Institution: EaStCHEM: The University of Edinburgh / University of St Andrews

Unit of Assessment: B8 Chemistry

a. Overview

EaStCHEM, the joint Chemistry Research School of the Universities of Edinburgh and St Andrews generates a large volume of internationally-leading, high-impact research, supported by an environment that:

- Integrates its recruitment activities to create an intellectually stimulating, scientifically vibrant and collegial environment whilst actively developing research leaders of the future
- Has grown critical mass by strategic investment in key research areas of international importance while retaining breadth across the chemical sciences;
- Pools and invests in research facilities and dedicated research officers to maximise productivity;
- Provides excellence in training and supervision in a world-leading scientific environment
- Is outwardly looking across the disciplines, industry, and society, providing leadership and solutions to current and future grand challenges.

EaStCHEM's research is strategically organised into four flexible, forward- and outward-looking themes:

- The Chemistry/Biology Interface
- Molecular Synthesis and Catalysis
- Materials Chemistry
- Experimental and Theoretical Chemical Physics

We have a critical mass of 82 research group leaders (80.6 FTEs) and are submitting more than 97 % of eligible staff to REF2014, excepting only the Head of College/RSC president and Dean for Quality Assurance: our expertise spans the entire spectrum of chemistry. The research themes are further enhanced by multidisciplinary centres that promote collaboration with academic and industrial colleagues in physics, engineering, environmental sciences, geology, biology and medicine as well as targeting impact in the commercial and policy-making sectors.

The continued success and sustainability of EaStCHEM has been augmented by major upgrades and investments in infrastructure, equipment and people. Our pooling model has been highlighted as best practice by both the 2009 EPSRC International Review of Chemistry and The External Review of Chemistry Pooling by the Scottish Funding Council, 2009.

b. Research strategy

EaStCHEM *performs world-leading chemistry research with global impact while developing the next generation of international research chemists by:*

- Strategically investing in research activity of the highest international calibre in major areas of existing strength, whilst nurturing emerging and complementary areas;
- Empowering our academics and researchers to perform at the highest possible level through provision of a supportive environment with excellent technical and administrative support;
- Providing world-class infrastructure and supportive open-door collaborative opportunities to promote our activities.

EaStCHEM's research strategy has been highly successful in enhancing the quality of our research as measured in metric, reputational, and impact terms with substantial improvement across all areas since RAE08 (see Figure 1).

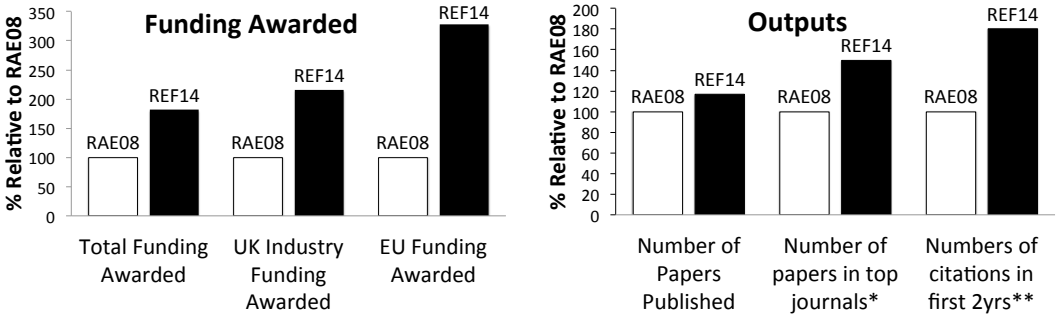

Figure. 1. EaStCHEM at a Glance. *Comparison of performance metrics during the REF2014 period with those from RAE08. Performance is normalised to RAE08. Notes: Funding is as % of value. * Top journals are defined as Science/Nature and associated journals, JACS and Angew. Chemie. ** Total citations in the first two years after publication (source ISI WoK, Aug. 2013).*

Key highlights of EaStCHEM's performance in the REF2014 period are.

