has been addressed and, as of 31/07/13, 207 PhD/EngD students (mainly on 4 year courses- includes writing up students) are registered in Chemistry, (114 were registered on the same basis in 2007). This growth in the number of PhD students has been achieved via the UCL college impact studentships (30 fund matched studentships in chemistry; mostly co-funded with industry), CASE awards, the EngD centre (>100 students over the period), strategic collaboration with international centres of excellence (A*STAR in Singapore, JAIST in Japan), and EU, Wellcome Trust, charity and direct industry awards. It has been departmental policy to actively explore and develop funding for new studentships, coordinated through the departmental management group, the PG tutor and the EngD coordinators.

The department has a yearly intake of *ca*. 120-140 into its undergraduate degree programmes, with student A-level scores averaging AAA or better. 300 of the 376 currently enrolled undergraduates are studying for MSci degrees, while the remainder are on the BSc track. The department also plays a pivotal part in the teaching of the Natural Sciences BSc and MSci degrees (360 undergraduates). About half of the intake for PhD/EngD degrees are UCL undergraduates. Undergraduate recruitment underpins the department's financial position and provides exceptionally well-trained graduates for the research school. The department's postgraduate school currently has an additional 29 students on taught one-year MSc courses (grown from 1 to 4 courses during REF). The department admitted 65 new PhD/EngD students in 2012. The EPSRC sponsored Industrial Doctorate Centre EngD program, which is focused on molecular modelling and materials chemistry, has been particularly successful and funding of this M3S IDC from the EPSRC has just been extended by 5 yrs. It has built on the EPSRC core funding of ten students a year through self-funding, institutional support, fully paid industrial scholarships, and CSC scholarships; this additional funding raised the EngD student intake in 2012 to 22 students. The EngD students each have an industrial company sponsor and spend at least 6 months in industry

(>40 companies to date). While the students are split equally between molecular modelling and materials chemistry projects, an emphasis of the program is the synergy between modelling and synthesis/characterisation. The UCL chemistry department also has 10 PhD students from the EPSRC-funded UCL Security Science Doctoral Research Training Centre (UCL SECReT). SECReT students spend a four-month period in industry and complete additional training courses relating to crime and security.

The current doctoral students come from 29 countries, including 15 countries from outside the EU, a number of whom are self-funding. The students are attracted to UCL via its international reputation; extensive work from **Guo** and **Tocher** who are/were pro-provosts for China and SE Asia, and have regularly visited both regions; Chemistry PhD open Days (2 per year); a significant web presence; and a dedicated full time administrator.

UoA 8 Research student FTE, by academic year

	2008-9	2009-10	2010-11	2011-12	2012-13
PhD	112.04	106.58	112.46	115.38	128.58
EngD.	10.10	11.96	12.48	19.97	20.78
SECRet PhD	-	-	-	0.87	1.55
MRes (EngD. track)	-	5.53	15.85	10.41	20.35
PhD Total	**122.14**	**124.07**	**140.79**	**146.63**	**171.26**

PhD submission rates within a year after end of funding have improved from ca. 75% in 2008 to 93% in 2012. The graduate tutor (**Hailes**) oversees PG progression. Each student is assigned a subsidiary supervisor who participates in assessment milestones and provides additional support. In their first year, students introduce their research topic to the rest of the department with a 5-minute oral presentation, and prepare a 20-page report 9 months after their start date. The subsidiary supervisor provides a short assessment that is then discussed with the student and the supervisor. MPhil to PhD transfer occurs during the candidate's 2nd year. Here a 40-page full research report with a timetable for completion of the PhD and an assessment of the student's progress by the primary supervisor are submitted to the upgrade panel prior to the upgrade viva. In the case of failure, the student is permitted a second attempt to upgrade 18-24 months from their original start date. After the viva, a poster presentation is made and their primary supervisor advises on the work needed to complete the thesis. The student gives a 25-minute presentation to the department or research section in the penultimate term prior to thesis submission.

