Institution: University of Bath



Unit of Assessment: 8: Chemistry

a. Overview

The Chemistry Department at Bath (which forms the UoA submission) has shown rapid and dynamic development in the REF period. Research in Bath Chemistry combines excellence in core fundamental research with a strategic approach to leadership and participation in large interdisciplinary research initiatives targeted at solving global grand challenges. This is reflected in our research groupings (themes), which cut across traditional chemistry sub-disciplines, emphasising our flexible approach: Catalysis & Chemical Transformations; Energy Materials; Sensing & Healthcare; Structural Chemistry; Sustainable Chemical Technologies.

Our research is supported by excellent infrastructure, strategic and sustainable staff growth, a growing PhD student cohort, an expanding funding portfolio and a wide range of UK and international collaborations. <u>Research outputs</u> have increased on all metrics in the REF period. <u>Income</u> has dramatically increased, e.g. an EPSRC portfolio of more than £30M in 2013. <u>Academic staff complement</u> has grown strategically, with an emphasis both on retention and on strong recruitment. <u>Infrastructure and equipment</u> has benefitted from substantial investments and more strategic operational arrangements. We have shown a high level of <u>leadership in research</u>, with our academics leading a range of large, high profile research consortia. Our <u>PhD student</u> cohort has substantially expanded, including the successful establishment and renewal of the Doctoral Training Centre in Sustainable Chemical Technologies. <u>Strong cross-disciplinary links</u> include a high degree of involvement in major collaborative projects and programmes, with substantial funding. <u>Excellence</u> has been rewarded by a range of Fellowships and Prizes.

b. Research strategy

Our aim over this REF period has been to enhance the quality, volume and impact of our research, and we have achieved this by developing a Research Strategy for Bath Chemistry that follows a distinctive focus around:

- Strongly *interdisciplinary approaches* to current scientific challenges, with close alignment with key strategic themes at the regional, national and international levels;
- Building, developing and supporting *critical mass efforts* both within and beyond the Department and University, while encouraging and nurturing individual excellence-led approaches to fundamental research;
- Leadership, partnership and participation in a wide range of *major research consortia*, with enhanced links to collaborators both in academia and industry, in the UK and overseas.

This strategy was introduced following a review of RAE2008 outcomes, which recognised the strengths and range of expertise within the Department, and identified how opportunities offered by strategic challenges mapped onto this excellence. Research is therefore grouped within Bath Chemistry using a flexible approach building on existing expertise and critical mass, encouraging interdisciplinary links and *focused around critical scientific challenges*. This has been coupled with retention and development of the academic staff cohort, which is discussed below. Building this research concentration has benefited from a strongly collegiate approach and supportive leadership throughout the REF period.

The vast majority of researchers are associated with more than one theme, reflecting our strongly interdisciplinary and collaborative approach. Cutting across the themes, technique focuses within the Department ensure that research in Bath Chemistry is at the leading edge of new methods for characterisation, including innovative applications of these. Particular strengths exist in catalysis, computational chemistry, dynamic structural science, synthesis, electrochemistry, sensing, analytical chemistry and in using central synchrotron, neutron and laser facilities.

The *interdisciplinary research themes/groupings* in Bath Chemistry offer an integrated approach to tackling key research areas. They have been developed to deliver the strategic aims outlined above, harnessing and growing research expertise and mapping this to high priority research challenge areas. They help create an environment in which collaboration and excellence are nurtured, building a *sustainable funding portfolio* by exploiting a broad distribution of funding sources. They have also helped us in establishing leadership and being pro-active in setting



research priorities for the University and offering a focus for **growing and grouping our PhD student portfolio**. By catalysing our involvement and leadership of major research efforts, we are enabled to support the development of further investigation-led excellent research, involving a wider range of co-investigators, particularly early career researchers. Within the research themes, there are active seminar and visitor programmes, and the themes also act as a focus for targeted recruitment of new staff and investment in PhD students.

<u>Catalysis and Chemical Transformations</u>: Activities in this theme range across transition metal, organic- and bio-catalysis. Among highlight outputs is work on the widely used borrowing hydrogen methodology [*JMJ Williams*; JACS (2009), 167 citations], mechanistic studies of hydroamination [*MS Hill*; JACS (2009), 95 citations], alkoxide initiators for ring-opening polymerisation of lactides [*MG Davidson*; ChemComm (2008), 84 citations] and catalytically active metal complexes [*MK Whittlesey*; JACS 2009, 64 citations]. This area is underpinned by leadership and major funding through the EPSRC **UK Catalysis Hub** and the **Catalysis in Sensing & Health** consortium and has led to significant impact, e.g. the Case Study in catalysis.