- Twenty new research leaders have been appointed since RAE08, including 4 professors and 14 Early Career Researchers (ECRs). There have been 463 PhD starts and 265 PDRAs appointed during the REF2014 period.
- The number of papers in top journals (Fig. 1) has risen by 60% compared with RAE08. The total number of citations within 2 years after publication has almost doubled, from 7700 in RAE08 to 14000 in REF2014.
- Funding award value has increased by more than 80%, with UK industrial funding doubling and EU funding more than tripling. Research awards announced for 2012/13 are in excess of £42 M (cf £12 M in 2007/08). Note that this is funding announced during the REF period and is not the same as research funding spent reported in REF4.
- The number of competitive grants in excess of £1 M has gone up from 6 during RAE08 to 38 during REF2014.
- Seven ERC Advanced Investigator grants (Attfield, Bradley, Leigh, Lloyd-Jones, Naismith, Nolan, O'Hagan), and four ERC Starter/Consolidator Grants (Cockroft, Lam, Michel, Smith) have been awarded to researchers in EaStCHEM during the REF2014 period. Two more ERC grants (Ashbrook and Goss, not included in graph) have been awarded in Nov 2013.
- Large, competitive, EaStCHEM-led, multidisciplinary grants have been secured for specific infrastructure and centres to develop leading science. These include;
  - £11.5 M (EPSRC at 100% FEC, PI: Bradley) for Molecular Sensing and Imaging,
  - £6.2 M (Wellcome Trust, £5 M, Scottish Funding Council £1.2 M, PI: Naismith) for the EaStCHEM-led Biomedical Sciences Research Centre.
- Fellows of national academies have been elected worldwide, include two new Fellows of the Royal Society (ECampbell, Lloyd-Jones), nine new Fellows of the Royal Society of Edinburgh, one Fellow of the Learned Society of Wales and one Fellow of the Academy of Medical Sciences. Internationally, EaStCHEM also has Elected Fellows to the Royal Society of Canada, the Royal Swedish Academy of Sciences and the European Academy of Science.
- Our Equality and Diversity policies have been recognised with Athena Swan Gold and Bronze Awards.

International Benchmarking. A central theme of our strategy has been to develop our research capabilities to compete on a global level, therefore international comparisons offer an important measure of the successful implementation of our strategy. Thus, the EaStCHEM *h*-index is 65 for papers published in the REF2014 period (up from 53 for RAE08), a metric that places EaStCHEM in an elite group of European Chemistry units (e.g. ETH has an *h*-index of 60 for the same period with similar sized output of just less than 3000 papers; TU Munich has an *h*-index of 56 with a slightly smaller output). During REF2014 we published 305 papers in the top journals (defined in Fig. 1), which is comparable with high-quality Chemistry departments of about the same size including ETH (293 papers), TU Munich (161) and UCLA (351 papers with a larger number of staff [~90]). All citation data are from ISI WOK, Aug. 2013.

Members of EaStCHEM have also received 11 international prizes with highlights that include the Akzo Nobel Science Award (2012) and the Wagener Award of the European Electrochemistry Society (2011) to Bruce; O'Hagan was awarded the American Chemical Society (ACS) Fluorine Chemistry Prize (2012). 11 PhDs and PDRAs have won prestigious international early career/postdoctoral fellowships including Fulbright and Presidential fellowships in the USA, JSPS and Marie Curie IEFs.

EaStCHEM's Investment Strategy is continually to look for opportunities to improve our provision of state-of-the-art infrastructure and facilities. During REF2014 2500 m^2 have been renovated and 3000 m^2 of new space constructed with University investment of £17 M. An important part of this strategy to lever University investment with competitively won external investment. Highlights here include (i) the £10 M investment in Chemical Biology in addition to £6.2 M external funds won from the Wellcome Trust/SFC (PI: Naismith), (ii) investment of almost £2 M to support the EPSRC Core Capability and Advanced Materials bids (total funding from EPSRC to EaStCHEM ~£4 M) with EaStCHEM finishing top of the priority lists for both of these EPSRC competitions.

EaStCHEM's Knowledge Transfer (KT) strategy was a priority area in EaStCHEM's RAE08 future planning section. This has been delivered by investment in three in-house Business Development Executives (BDEs) who actively promote commercialisation, joint industrial studentships and consultancy activities. These BDE activities have led to significantly enhanced activity in this area, with the award of significant translational grants such as proof of concept (8 PIs, > £2m total) and RCUK follow on funding (5 PIs, > £4M) arising from our research.