EngD students follow traditional PhD type research but have a wide range of additional training, lecture courses, a dissertation, poster presentations, industrial days and schools events, and are awarded a MRes degree at the end of year one. All EngD students receive training in project management from the Association for Project Management in year two. Many students have received the Certificate of Project Management, which is in demand in industry. Three such EngD students have taken on project management careers (e.g. Waugh, Credit Suisse). EngD students are regularly employed by their sponsor or related companies on graduation (> 40%).

All doctoral candidates must update and complete their electronic Research Student Log, which is monitored by their supervisor and provided by the UCL Graduate School. The Log provides a flexible way of recording the details of the candidate's research programme, scheduled formal supervisory meetings and development of academic and discipline-specific key skills. This monitoring allows PG students to assess, plan and chart their progress during their studies, and it equips all candidates with the ability to manage their continuing professional development in their future careers. Staff advise on the fundamentals of job applications (application forms, CVs) and graduate school courses are available on career planning.

Specific activities are logged and monitored via the Graduate School's Skills Development Programme, which enables research students to view and register for training available to them both at the Graduate School and within the Chemistry department. Each training course or activity is awarded a pre-specified number of points upon completion; students must collect a total of 60 points before submission of their thesis. Students are also encouraged to log their involvement in non-structured activities including conference attendance, paper preparation, external training and research, and extra curricular activities within UCL, for which they also receive points.

d. Income, infrastructure and facilities

4.1 Infrastructure

The Chemistry department currently operates over two sites. The main site, the Christopher Ingold

Building (CIB; 9000 m^2), houses all undergraduate teaching and the majority of the department. A smaller site exists in the Kathleen Lonsdale building (KLB; 800 m^2) where computational, synthetic organic, nuclear and flow chemistry take place. The department has led a successful EPSRC bid for a research facility for catalytic science, located within the research complex at Harwell. The department is a major user of central facilities, particularly at Diamond. It has some joint laboratories in the LCN, especially for PCCP measurements.

The department has seen substantial university investment in infrastructure since 2008. To underpin its research goals, the department has sought to provide the best laboratory space, state of the art instrumentation, and a dedicated support infrastructure of workshops, glassblowers, microanalysis and instrument specialists. The undergraduate laboratories, connecting corridors and central space within the CIB have all been refurbished (2009-13). A new front entrance (2010) has provided significantly enhanced security while also enhancing the aesthetics of the building.

The department has developed a new 8-person lab in the KLB (2012) and a 4-person lab in the CIB (2011) to enable radioactive experiments, especially tracer studies for **Howorka** and **Arstad**. In 2013 a new 12-person biochemistry lab for **Battaglia**, new Mössbauer, SEM/TEM laboratories and labs for medical imaging have also been constructed. In computing, the department/College has invested in excess of £2M in new resources including expansion of five new chemistry clusters. The department also houses a large (60 space) computer cluster accessible for research students.

The department has a mechanical workshop (350 m^2) equipped with lathes, milling machines and precision instrumentation. The instrumentation is regularly serviced and renewed. Three full-time technicians work in the facility and are able to provide advice, guidance and a bespoke service for equipment manufacture. The department's two glass blowers provide a high standard of work and consultation and design services. An electrical support group (3 technicians) provides routine and preventative maintenance as well as construction of equipment. In computational science the six local computer clusters are maintained by three support officers.

The department has taken a leading role both within UCL and the UK in reducing our environmental footprint and fully adopting a "green agenda" for our research. This activity has been coordinated by **Sella** and has included reducing our water usage by 70% from 2009-12 by changing to turbopumps, using water re-circulators, avoiding sending water to waste (especially from condensers) and monitoring our water usage. We have also reduced electricity usage through accurate metering and running fume cupboards at lower velocity. The department's efforts have been recognised with a commendation by the UK national S-Lab Awards (2012).