Energy Materials: Energy materials research covers diverse experimental and computational approaches, with a focus on future sustainable and renewable energy sources, including energy storage applications. Highlight outputs in this theme include work on controllable band gap oxide materials [*AR Walsh*; Phys Rev Letts (2008), 183 citations], lithium battery materials [*MS Islam*; Chem Mater (2008), 140 citations] and nanostructured materials for energy applications [*KC Molloy*; Nano Letts (2010), 70 citations]. Substantial funding and partnerships in this area include leadership in **SUPERGEN** projects in **Energy Storage & Excitonic Solar Cells**, EPSRC **Programme Grant in Computational Materials**, and the **Grand Challenge in Nanomaterials for CO₂ storage**, and participation in the **SUPERSOLAR** consortium and the **EU ITN** in Photovoltaics.

<u>Sensing and Healthcare</u>: A rapidly growing focus area within Bath Chemistry, novel sensing research has led to high impact applications in a range of areas, from biosensors to molecular switches and thin film systems for energy conversion. Linking core synthetic chemistry to applications in Healthcare and associated technologies is key. Highlights include outputs on dye-sensitised solar cells [*LM Peter*; JACS (2008), 345 citations & JACS (2008), 134 citations] and in boronic acid sensor molecules [*TD James*; JACS (2009), 79 citations]. Substantial funding partnerships include **SUPERSOLAR**, **PV21** and **EU ITN** in cancer diagnostics, and substantial **industrial funding** and **KT partnerships**; a high degree of translation into application is reflected in three REF Impact Case Studies from this theme.

<u>Structural Chemistry</u>: The critical mass in this area has a broad-ranging approach targeting materials via synthesis, characterisation and computation. Highlights include work in post-synthetic modification of metal-organic frameworks (MOFs) [*AD Burrows*; Angew Chem (2008), 95 citations], computational approaches to functional materials structure [*MS Islam*; J Mater Chem (2008), 86 citations] and supramolecular combinatorial chemistry [*GD Pantos*; JACS (2011), 41 citations]. Substantial funding and partnerships in this area include leadership of EPSRC **Programme Grants** in **metastable state materials** and in **computational materials**, the **Dynamic Structural Science** Consortium at Harwell Research Complex and the EPSRC **Grand Challenge in Directed Assembly** of Materials.

<u>Sustainable Chemical Technologies</u>: Underpinned by the Centre for Sustainable Chemical Technologies (CSCT), research in this area also includes green chemistry, flow chemistry and water research. Key outputs include those from wastewater analysis [*B Kasprzyk-Hordern*; Water Res (2008), 210 citations & Water Res (2009), 183 citations] and sustainable chemical processes [*JL Scott*; Green Chem (2009), 99 citations]. Strategic elements include leadership of the **DTC/CDT** in SCT, the EPSRC **Sustainable Chemical Feedstocks** collaboration and the **EU ITN** in **Sewage Epidemiology**, and partnership in the EPSRC **Centre for Innovative Manufacturing** in **Continuous Manufacturing and Crystallisation** and in the **Wessex Water-Bath** collaboration.

These themes involve strong cross-disciplinary links both within the University (Chemical Engineering, Pharmacy & Pharmacology, Biology & Biochemistry, Physics) and beyond. The latter include substantial involvement in major funding initiatives including both national and international consortia. Many of these are led from Bath and are detailed in "Collaborations" below. The Department of Chemistry has led the drive within the University of Bath to move towards larger, interdisciplinary research efforts. The excellence of our staff, our awareness of the importance of such larger, often multi-institutional, research efforts and our support for staff involved in such



consortia has led to great success in placing Bath Chemistry at the centre of many high profile research programmes, with a *total project value of well over £130M* during the REF period.

Increasing *internationalisation* has been achieved, building on both the international profile of staff and University efforts in this area. Major project-led links include those associated with the Centre for Sustainable Chemical Technologies (RWTH Aachen, Ohio State, Universita' Ca Foscari Italy, Yale, Osaka, Sydney, Monash), involvement in three Marie-Curie ITN Networks, including one led from Bath Chemistry, and with the Catalysis for Sensing and the Environment initiative (ECUST, China), with many benefits including recruitment of overseas PhD students bringing a range of scholarships to Bath. University strategic links with the Universities of Sao Paolo (Brazil), Tsinghua, Zhejiang (China), Stellenbosch (South Africa), Yonsei (Korea), Ohio State (USA) provide funding for exchange visits and growing research collaborations. Bath Chemistry also has a range of *direct industrial links*, with around 50 companies, including both multi-nationals and SMEs and a dozen *direct clinical collaborations*. These involve varying levels of collaboration and funding, and are harnessed extensively to identify research targets, funding opportunities and advising our research strategy, including *via* our *Stakeholder Advisory Board* (Chair, Dr Will Barton, TSB), that provides a valuable external perspective on our current research activities and future directions.

Substantial advances are evident with respect to the research position described in RAE2008:

<u>High quality research</u>: Outputs have increased substantially both *in number and in quality* in the REF period. This can be measured by indicators such as number of papers in the highest profile journals including Science, Nature family, JACS, PNAS, Angew Chemie, Chemical Science, Chem Eur J, Chem Comm, Org Letters, PRL and by a substantial increase in citation measures. To indicate this, 50% of those in this return have published >50 papers during the REF period, and 33% of staff have h-index of >30, one of the main measures of eminence internationally.