Strategy development and delivery is led by a committee of a director, a deputy director and two research leaders (currently Woollins, ECampbell, Arnold and Morris) with staggered, 5-year tenure periods and an International Steering Group that currently consists of a senior UK academic, the CSO of a highly successful UK company and two overseas academics. Regular 'away days' involve all academic staff in the development of research strategy.

Current Research Position and Future Strategy. Our research strategy, in line with that outlined in the RAE08 documentation, is to have four strategically aligned research themes that provide support for excellent individuals where critical mass can enhance, promote and accelerate their research. Staff members participate flexibly in one or more themes as appropriate.

The Chemistry/Biology Interface.

Research within this theme encompasses the study of protein structure and function, mechanistic enzymology, proteomics, biocatalysis and biotransformations, the application of biophysical techniques to complex biological systems, and the application of chemical tools, including high-throughput approaches, to answer and address important biomedical questions and needs. Key strengths include (i) Structural and molecular biology (Barlow, Bode, Botting, Daff, Dryden, Lovett, Mitchell, Mowat, Naismith, Uhrin) focused on understanding how proteins control their function in problems ranging from cancer to microbial infection, (ii) Total synthesis, and the application of biologically active molecules and materials (Bradley, CCampbell, Campopiano, Florence, Goss, Hulme, Lawrence, Lilienkampf, Mount, Nudelman, O'Hagan, Smith, Westwood). (iii) The application of the tools of chemistry to control stem cell fate and cellular regeneration, and in the area of optical and electrochemical molecular sensing and imaging (Bradley, CCampbell, Lilienkampf, Mount, Vendrell).

The research activities include three complementary and multidisciplinary research consortia: the Biomedical Sciences Research Complex (BSRC, director: Naismith); the Centre for Translational and Chemical Biology (CTCB, co-director Barlow) and the Interdisciplinary Research Collaboration (IRC) in Molecular Sensing and Imaging (PI: Bradley), conceived to enhance synergistic interactions between chemistry, biology, medicine, engineering, and physics. We view this cross-disciplinary focus as pivotal for our future growth. The foundation of the centres combined with strategic recruitments (Bode, Gloster, Goss, Lawrence, Lilienkampf, Lovett, Nudelman) has provided critical mass of activities within these key areas, as highlighted for development in RAE08.

Research Highlights since 2008
Selected highlights include a new model of an ion channel gating mechanism (Naismith, *Science* 2008), palladium-mediated intracellular chemistry (Bradley, *Nature Chem* 2011) and protein-directed dynamic chemistry (Campopiano, *Nature Chem* 2010). Naismith determined the structure of a RING E3 ligase bound to ubiquitin-loaded E2 (*Nature* 2012). Barlow and Uhrin determined the structure of complement factor H (CCPs 19-20) bound to C3d (*Nature Struct. Bio* 2011).

Molecular synthesis and catalysis.
Research covers a wide range of synthetic organic and inorganic chemistry, with a significant strength in catalysis. Recent senior (Lloyd-Jones, Nolan, Vogt) and junior (Cazin, Cowley, Inglis, Kay, Schneider, Shaver, Thomas) appointments have particularly strengthened activities related to the synthesis and reactivity of organic and inorganic compounds (Arnold, Cowley, Kilian, Lloyd-Jones, Love, Woollins) in homogeneous catalysis (Cazin, Clarke, Cole-Hamilton, Kamer, Nolan, Schneider, Shaver, Thomas, Vogt, Westwood), to complement activities in organocatalysis (Philp, Smith) and supramolecular chemistry (Cockroft, Lusby). Structure-informed research on, and dynamic approaches to, large single molecule magnets, luminescent molecules, and functional nanomolecules (Brechin, Kay, Slawin, Inglis) have also advanced through recent appointments.