4.2 Facilities

The department has maintained and significantly enhanced its facilities during the REF period. The UCL budget is organized by faculties, with each faculty given a target for its contribution to central costs. This structure filters down to departments being given a specific monetary target. The chemistry department has hit its targets during the REF period and has produced an annual surplus of ~£200-300k (2011, 2012). This surplus was reinvested in the equipment infrastructure, including purchase of open access departmental ATR-FTIR, XPS and UV-Vis machines.

The department has outstanding library facilities with online access to >1900 chemistry journals. Chemistry at UCL also makes extensive use of the British library (5 minutes walk from the department) which is the UK's national library.

Materials and computational chemistry facilities in particular have been radically improved since the last RAE. The department now has 13 mass spectrometers, 5 high field NMR instruments, 3 SQUID magnetometers, and 3 SEMs. The department was recently successful with an EPSRC equipment bid (£1.5M in 2013; £1M in 2014, £0.5 M in 2015) and has had an additional college contribution of £900k. The department is acting as a central equipment hub for 6 universities (Kent, OU, Greenwich, Kings, QMUL, IC) through this initiative. This has enabled the installation and use in the chemistry department of: a high resolution TEM instrument with EDX and Gatan camera (£0.5M); a new Thermo XPS spectrometer (£0.35M) which can handle over 60 samples a day, with full analysis and depth profiling; two new X-ray diffractometers – a Stoe system with dual ports and the ability to heat samples to 1000 °C, and a Bruker thin film system; two upgrades to another Stoe system; and a new detector for the existing Bruker D8 system. A new single crystal instrument with dual radiation source (Mo/Cu; Agilent, July 2013) underpins research in synthetic chemistry. Two new mass spectrometers have been installed, one GC-MS and one for looking at real-time gas-phase reactions. Two new AFM systems have also been

installed. The department has also invested £800k in a new 600 MHz cryoprobe NMR system that is particularly sensitive for ^{13}C.

Four new laboratory manager positions created during REF oversee the efficient running of computing, X-ray facilities, instrumentation and organic chemistry, and have developed centralised booking procedures for instrumentation. They have also implemented a system to track chemicals in the department (Quartzy), provided expert student training and spread best laboratory practice. Our introduction of the Quartzy web-based labelling system has reduced duplication, prompted chemical sharing and enables us to track every chemical, thereby reducing waste. The department has championed this free program and has advised IC, Kent and UCL Pharmacy on usage.

The department covers maintenance contracts on selected equipment with the rest maintained by a team of in-house technicians and workshops. These technicians train the PDRAs and students in the use of equipment. The departmental ethos is that all students and PDRAs should acquire their own data from instruments – overseen by lab managers and supervisors through problems classes, hands on training and allied modules. The technicians are also active in research and regularly co-author papers. The close interaction between academic staff and the workshops means that apparatus can be quickly optimised or upgraded.

The department aims for all facilities to break even on a cost basis. However, we are also mindful of getting maximum use from our public investment and are very efficient in using machines on a full time basis. We aim to support all research work and enable all staff to have an active research presence. No academic has been prevented from doing research for lack of funds; those who have difficulties are helped with advice on grant proposals and extended loan facilities for staff to use for chemicals, equipment and facilities.

4.3 Income

The department is supported through extensive grant funding. As of 1/7/2013 it had an EPSRC portfolio of £39.5M the largest portfolio of any chemistry department in the UK (EPSRC GoW). It is further subcontracted on other EPSRC grants as Co-I for example the work of **Guo**, **Slater**, **Cora**, **Hailes** and **Tabor** (>£7M**)**, and in a programme grant with Sheffield University (UCL award £1.3M). It has had extensive additional support during the REF period and held the following grants: Leverhulme Trust (13 grants); Wellcome Trust (13 grants); MRC (10 grants); BBSRC (10 grants); NERC (2 grants + fellow) and the European Commission (23 grants) that contributed a further £8.9M of support. These grants support the work of *ca.* 60 PDRAs at any one time as well as 5 senior research fellows. In total the department has over 70 companies who sponsor PhD studentships, across a wide cross-section of industry. Total expenditure from research grants has increased from **£36.5M** in the previous RAE (over 7 yrs) to >**£55M** in this REF submission (over 6 yrs). The major expenditure was from research council, charity, EU and industry that amounted to >**£43.1M**. This is closely followed by central computing expenditure that exceeded **£6.5M**. Further central experimental usage, especially Diamond, ESRF, ISIS and ILL, amounted to >**£5.4M**.