Income: Bath Chemistry has dramatically increased its research income, typically holding and maintaining an EPSRC portfolio of *ca.* £20M, increasing in 2013 to more than £30M (in a unit of just over 30 academics), representing *an increase of around 250%* since RAE2008.

<u>Growth</u>: Academic staff complement has *grown at all levels* (25 FTE submitted to RAE2008, 33.1 to REF2014), through recognising excellence (for example, by attracting and retaining Fellowship holders) and by balanced high quality appointments at both early career and established levels. This strategy has been supported by significant investment in posts from the University including establishment of early career Fellowship positions and funding for senior appointments, including Chair positions.

Infrastructure and equipment: Substantial investments in laboratories, building improvements and major equipment purchases (*more than £4.5M* in REF period) have ensured that the research environment in the Department has continued to develop to deliver the facilities required for this rapidly expanding research effort. A Chemical Characterisation and Analysis Facility (CCAF) has been established within the University to operate, support and develop key research equipment, and new laboratories have been established for the theme areas of Sustainable Chemical Technologies, Catalysis and Sensing & Healthcare.

<u>Leadership in research</u>: Bath Chemistry academics lead a range of *large, high profile research consortia*, in the UK and internationally, with funding of *ca. £50M* in the REF period, augmented by partnership in a wide range of other major critical mass consortia, and enhanced industrial links.

<u>PhD student expansion</u>: PhD cohort has substantially expanded (~50% increase to ca. 125) in the REF period, funded through various routes including CASE awards, University and overseas scholarships, direct industrial funding, EU Training Networks and Centres for Doctoral Training, including the successful establishment of the *Doctoral Training Centre in Sustainable Chemical Technologies*. Through the growth in PhD cohort, the DTC programmes and the establishment of a Faculty Graduate School, Bath Chemistry now offers a dramatically enhanced PhD experience, in terms of research opportunities, interdisciplinary approaches and transferable skills training.

Future Strategy

Bath Chemistry has built its growth in the REF period on the establishment and support of viable, cross-disciplinary themes supporting collaborative research that encourages involvement in larger and longer projects with substantial funding. This approach has led to a sustainable model that will continue in the period beyond REF. Our themes will continue to lead to scientific excellence, high achievement and the development of impact.



Our strategy is driven by underpinning excellence, and a proven ability to apply this excellence in developing and leading further critical mass efforts, tackling current and future topics of scientific and societal relevance. An increasing emphasis on growing our international links will harness both the framework of University partnerships and Chemistry-led collaborations, and will target diversifying funding streams, for example by securing more EU/ERC funding. We are well placed to benefit from the recent establishment of the GW4 alliance, a research-led partnership between the Universities of Bath, Bristol, Cardiff and Exeter established in April 2013, which has already galvanised funding for Centres for Doctoral Training. Our strategy for growth is supported by plans to develop further Chemistry estate on the Bath campus, adding to recent substantial additional provision in this area, along with enhanced equipment provision, driven by Faculty plans for growth of the CCAF. Staff expansion will be maintained, as we achieve the targets set for Chemistry within the University Strategic Plan. Continued growth of our PhD student complement will be supported by the recent successful renewal of the DTC in Sustainable Chemical Technologies, together with ongoing partnership in four other CDTs, three of which are newly funded.

c. People, including:

i. Staffing strategy and staff development

The Bath Chemistry staffing strategy is based around a balanced approach to growing our staff profile, by *retaining, developing, rewarding and recruiting.* We have a strong record in retention of talented researchers throughout the REF period, augmented by recruitment of excellent new appointments at both established and early career levels, including Fellowship holders. This excellent recruitment has been targeted towards the strategic research Themes: *Catalysis* – *Webster* (Bath Prize Fellow), *Hintermair* (Whorrod Fellow); *Energy Materials* – *Walsh* (Whorrod Fellow, ERC & Royal Society URF, promoted to Reader), *Weller* (Chair in Energy Materials); *Sensing* – *Pantos* (Lecturer); *Structural Chemistry* – *Sartbaeva* (Royal Society URF), *Thomas* (Research Fellow & Programme Manager), *Wilson* (Chair of Physical Chemistry); *Sustainable Chemical Technologies* – *Buchard* (Whorrod Fellow), *Kasprzyk-Hordern* (Lecturer, *promoted* to Senior Lecturer), *Scott* (Senior Research Fellow & Group Leader). Our *Bath Prize Fellow* appointment was enabled by a 2012 University initiative creating new investment posts supporting areas of research strength. Prize Fellows are permanent academic staff, whose posts start with a two year dedicated research period, supported by training and career development.