Major research successes during REF2014 in homogenous and organo-catalysis have resulted in the recent EPSRC Catalysis Critical Mass (£3 M), and EU ITN (€1.5 M) awards, generating a catalysis hub for the North of the UK. This is enhanced through intellectual interaction with SASOL Technology UK. Next generation refrigerants based on molecular clusters are being integrated into chips as cooling platforms for analytical and astronomical cryo-sensors, and a long-term replacement for dwindling resources of ^{3}He.

Research Highlights since 2008
More than 100 papers have been published in the top journals (as defined above) during the REF2014 period. Major contributions have been made to the general synthesis of biaryls using gold catalysts (Lloyd-Jones, *Science* 2012) and to the chemistry of f-block elements, including the first covalent bond formation of the uranyl oxo group (Arnold, Love, *Nature* 2008). Other highlights include the delineation of design principles for magnetic cryocooling (Brechin, *ACIE* 2012) and the development of efficient and general NHC-supported catalysts for hydrocarbon transformations (Nolan, *JACS* 2009).

Materials Chemistry.
The membership of the materials chemistry theme includes a wide range of expertise with particular emphasis on energy materials including battery and fuel cell materials and devices (Bruce, Irvine, Baker), porous solids for catalysis, gas storage and medicine (Morris, Wright), the synthesis and characterisation of electronic and solar materials (Attfield, Lightfoot, FMorrison, de Vries, Robertson, Zysman-Colman), the study of materials at extreme pressures and temperatures (Moggach, Parsons, Pulham) and advanced characterisation (Ashbrook, Zhou).

The strength of the materials chemistry theme was recognised in the RAE08 submission, and our REF2014 strategy has been to enhance the capability of this group through targeted investment in infrastructure and facilities (see section d). A key target stated in RAE08 was the development of new functional materials of relevance to industry – the success of this goal is exemplified by vastly increased funding from UK and overseas industry of almost £4 M. The impact of this group is also clear from the 3 impact case studies listed in REF3b, which includes two new start-up companies and significant impact on technology used in energy technologies and policy. The theme includes research infrastructure that is unique in the UK, such as the Centre for Science under Extreme Conditions that allows the study of fundamental chemistry under conditions of extreme temperature, pressure and radiation.

Research Highlights since 2008
Selected highlights include the development of reversible and higher-rate lithium-air battery technology (Bruce, *Science* 2012), which offers a step change in the energy capacity of Li-batteries. Attfield (*Nature* 2012) provided fundamental evidence for charge order and distortions that have major implications for the properties of metal oxides. Unusual chemistries of porous metal-organic frameworks have been developed to provide ultra-selective adsorption properties of toxic gases (Morris and Zhou, *Nature Chem*. 2009), and Irvine (*Nature Mater*. 2012) has

developed metal oxide chemistry to produce efficient photocatalysts.

Experimental and Theoretical Chemical Physics.

The strengths of this theme include complementary experimental and theoretical activities in the development of advanced analytical and modelling techniques (Botting, Buehl, Langridge-Smith, Michel, CMorrison, van Mourik), ultra-fast optical spectroscopies (ECampbell, Jones, Kirrander), laser-induced nucleation (Alexander), surface chemistry (Buck, Baddeley, Haehner, Richardson, Schaub), atmospheric chemistry (Heal), and complex fluid dynamics (Camp).

A new ultrafast spectroscopy laboratory, as highlighted for development in RAE08, was supported with £1.5 M of University funding, and Kirrander was recruited to add theoretical expertise in time-resolved dynamics and spectroscopy. Other new appointments (Buehl, Michel), also in line with plans presented in RAE08, further expanded theoretical research to complement and add critical mass to strong experimental activities within NMR technique development, drug development and homogeneous catalysis. This area is strongly supported by advanced experimental infrastructure and expertise within SCISS (the Scottish Centre for Interdisciplinary Surface Spectroscopy) and COSMIC (the Collaborative Optical Spectroscopy, Micromanipulation and Imaging Centre) as well as the facilities available within EaStCHEM's research computing facility and HECToR, the national high–performance computing service for the UK academic community.