The external advisory board to the department and the faculty in their strategic review recommended diversification of research funding to include sources other than EPSRC. This has been achieved, with a greater proportion of the department's research income now coming from other sources despite the substantial increase in EPSRC funding. The increase in non-EPSRC grant spend per annum (from 2008/09 to 2012/13) comes from increases from EU government bodies (£613k to £1.56M), NERC (£2k to £125k), MRC funding (0 to £186k) and UK industry (£92k to £421k). The total grants administered in the department has increased from 170 (2008) to over 200 (2012). Staff have won 10 Leverhulme grants during REF (ca. £250k each). There has been a significant uplift in EPSRC awards to the department in 2013, from **£5.3M** in 2012 to **£13.9M**. This increase has been particularly marked in computational and materials science, from 6 awards totalling £1.5M in 2012 to 14 totalling £12.9M. Six professors in these sections (**Catlow, de Leeuw, Guo, Parkin, Price, Coveney**) have now collectively spent >£20M from awards as PI over the REF period; this funding has enabled them to collectively publish >250 papers in that time (including many high impact publication). As of 1/7/2013 UCL chemistry held the largest grant portfolio in its history with many awards starting in 2013 with 4-5 year award periods- ensuring baseline funding sustainability with the current uplift in funding reflecting our research vitality.

The department aims to maintain and consolidate its recent grant successes and will further aim in the next REF period to continue the successful policies that have enabled it to have a substantial portfolio, including diversification of funding sources. We will be continuing our extensive internal review of grants, sabbatical leave, developing closer industry links (through

symposia and events), collaborative applications with other institutions (especially at programme grant level) and looking to further expand our EU-related funding.

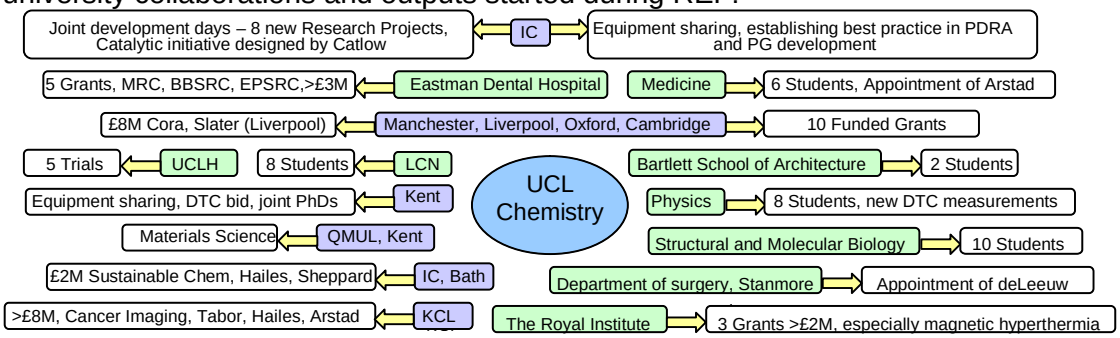
The dean of MAPS has invested more than £1.4M in chemistry equipment and infrastructure over the REF period and is committed to future improvements at the same level- with investment plans around facilitating chemistry's strong and developing presence with the Crick and Harwell Campus. A key development consolidated during the REF is the Centre for Materials Research (based in Chemistry) which brings together >100 investigators from several departments. Prof Choi will be appointed in Feb 2014 to head a new materials discovery institute with research space provided in engineering – to strengthen the chemistry and chemical engineering interaction.

e. Collaboration and contribution to the discipline or research base

5.1 Collaboration

Staff are encouraged to collaborate through the use of workshops, scientific "speed dating" events, industrial days, sectional meetings, "corridor moments" - coffee room chats and through networking events. In the past year alone, "speed-dating" events held with the LCN, UCL Medicine, the School of Pharmacy and IC Chemistry have led to more than 20 new research interactions. The IC Chemistry interaction – though three one-day workshops (2011-13) led to funding 15 summer research studentships (2012), 4 publications and two grant applications.