We have an outstandingly successful track record in *developing Early Career Researchers* (ECRs), who benefit from our interdisciplinary approach to research and whose success (evidenced by securing external funding, producing high quality publications, winning external Fellowships and recognition) reflects well upon the nurturing environment Bath offers for mentoring and development. The support and development opportunities offered to our growing cohort of post-doctoral researchers (PDRA numbers have doubled since 2008) mirror this environment. Our strategy also reflects *retention and reward of established researchers*, reflected in rewarding excellence by internal promotions to all levels including Chair. This approach is underpinned by a positive and supportive Staff Development and Performance Review scheme, based on ambitious objective setting, identification of challenging but realistic targets, and achievement of full potential. Our research-focused workload model and strategic appointment of talented Teaching Fellows enables the workload balance of our talented researchers to be managed to best effect.

<u>Consistent development of Early Career Researchers</u>: All externally-funded Fellows (RS URF, ERC, Whorrod) have attained permanent positions in the Department, including to promoted positions (*Jones, Walsh*). This reflects our strong and pro-active approach to scientific and professional mentoring. In addition to the allocation of reduced teaching and administrative workloads, early career appointees are supported by priority allocation of PhD students, open access to analysis facilities, and by provision of appropriate laboratory space. ECRs are supported in developing their independent research but are also encouraged as key partners in larger projects in which Bath Chemistry is involved.

<u>Policy aspects</u>: The retention, development and success of our ECRs, and our actions in supporting this, reflects our implementation of the Concordat to Support the Career Development of Researchers, to which we are fully committed and which aims to provide a productive and supportive working environment for researchers. As a recognition of this the University of Bath was awarded the 'HR Excellence in Research' badge from the European Commission and has already undertaken steps to ensure that its principles are embedded across the University. As part of the



strong University-wide commitment to staff development, the Department of Chemistry also embraces the central Bath approaches to Equality and Diversity issues, rooted in a high degree of institutional emphasis on the importance of these issues and reflected in continued good practice and the provision of compulsory diversity training. In terms of gender equality, we have, through excellent recruitment and staff development, improved the gender balance within the Department, including in more senior roles (e.g. *Edler*, Head of Physical Chemistry). We actively promote equality and diversity within the Unit, operate within the framework of the University Athena Swan Bronze award and, in 2013, have applied for Departmental Athena Swan recognition.

<u>Recognising and Rewarding Excellence at all levels</u>: During the REF period, there has also been a healthy throughput of internal promotions to Chair, for *Frost, Hill, James, Marken, Whittlesey*.

<u>Visiting Professorships & Sabbatical Research Leave</u>: The Department and the University also encourage research development of staff at all levels, by supporting colleagues with these schemes. Visiting Professorships have been held in the REF period by *Bull* (China), *Burrows* (Brazil), *Edler* (Sweden), *Frost* (China), *James* (China, Japan), *Walsh* (China), *Wilson* (Adjunct, USA), while *Edler* and *I Williams* have benefitted from the award of Research Sabbaticals. Bath Chemistry also regularly attracts high profile visiting scientists, including Bond (Aus), Anslyn, Chisholm, Ozin, Power, Sessler, Stoddart (all US), Fujita, Harada, Ishihara, Maruoka (all Japan).

ii. Research students

The importance of PhD students in a successful and expanding research effort in Chemistry has been reflected in the *strong growth in PhD numbers* within Bath Chemistry in the REF period. Recruitment in each of 2011-2013 amounted to *ca.* 35 to PhD, with typically an additional 4-7 to the MRes programme. The current total PhD cohort amounts to around 125 (*cf.* ~80 at time of RAE2008, a *50% increase*, with consistent growth as follows):

Year	2008/09	2009/10	2010/11	2011/12	2012/13	2013/14
Recruited	25	26	28	34	35	36
Cohort	80	85	90	100	110	125

Our ratio of PhD students to staff (~3.5) has grown in the REF period in spite of substantial ECR recruitment and at a time of contracting sources of PhD funding from the research councils and industry. Bath Chemistry's success in this area has been aided by: the establishment of the EPSRC Doctoral Training Centre in Sustainable Chemical Technologies and partnership in other DTCs; University studentship schemes including research scholarships and the rewards scheme supporting successful large grant applications with PhD funding; increased number of overseas students (notably links with China, funding PhD students through government scholarship schemes); CASE awards and other funders including industry, government laboratories and central facilities. Internal co-funding of PhD studentships is also guaranteed where 50% external contribution has been obtained, for example from industry, This growth has been targeted in our research themes, growing critical mass PhD cohorts in key areas.

Our expanding cohort of PhD students have benefitted from the establishment of Faculty Graduate Schools, offering additional support opportunities, such as co-ordinated skills training, within a full research-focused PhD training programme that offers both scientific and personal development. coupled with valuable transferrable skills. The University also promotes a vibrant, sustainable and supportive research community, within which the Researcher Development Unit provides development opportunities, workshops and projects. It also participates in the Higher Education Academy's Postgraduate Research Experience Survey (PRES), with 94% of respondents indicating they would recommend the University. Commitment to excellence in research student supervision is emphasised by recent University Awards given for PhD supervision (Bull), and for embedding research into teaching (Lewis). Our PhD students also benefit from extensive opportunities to attend international conferences (their excellence has been rewarded with a large number of Prizes at these), supported by a Departmental bursary scheme, and from strong collaborative programmes and industrial links. This contributes to the strong destination record of our PhD graduates into positions in academic, industrial and clinical environments. Bath Chemistry PhD students also run a high profile Millennium Lecture Series, established in 2009, with lecturers including Prof. Lord Robert Winston, Prof. David Nutt, Prof. Phil Jones, Prof. Steve Jones, Prof. David Phillips and Prof. Alice Roberts.