Research Highlights since 2008

Major contributions include a flexible method for creating ordered structures with nanometre precision by functionalising hydrogen-bonded surfaces (Buck, *Nature* 2008), the use of laser-induced nucleation to give precise spatial control over crystal formation in gels (Alexander, *JACS* 2009), the demonstration that carbon nanoclusters are precursors to the growth of epitaxial graphene (Schaub, *Nano Lett.* 2011), and the use of femtosecond photoelectron spectroscopy to probe the properties of exotic electronically excited states of fullerenes (ECampbell, *PRL* 2012).

Beyond REF2014 - Future Strategy for Leading Cross-disciplinary Research.

The theme covering the Chemistry/Biology interface is well placed to continue its already highly successful and high-profile engagement with the translational science agenda and we will further strengthen interactions with Medicine and Engineering specifically for the development of new functional materials and sensing systems for application in regenerative and clinical medicine, led by EaStCHEM PIs within the MRC Centre for Inflammation Research (Bradley, CCampbell, Vendrell) and the Scottish Centre for Regenerative Medicine (Bradley, Nudelman). The recent major funding awards to the EaStCHEM-led Biomedical Sciences Research Complex and Interdisciplinary Research Collaboration in Molecular Sensing and Imaging (both described above), plus others such as the EPSRC-funded programme grant IMPACT (PI Murray (Engineering) with Bradley, Mount) for cancer sensors offer a roadmap for the development of the theme, with activities strengthened by recent new appointments and infrastructure investment in areas such as high field NMR and mass spectrometry of complex systems.

We will ensure that the significant investment into the synthesis and catalysis theme made during the REF2014 period in new staff, infrastructure and equipment (see section d) will lead to a further step change in activity. New appointments offer significant opportunities to develop new areas in molecular nanotechnology as well as developing existing strengths in synthetic molecular chemistry and catalysis. We will leverage funding from new areas through more collaborative projects both within and outwith EaStCHEM: Kamer is leading a Global Engagement partnership in catalysis with Dutch universities; a new joint EaStCHEM/TU Munich catalysis PhD programme (Arnold, Love), is being extended to Singapore universities. Functional building-block approaches to combine optical and magnetic properties in new materials are being developed for photonic and nanotechnological developments.

Within the area of theoretical chemistry we will develop methodology to predict and interpret a new generation of experimental studies of fundamental electron dynamics and time-resolved structural techniques, making us key players in international collaborations based at x-ray Free Electron Laser facilities e.g. DESY, Hamburg and LCLS, Stanford. Fundamental and applied experimental nanocarbon activities will be enhanced with more coordinated collaboration within EaStCHEM and with related disciplines (Engineering and Medicine) to boost funding opportunities

and develop new materials and devices for applications within medicine and organic electronics.

Investment is planned in several areas of the materials theme that link them to other key strengths. The appointment of McKeown from 01/01/14 opens up opportunities in organic materials that complement our existing strengths, especially in the development of carbon capture and other gas storage solids, where we are strong contributors to the Edinburgh-based UK Carbon Capture and Storage Centre, and where we already benefit from joint EaStCHEM/Engineering funding of more than £3 M from the EPSRC. Planning permission has been granted for a new 3000 m^2 building aimed at providing new infrastructure for Advanced Materials Research. This will be accompanied by a senior appointment in the Energy Materials area. We will significantly invest in our electron microscopy facilities (having recently won £2 M from the EPSRC) to develop a state-of-the-art suite of equipment for materials study. Increasing impact will also be a priority in this theme, building on recent successes summarised in REF3a.

Identifying and Responding to Global Grand Challenges: The breadth of expertise in the chemical sciences and the flexibility of the research groupings allows EaStCHEM to respond rapidly to emerging priorities at the national and international levels and makes it a hub of cross-disciplinary research. Much of our future strategy takes account of the central position of chemistry and how we interact with many different disciplines. The expansion of the Centre for Science at Extreme Conditions (CSEC), through a rise in external funding of £4.3 M to £12.6 M, further embeds our links with Physics and Engineering. The Joseph Black CO_2 laboratory (JoBLab, Arnold, £1.1 M) has brought CO_2 chemistry into the UKCCS (UK carbon capture and storage) network headquartered in Edinburgh; we now work with engineers in sensing, capturing, and converting CO_2 into new materials. It has been integral to recent EaStCHEM homogeneous catalysis success (EPSRC, £3 M) and involvement in the UK Catalysis Hub (EPSRC, £11 M). Further investments designed to enhance our four research themes will expand our capability to work across boundaries with other sciences, and with industry and national labs. Examples include the development and application of mass spectrometry, to be supported with a new senior appointment in 2014, the strengthening of medical materials expertise with new appointment Nudelman, and increased interactions with the National Nuclear Laboratory on nuclear waste monitoring and reprocessing (Mount). New university-funded tenure-track fellows will be allocated to EaStCHEM in 2014 for strategic recruitment activities across these areas.