Key new university collaborations and outputs started during REF:



The department very positively supports collaboration and a wide range of external researchers from academia and industry regularly use our equipment and facilities. The interaction with the Eastman Dental Hospital on antimicrobial coatings in particular has flourished over the REF period (**Parkin, Carmalt, Blackman**) and has led to over 25 publications, a granted patent, newspaper articles (Telegraph, Times, Evening Standard), five joint research grants (>£3M), seven PhD's, investment of > £1M from Ondine for research (PDRA and PhD student in chemistry) and four clinical trials. This has underpinned the commercialisation of Periowave, a treatment for periodontal disease that has been used by 100,000 patients. **McMillan** has a number of projects funded with the Royal Veterinary College – these have resulted in a new patented diagnostic for knee damage based on Raman spectroscopy. This treatment method has been trialled on animals and in 2013 on human patients. One other notable success is that **SL Price** has recently obtained £1M from EPSRC for a joint grant with Pharmacy for the prediction of new structural polymorphs. In addition **Guo** is Co-I or PI on 6 large national (supergen) consortium grants on energy storage (>£10M); and **Coveney** is the coordinator of 4 EU grants (>£4M UCL component).

In larger collaborative initiatives, UCL Chemistry has had a key role in the development of the scientific strategy of the UK Crick Institute and will be actively and extensively involved in the Institute in the years to come. The Crick will have the largest concentration of biomedical researchers in Europe and is supported by > £1Bn in funding from Wellcome, MRC, Government and UCL, IC and Kings. **Caddick** has acted as the UCL coordinator for large parts of this initiative and **Hailes** has designed the Institute's chemistry lab space. **Caddick** is currently a member of the Crick Coordination Committee. Due to the department's input, it was recognised that the best way for the Crick Institute to engage with the strong academic chemistry community at UCL was to create dedicated facilities for chemistry at the Institute. These will provide space for around 30 researchers. The joint PhD programme funded by the Wellcome Trust in structural molecular, chemical and computational biology will form a major part of the Crick Institute. Where appropriate, secondments to the Institute will be arranged. Two Crick Research Fellows (**Christie** and **Bucar** (tenure track)) were appointed in Oct 2013. The department also anticipates the creation of one or more satellite groups closely aligned with the work that will take place at the Institute.

Chemistry has played a key role in developing the new UK Catalysis Hub at the Harwell

campus (Diamond), a £12.9M EPSRC-funded initiative to establish a strong centralised presence for catalysis research. **Catlow** has obtained substantial funding for this initiative and plays a key national role in coordinating the activities. He is also leads the development of the catalysis design centre (>£4M in funding), which will focus on developing molecular understanding of catalyst processes. **McMillan** designed the chemistry labs at Diamond and **Thornton** chaired the Scientific Advisory Committee of the Diamond Light Source (2007-9). The department will take advantage of its involvement in the hub through new grant applications, training of students/PDRAs, access to new equipment and strengthening links with Engineering and the other lead universities (Cardiff, Bath and Queens University Belfast). UCL Chemistry also has joint appointments with Diamond (**Scanlon, Beale**) that will be strengthened through the Catalysis Hub. UCL has appointed the ex-director of Diamond (Materlick) to foster stronger links with central facilities.

The department has played the lead role in the establishment of the Thomas Young Centre (TYC) - an alliance of about 80 London research groups in theoretical and computational chemistry based mainly at IC, KCL, UCL, and as of 2011 QMUL, and which has received financial support from the UCL central and MAPS Faculty funds. The National Physical Laboratory is also an affiliate member. **Catlow** was one of its founding members, **de Leeuw**, **Guo**, and **Michaelides** sit on its executive committee and since 2011 **Michaelides** has been Director. One of the core aims of the TYC is to coordinate a world-class visitor programme and programme of scientific events for researchers with an interest in the theory and simulation of materials in the London area. Since 2009 it has hosted over 230 events, 8 international workshops, and published over 160 papers. The TYC also acts as a portal for industry, government, and international research institutions, establishing funded research programmes with BP and Argonne National Laboratory. UCL has committed core funding to underpin the centre over the next REF period.