Centres for Doctoral Training: A Doctoral Training Centre in Sustainable Chemical



Technologies (Davidson) was established in 2009 with an initial £7.5M from EPSRC; this DTC has leveraged £4.5M of additional funding to date, and has recently had its funding renewed to 2022/23, with a further award totalling £7M. It offers a four-year integrated PhD programme in Sustainable Chemical Technologies (coordinated by Scott) and is training >140 PhD students in ten cohorts beginning in October 2009, including a commitment of 30 University funded PhD positions over the lifetime of the DTC. The DTC, one of only a handful awarded to UK Chemistry Departments in the initial 2008/9 round, has established substantial international and industrial collaborations. The DTC cohort model, which cuts across conventional discipline boundaries, has provided a welcome additional option to the traditional group-based PhD approach, giving many benefits including enhanced recruitment and monitoring of student progress and achievement, all of which are more efficient for cohorts than individuals. The establishment of the DTC has also had significant benefits across the whole PhD cohort, with good practice and the evident dynamic approach to postgraduate training being invigorating for all Bath doctoral students; it also supports a key aim of the University Research Strategy to strengthen the research base by increasing postgraduate research student numbers. Bath Chemistry (Wilson) is also a partner in the seveninstitution, multi-disciplinary industry-facing DTC established as part of the EPSRC Continuous Manufacturing and Crystallisation Centre (in addition to Bath-based PhD students, this involves a mobile 15-strong cohort who visit Bath for two periods of consolidated training). We are also partner in three further newly-funded Centres for Doctoral Training: CDT in Catalysis (Cardiff, Bristol, Bath), CDT in Water Informatics (Exeter, Bristol, Bath, Cardiff) and the CDT in New & Sustainable Photovoltaics (seven partners including Bath).

d. Income, infrastructure and facilities

The REF period has been characterised by *strong growth in research funding* within Bath Chemistry, including substantial involvement in larger, longer projects, offering leadership of and involvement in critical mass efforts and a more strategically-managed approach to research planning and partnership. This is underpinned by substantial investments in equipment, a coherent approach to the management of chemical analysis facilities, an extended technical support framework and an expansion of the Department beyond its previous estate, to accommodate research growth. Bath Chemistry provides a vibrant, highly active environment, within a rapidly growing research effort, with a wide-ranging and diverse programme of seminars, workshops, academic, international and industrial visitors, workshops and industrial forums, including sandpit events led by application-focused problems, e.g. Sustainable Water in 2011.

Strong and consistently growing funding: Over the REF period, research funding held within the Department has increased by **a factor of more than 2.5**. In terms of grant awards, EPSRC funding has been consistently at or above the £20M level since 2010 (increasing from *ca.* £12M in 2007), reaching a current value of **more than £30M** in 2013. While this includes elements of funding for consortia, and National Hub funding (detailed below), the resource held for direct spend within Bath Chemistry in 2013 is £20.1M, the highest for any Department within the University. Bath is among the highest earning UK Chemistry Departments for EPSRC income, and regularly highest per academic FTE, currently approaching £1M. This reflects the fact that the majority of research active staff hold current PI grants.

<u>Wide range of funding sources</u>: In addition to healthy levels of EPSRC funding, *diversity of funding streams* has been increasingly evident in the REF period, with significant research income from the EU, BBSRC, MRC, TSB, Industry, Wellcome Trust and others. EU funding led by Bath amounts to more than €10M including FP7 project funding, ERC fellowship awards at both starter and consolidator level, and Marie Curie Training Networks, including a major new €4M+ network (SEWPROF; see below) led from Bath Chemistry, funded in 2012.

<u>Endowment income</u>: In 2010, Bath Chemistry secured the then *largest individual endowment* ever for the University, of £1M, to establish an endowed chair (Whorrod Chair in Sustainable Chemical Technologies, held by DTC Director *Davidson*) and a Fellowship Scheme for early career researchers. Four five-year fellowships in sustainable chemical technologies have been awarded to date, three in Chemistry (*Buchard, Hintermair, Walsh*), with others to be awarded in the period to 2015. The CSCT has leveraged a further £2.8M based on this endowment income.