c. People

i. Staffing strategy and staff development

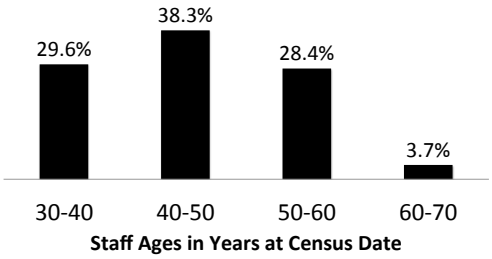

Fig 2. EaStCHEM Staff Age Profile

EaStCHEM's age profile (see Fig. 2), with an average age of 45 years, reflects our sustainable staffing strategy. 15% of our professoriate are female and 100% of our new staff since 2008 were under 50 years of age on appointment. EaStCHEM's overall staffing policy is to attract world-class academic staff to enhance strategic areas of research, and to offer a highly supportive research environment and an attractive career path. Twenty new members of staff have been appointed since RAE08. New recruitments include four at the professorial level from inside (Lloyd-Jones) and outside the UK (Nolan, Buehl, Vogt), with a fifth appointment from 1/1/2014 (McKeown; Cardiff). New fellows and lecturers have been appointed from Europe (Bode, Cazin, Cowley, Nudelman), North America (Kay, Kirrander, Shaver, Zysman-Colman), Australia (Lawrence), Singapore (Vendrell) and Japan (Schneider), as well as from within the UK (de Vries, Michel, Lovett, Lilienkampf, Thomas). These appointments have served to increase critical mass in the general field of synthesis and catalysis, and have brought complementary expertise to increase the synergy and international competitiveness within theoretical chemistry, green chemistry and biomedical imaging and materials.

The substantial success that EaStCHEM has achieved, and the leadership quality it has developed in its members has led to the recruitment and secondment of senior staff to prestigious posts in the UK and internationally, e.g. Yellowlees: President of the RSC; Chapman: Principal and VC of Heriot Watt University; Madden: Master of Queen's College, Oxford; Harrison: fulltime secondment as Director of the ILL, Grenoble (from Jan. 2014, CEO of Diamond). This is evidence of a vibrant and supportive environment that allows staff to flourish. Locally, staff have also taken on significant leadership roles; Yellowlees: Head of College of Science and Engineering (UoE);

Richardson: Vice-Principal and Master (StA); Woollins: Vice-Principal Research (StA from 2014); Mount: Dean for REF2014 (UoE); McDougall: Dean Quality Assurance (UoE); Tasker: Director of ScotCHEM, the pan-Scotland research pool organisation, providing leadership and best practice for Chemistry research in Scottish academia. Senior group leaders are actively encouraged to enhance the research environment through participation in major research initiatives, identifying and leading new initiatives to solve Grand Challenge problems through the application of new chemistry, and through advisory and mentoring activities.

A key measure of vitality is the award of competitive externally-funded fellowships to permanent academic staff. As examples, during the REF2014 period our staff won: EPSRC/BBSRC Senior Research Fellowships (Arnold, Greaney, Lam, Leigh, Morris), Leverhulme Leadership Fellowship (Florence), RS Industry Fellowships (Morris, Clarke). We encourage applications and enable successful fellowship holders to concentrate on their research activities with a policy of recruiting temporary teaching fellows to provide teaching cover for successful fellowship applicants.