The department has taken a UK lead in establishing jointly funded PhD programs with leading international Industrial research institutes. These starting in 2013 include JAIST in Japan (4 PhD p.a. for 4 years), A*STAR in Singapore (4 PhD p.a. for 4 years) and Saudi Arabia (3 PhD start in 2014). We have also developed close links with Yale university, including meetings of staff, and four new joint research programmes where PhD students are exchanged on six-month rotation.

UCL Chemistry staff have played leading roles in industry and with the legal profession. **De Leeuw**, **Di Tommaso** and **Sankar** have all recently held RS-industry fellowships. **Sankar** played a lead role with JM in the use of advanced characterisation methods for analysing nanoparticle catalysis and in the development of a new research institute for JM in Singapore. **Cockcroft** has been an expert witness on six legal cases since 2008.

UCL chemistry staff have contributed to the development of chemistry in developing countries. **Catlow** played a leading role in establishing a materials modelling centre in South Africa (Royal Society funded, from 1996-2010) and **de Leeuw** has played a mirror role in Ghana (2011-5). The department was awarded three British Council awards in 2013 for collaborations with India. UCL chemistry staff have more than 100 international research collaborations and use central facilities in over 15 countries, especially for diffraction (NIST, Oakridge, ILL, ESRF) and large laser usage.

5.2 Contribution to the discipline

UCL chemistry staff have given over 500 invited lectures and seminars over the assessment period in over 40 different countries, including 5 lectures at Gordon Research Conferences and 25 plenary/keynote lectures – for example **Parkin, Darr** and **Sankar** at ICMAT7 in Singapore, **de Leeuw** at SEADIM 9 in Cuba, **Michaelides** at ICAMM-2012 in France and **Cora** at CHITEL 2010 in France. Staff have been on the advisory boards and organising committees for more than 50 international conferences and workshops, including the 2009 IUPAC Main Group Symposium, the 2009 International Conference on Laser Spectroscopy, the 2010 Goldschmidt Conference, a 2011 Lorentz Center workshop, a 2011 Thomas Young Centre workshop, Electrochem 2012 and the spring 2013 meeting of the European Materials Research Society. They are also editors or board members for over 25 international journals, including Dalton Trans., Tetrahedron, J. Mater. Chem., Faraday Trans. and JACS. Furthermore six staff currently hold visiting professorships.

Chemistry staff have played a leading role in examining PhD theses. They have also refereed proposals for over 30 international research councils and charities, including the US National Science Foundation (**Di Tommaso**, **Fielding**); US Department of Energy (**Kaltsoyannis, Scanlon, Thornton**); ESRF (**McMillan**, **Thornton**); Romanian Research Council (**Beale**, **Lewis**); Dutch Research Organisation (**Beale**, **Howorka**); Greek Education Ministry (**Grau-Crespo**, **Lewis**), Czech Science Foundation (**Scanlon, Howorka**); Portuguese Science Foundation (**Carmalt,**

McMillan, Caruana); Polish National Science Centre (**Kerridge**); and the US-Israel Science and Technology Foundation (**Fielding, Howorka, Parkin**). Thirty members of the department have refereed for EPSRC in the last year as college members. Staff contribute directly to UK learned societies. **Fielding** is a member of the RSC Council and 12 other staff sit on RSC committees. The department also has members who sit on SCI, IOP and IOM committees. **Parkin** has been a lead chemistry evaluator of RS Newton fellowships (since 2010) and RS equipment awards; **Kaltsoyannis** is a panel member of the RSURF (2010-13); **Catlow** chairs the Ramsay Fellowship panel (2008-13) and the chemistry committee of the Royal Society (2008-2010). **Bell** and **Lewis** are the current Chair and Secretary, respectively, of the British Zeolite Association, while **de Leeuw** is on the UK Association of Engineering Doctorates executive committee and the Royal Society International Networks panel and was the Chair of the British Association for Crystal Growth. **McMillan** (2013) co-founded the Shock Waves group of the Institute of Physics.