<u>Infrastructure</u>: Bath Chemistry is well-equipped to support our growing research effort. As expected for a leading Chemistry Department, we have access to state-of-the-art facilities and equipment. Building upon our grant income successes, there has been significant recent



expansion in estate and equipment. We benefit from:

- Excellent, state-of-the-art provision in modern buildings (constructed 2001 and 2003);
- Fit-for-purpose laboratories, with modern design and infrastructure;
- Recent expansion of estate occupied by Chemistry research to accommodate growth, offering 300 m² of additional well-appointed research space in building 5-West on the Bath campus, which includes fully refurbished laboratories equipped with fume hoods and analytical equipment, accommodating key critical mass research units in Sustainable Chemical Technologies, Catalysis and Sensing & Healthcare;
- Excellent equipment to support research key facilities for Chemistry research include: NMR (x 5), Mass Spectrometry (x 5), X-Ray Diffraction (x 7), together with full provision of spectroscopic, thermal and computational capabilities. High level dedicated scientific support is provided by experts in Mass Spectrometry, NMR and X-ray diffraction and glassblowing.
- These are integrated into a *Chemical Characterisation & Analysis Facility* (CCAF) across the Faculty, led from Chemistry, providing integrated access to research facilities and a strategic approach to operation and development. A parallel, complementary, Microscopy Analysis Service (MAS) is also established.
- The recent integration of a Faculty Technical team of 30 staff covers all elements of technical support; the enhanced support available is recognition of the need of the growing Chemistry research effort for more resource.

Investment in equipment and infrastructure

The expansion of infrastructure and facilities to support the growing Bath Chemistry research effort has been enabled by substantial internal investments in the REF period, totalling £4.5M. These have included enhancement of Mass Spectrometry facilities (£350k), NMR (£150k), X-ray diffraction (£450k), Circular Dichroism (£50k) and an EPSRC-funded minor equipment award (£600k). Infrastructure improvements have included the construction of Structural Chemistry and Crystallisation laboratories (£150k), analytical equipment laboratory (£100k), Microbiological laboratories (£50k), a dedicated Hub for the Centre for Sustainable Chemical Technologies (£0.75M) and the provision of additional bespoke Chemistry research space on campus (£1.8M).

Major involvement in central facilities

Researchers in Bath also benefit from substantial exploitation of *central facilities* (including X-ray, neutron and lasers) provided through STFC and others. At the strategic level, Bath Chemistry academics are heavily involved in £multi-million EPSRC-funded groups at the Research Complex at Harwell (RCaH), including leadership of the Dynamic Structural Science consortium (*Raithby*) and the UK Catalysis Hub (*Davidson*) and partnership in the Imaging (*Pascu*) grouping at this new central facility hub for physical sciences research. Our significant footprint at the RCaH offers substantial laboratory space and access to further excellent infrastructure and equipment. Bath academics also gain substantial peer-reviewed access to Diamond, ISIS, ESRF, ILL and other facilities, notably in the US, with >500 days allocated to Bath PIs (principally *Edler, Mahon, Pascu, Raithby, Thomas, Wilson*) in the REF period (with *total value well over £5M*). This enhances research quality and capability, with a range of Bath research also selected as Facility Highlights. Involvement at these facilities also includes more strategic and senior roles, including Chairing the Scientific Council of the ILL, Grenoble (*Wilson*), and involvement in a range of instrument development, strategic and peer review roles at the various facilities (*Edler, Raithby, Wilson*).

e. Collaboration or contribution to the discipline or research base

Bath Chemistry has a strong record of collaboration with fellow academics, with industry and, increasingly, with clinicians. Levels of collaboration have accelerated during the REF period, with a very high level of involvement in major funded collaborations, including extensive interdisciplinary partnerships. This has involved Bath Chemistry academics both in leading such initiatives and as partners in consortia led from elsewhere, with a total value of more than £130M.

Leadership of major funding and consortium initiatives include the following:

- Centre for Sustainable Chemical Technologies (including Doctoral Training Centre; EPSRC, Industry, Benefactors; >£19M including follow-on and leveraged funding; *Davidson*)
- SUPERGEN Energy Storage Consortium (8 HEI; £5M; EPSRC, Industry; Islam);
- UK Catalysis Hub (4 HEI; £3M; EPSRC, part of £13M National Hub; Davidson)
- SUPERGEN Excitonic Solar Cell Consortium (5 HEI; £4.5M; EPSRC, Industry; Peter)



- Programme Grant in Metastable State Materials (£3.5M; EPSRC; Raithby, Wilson)
- Programme Grant in Computational Energy Materials (3 HEI; £3.3M; EPSRC; Islam)
- Sustainable Chemical Feedstocks consortium (3 HEIs; £2.7M; EPSRC; Davidson)
- **SEWPROF** International Network on Sewage Epidemiology (11 academic, 5 industry partners; **€4.2M**; EU Marie-Curie ITN; *Kasprzyk-Hordern*)
- Dynamic Structural Science Consortium RCaH (7 HEI; £1.7M EPSRC; Raithby)
- Nano Grand Challenge Project CO₂ Reduction (3 HEIs; £1.6M; EPSRC; Marken)
- CCP5 Computational Chemistry Project (£500k; EPSRC; Parker),
- Grand Challenge Network in Directed Assembly (8 HEI Theme leaders; 600 Network members; £800k; EPSRC; *Raithby*)

plus others including **CASE** – Catalysis for Sensing and the Environment (3 HEIs, UK-China, including largest ever Bath KTP award of **£350k** with Quotient Diagnostics; *James, Bull*), **CMAC-SPIRIT** – SFC Demand-Led Knowledge Exchange Scheme (5 HEI, **£1.2M** SFC, Industry; *Wilson*).

Participation and Partnership in major funding and consortium initiatives:

- CMAC EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation (7 HEI; >£50M; EPSRC and Industry; Node led from Bath; Wilson)
- Innovation and Knowledge Centre (IKC) SPECIFIC, Sustainable Product Engineering of Industrial Coatings (6 HEI; EPSRC, TSB, Industry; £16M; led from Swansea; *Davidson*)
- RCaH Catalytic Science (9 HEI; £1.6M; EPSRC; led from UCL; Davidson)
- SUPERGEN PV21 Photovoltaics (£8M; led from Durham; Islam, Marken, Peter, Molloy)
- SUPERSOLAR Solar Energy Hub (£4M; led from Loughborough; Hill, Walsh)
- **PVTEAM** EPSRC Solar Cell Consortium (£2.5M; led from Bristol; *Molloy, Peter, Walsh*)
- **DESTINY** Dye Sensitised Solar Cell Consortium (EU Marie-Curie ITN; €4M; led from Bath Physics; *Cameron, Walsh*)
- Wessex Water/Bath partnership in Water Research; (Wessex Water; £3M; led from Bath Chemical Engineering; *Kasprzyk-Hordern*)
- **PROSENSE,** EU Marie-Curie ITN on Cancer Diagnostics (€4M; led from Bath Chemical Engineering; *Frost, Pascu*)
- EU FP7 Project EMBEK1 Development and analysis of polymer based multifunctional bactericidal materials (6 HEI, ca. €1M; led from MPI Mainz; *Jenkins*)
- EU FP7 Project Bacteriosafe Active Wound Dressing (7 HEI, ca. €1M; Mainz; Jenkins)
- ERI ALISTORE Advanced Lithium Energy Storage Systems (ca. €1M; Islam)

plus others including **RCaH Sensing** (led from Oxford; *Pascu)*, EU **COST Action D40** – Innovative Catalysis (*Frost*) and **CM083** – Foldamers (*Bull*); three new **Centres for Doctoral Training**, as noted above.

<u>Non-academic links and collaboration – Industrial and Clinical partnership</u>: The substantial industrial links of Bath Chemistry researchers are noted in the Impact Statement. We hold funding from, or collaboration with, more than 50 partner industries, while research and clinical testing links are established with 12 collaborating clinical units. These have had major benefits in developing our research portfolio, and have helped form our strategy of major research collaborations, often academic / industrial / clinical, ensuring we have an appropriate focus on developing excellent basic research solutions to real-world problems, and creating an ideal environment for building sustainable approaches to future research funding. In addition to individual industrial advisory panels on our large research projects, our strong links to industrial researchers have recently been enhanced by the establishment of a **Stakeholder Advisory Board** for Bath Chemistry.

Engagement with Funders and Policymakers: The vast majority of Bath Chemistry researchers are EPSRC Peer Review College members and regular referees. Further involvement with EPSRC at a high level include: Chairing and Membership of Prioritisation Panels (*Various*); Membership of TOP and its successor Strategic Advisory Network (*Raithby*); Transformative Research Strategic Advisory Group, Manufacturing the Future SAT, Grand Challenge Advisory Group & Directing IDEAS Factories (*Wilson*); Chairing Management Advisory Panel for National Mass Spectrometry Service (*J Williams*); Management Advisory Panel for Chemical Database Service (*Raithby*); Review of Materials Science (*Islam*).

High level involvement with other funders and policymakers includes: DEFRA Consultancy (*Davidson*); Preparing CS3 Sustainable Materials White Paper (*Davidson*); CIKTN Sustainable



Technology Advisory Board (*Scott*); Chair of STFC PALS Committee, membership of STFC Science Board and Chair of Scientific Council of the Institut Laue-Langevin, Grenoble (*Wilson*); Cambridge Crystallographic Data Centre Board of Governors (*Raithby*); REF2014 Chemistry Subpanel (*Davidson*). Bath Chemistry academics are also significantly engaged with the newly established Bath Institute for Policy Studies, augmenting our strategic approach.