Chemistry department staff were awarded more than 20 national and international medals and awards during the assessment period, including **Parkin** (CGI international award, IOM^3 Kroll medal), **Thornton** (Humboldt Research Award), **Hailes** (RSC Cornforth and IChemE innovation awards) and **Powner** (ISSOL Stanley L Miller Award). Recipients of individual RSC awards since 2008 include **Michaelides** (Marlow 2010), **Catlow** (Liversidge 2009), **Slater** (Barrer 2008), **Holt** (Harrison Memorial 2008), **McMillan** (Peter Day 2011) and **Thornton** (Surface and Interfaces 2011). **De Leeuw**, **Michaelides** and **Thornton** have all won Royal Society Wolfson Research Merit Awards during the assessment period (2009, 2012, 2013). In 2008 **Clark** was awarded the Franklin-Lavoisier Prize and Medal and the Royal Society Bakerian Medal. In 2011 **Powner** was awarded the 1st prize of the Origin of Life Challenge in collaboration with Sutherland of the MRC Laboratory of Molecular Biology, Cambridge, for which they received a $150k research grant.

Chemistry staff play a major role in shaping government policy and in administration of key initiatives/evaluations. **Catlow** is the UK chemistry lead for the current REF exercise and has advised chemistry heads of department and the chemistry community on putting together their REF submissions. **Hogarth** has assessed the chemistry degree programme quality of 7 UK and international institutions as part of the RSC Committee for Accreditation and Validation since 2010. **Coveney** (high performance computing (HPC)) and **Parkin** (nanotechnology) served on UK advisory committees that were chaired by David Willetts MP. For example, in 2011 **Coveney** was appointed by the UK e-Science Institute to lead on the publication "Strategy for the UK Research Computing Ecosystem", which later fed into a key policy document published by BIS in January 2012. As a result of the Strategy and the Vision reports' specific recommendations, policy changes and shifts in priority expenditure have already been made by the Government. £165M has been earmarked to implement recommendations that improve the UK's HPC capabilities and wider e-infrastructure, and a UK E-Leadership Council (ELC), which has the responsibility to advise the UK Government on the development of the e-infrastructure and to develop a wider plan for stakeholder engagement, has been established. **Caddick** gave evidence to the UK Government Science and Technology Select Committee investigation of the "Valley of Death", gave evidence at the House of Lords Select Committee on STEM skills supply and was a member of the Government's Tech City advisory panel. **Lewis** was a member of the consultancy panel for EDEXCEL's A-level syllabus reform and the Ofqual review panel for GCSE science. **Parkin** was the lead academic on an EU science mission to SE Asia which resulted in a £10M funding call and four consortia grants. The department is also regularly represented at parliamentary science events (**Powner** won the 2012 SET for Britain gold medal) and through POST secondments of PhD students (8 during REF).

Chemistry staff play a leading role nationally in the public understanding of science through the media. This is championed by **Sella**, who has held two EPSRC Senior Media Fellowships and made over 150 appearances on TV and radio during REF, from offering expert advice on radioactive poisoning and explosions to the BBC news to children's TV. He has also written a regular monthly column in Chemistry World (>50k circulation) on the use of chemical apparatus and is an organiser of the Cheltenham Science Festival. In 2008 and 2011 the department displayed stands at the Royal Society Summer exhibition; **Evans** highlighted the role of materials in society and **Slater/Michaelides** on the chemistry of ice, including downloadable phone applications. The department's web site provides links to school presentations that have been developed at UCL some of which have had >100k downloads. These videos cover many aspects of research from the department and highlight key achievements and techniques (CVD, plasma, electrochemistry of flames).