Engagement with learned bodies, Editorial Board Membership: Chair, SCI Young Chemists Panel (*Carbery*); Diamond User Comm., ESS Scientific Advisory Panel (*Edler*); RSC Dalton Division Council (*Davidson, Hill*), Chair, RSC Main Group Chemistry Group (*Hill*); Council, Int. Soc. Solid State Ionics, Executive Comm., RSC Materials Chemistry Division, RSC Energy Storage Steering Group (*Islam*); Secretary, RSC Electrochemistry Group (*Marken*); President, British Crystallographic Association, IUCr Comm., Struct. Chem. (*Raithby*); RSC Solid State Group Comm. (*Walsh*); Chair, RSC Solid-State Group (*Weller*); RSC Phys. Org. Chem. Group Comm., IUPAC Sub-Comm., Struct. & Mech. Chemistry, UK Rep, EuCheMS Div. Computational Chemistry (*I Williams*); RSC Perkin Council (*J Williams*); IoP Membership & Qualifications Board (*Wilson*); Royal Society Committees (*Pascu, Islam*). Bath academics are also heavily engaged in a range of Editorial Boards, and as Editor (e.g. *Peter*, Editor-in-Chief, RSC Energy & Environment Series) and Guest Editor roles (e.g. *James*, Chem Comm), with RSC, ACS and other major publishers. Bath Chemists are also lead authors on two current world-leading Chemistry textbooks – **Chemistry³** (general text: *Burrows*; OUP) and **Inorganic Chemistry** ("Atkins" 6th Ed.: *Weller*, OUP).

Conference Organisation & Participation

Main Organisers, Conference Chair: CASE'08, Bath; CASH'11 Bath, 200 participants; MASC-11, 145 participants, Bath, 2011; 21st IUPAC International Conference on Physical Organic Chemistry, Durham, 2012; Electrochemistry 2011 (250 participants), Bath, 2011; RSC Main Group Chemistry (Annually); Frontiers in Modelling Optical Excitations 2013 (Royal Society). Bath Chemists are also widely involved as Session organisers and in Advisory/Programme Board membership at a range of National and International Conferences – more than 40 in the REF period.

Bath Chemists are regular Invited Keynote Lecturers at International Conferences, with a total of more than 50 of these, including MRS Fall, 2008, USA (Islam); XXIII International Congress on Organometallic Chemistry, France, 2008 (Whittlesey); EuCheMS-12 International Conference on Chemistry and the Environment, Sweden, 2009 (Kasprzyk-Hordern); European Solid-State Conference, Germany, 2009 (Weller); Pacific Polymer Conference, Australia, 2009 (Jenkins); Asian Chemical Congress, China, 2009 (Bull, James); MRS Photovoltaic Conference, USA, 2010 (Walsh); EUCHEMS-3, 2010, Germany (Whittlesey); Pacifichem, USA, 2010 (Bull, Burrows, Hill, James); CGOM, Crystal Growth of Organic Materials, Ireland, 2012 (Wilson); European MRS, France, 2012 (Islam); MRS Annual Meeting, USA, 2012 (Walsh); ACS National Meeting, 2012 (Whittlesey, J Williams); Int. Conf. on Physical Organic Chemistry, 2012 (J Williams); MRS Boston, 2012 (Islam); 16th Congress of the International Society for Burn Injuries (ISBI) 2012 (Jenkins); 26th Conf. European Colloid & Interface Society, Sweden, 2012 (Edler); E-MRS, Strasbourg, 2013 (Weller); ISACS10: Japan, 2013 (James); RSC Inclusion Compounds, 2013 (Raithby). Bath Chemists have delivered a total of more than 300 conference invited talks in the REF period. Recognition of Excellence – Fellowships: across the themes, in the REF period our academics have won or held Fellowships at all levels, including Royal Society URF (Pascu, Sartbaeva, Walsh), RCUK (Cameron, Jones), ERC Starter (Walsh), ERC Consolidator (Pascu), Whorrod (Walsh, Buchard, Hintermair), Industrial (Frost, James), EPSRC Senior (Raithby), EPSRC Dream (J Williams), Royal Society Wolfson Merit Awards (Islam, J Williams) and Bath Prize (Webster). Evidence of Excellence: our staff are regular recipients of external Prizes & Awards for research excellence, including: RSC Structural Chemistry 2008 (Raithby); RSC Francis Bacon Medal 2008 (Islam); RSC Hugo Muller 2008 (Weller); Elsevier Journal Award 2008 (Kasprzyk-Hordern); RSC Theophilius Redwood 2009 (Marken); RSC Parkin Lecturer 2009 (Wilson), BCA Cruickshank 2009 (Thomas); ARC International Research Fellowship 2010 (Bull); RSC Homogeneous Catalysis 2011 (J Williams); Royal Society Wolfson Merit 2011 (J Williams); Royal Phil. Soc. Glasgow Thomas Graham Medal 2011 (Wilson): RSC Materials Chemistry Lecturer 2011/12 (Islam): BCA Parkin Prize Lecture 2012 (Thomas); Thieme Journal Award 2012 (Lewis); Global Young Academy Member 2012 (Walsh), RSC Harrison-Meldola Medal 2013 (Walsh), RSC Sustainable Chemistry 2013 (Islam), Daiwa Adrian, Japan, 2013 (James); Royal Society Wolfson Merit 2013 (Islam).