During the REF2014 period, 23 early career researchers gained competitively won *independent* junior fellowships bringing our total number of early career fellows to 39 in the period: Bode (EaStCHEM Fellow 2011), Cazin (RS URF 2011), Dong (Wellcome Fellow 2009); Flors (RS URF 2010), Gloster (Wellcome Fellow 2012, L'Oreal UNESCO Fellowship, 2013), Kay (RSE Fellow 2011), Killian (EaStCHEM Fellow 2009), Lovett (RS URF 2010), Michel (RS URF 2010), Moggach (RSE 2008), Rogers (Edinburgh Beltane Public Engagement Fellowship 2010), Sek, Viguier, Xiao (Scottish Enterprise/RSE fellowships 2008), Wann (EPSRC Career Acceleration Fellow 2010), Kirrander, Shaver, Thomas (all EaStCHEM Fellowship 2012), Vendrell (MRC Academic fellowship, 2012) Cowley, Nudelman, Zysman-Colman (all EaStCHEM Fellowship 2013), Inglis (RSE/Scottish Government Personal Research Fellowship 2013). EaStCHEM fellowships are University-financed 5-year tenure-track positions, with initially low teaching and administration loads. All fellowship holders are treated as members of staff with the same privileges and rights with respect to laboratory infrastructure and access to PhD studentships. Our transparent policy of reviewing the tenure of fellows after three years is an important part of our supportive research environment. So far ten of the above fellowship holders have progressed to permanent positions with us or other internationally renowned Universities.

EaStCHEM is a very attractive place to hold international fellowships, such as Marie-Curie awards. During REF2014 we have hosted 18 such fellows; e.g. 9 Marie-Curie fellows (not included in the staff member submission) are being hosted by our PIs at the staff census date.

In order to allow our researchers (particularly early career) to interact with world-leading scientists, we run an EaStCHEM International Visiting Fellowship Scheme with international research leaders visiting for one to two weeks, giving several lectures and interacting directly with research groups at postgraduate and postdoc levels. E. Carter (materials modeling, USA); B. Koel (surfaces, USA); J. Barton (bioinorganic, USA); M. Chisholm (inorganic materials, USA); J. Marie-Lehn (supramolecular, France, Nobel laureate); F. Stoddart (supramolecular, USA); R.D. Levine (theoretical, Israel) and A. Powell (molecular magnetism, Germany) have made such visits since 2008. This EaStCHEM activity has benefited strongly from dedicated videoconferencing facilities on the two sites that allow live, interactive broadcasting between our lecture theatres and to personal computers/tablets.

Staff professional development: We recognise that our staff members are the key asset of a successful research-led school. Career progression and professional development for all research support and administrative staff are strongly supported via appraisals, work-load modelling, mentoring, CPD courses, and the provision of a stimulating and well-resourced environment. Support is provided by the EU-accredited Institute for Academic Development (IAD) and Centre for Professional Development (CAPOD), with research ethics and integrity a core principle.

We were awarded the *HR Excellence in Research Award* (2010) by the EC in recognition of the steps we have taken to implement the principles of the Concordat to Support the Career Development of Researchers, and the support we give to students (see section c). New academics attend induction training and all discuss training, development and progression during their annual reviews. All researchers are offered innovation and commercialisation training and we offer PDRAs appraisals from industrialists as well as academics, and an entrepreneur's club.

Early career researchers are strongly encouraged to work towards a postgraduate certificate in teaching. A postdoctoral led (and staff mentored) cross-college team organises collaboration-generating events around major colloquia and other events, giving valuable experience and exposure to the PDRAs.

Research support staff: Adequate research support is essential for our success and there are currently 28 research support staff within EaStCHEM - 8 new research officers since RAE08. We have invested in apprentice technical support schemes that offer training across chemistry. Since 2011 four such apprentices have been trained by EaStCHEM. Our investment in skilled support for X-ray diffraction, mass spectrometry, NMR, surface analysis, and other major techniques (making a total of 20 for dedicated facility support) has produced valuable research contributions and brought in many new industrial users to our facilities (see REF3a).

Equality and diversity: In EaStCHEM 23 out of the 82 group leaders are from outside the UK. Early career PDRA researcher origins are even more international with >30 countries represented. The emphasis on equality, diversity and transparency within EaStCHEM has led to an Athena Swan Gold Award (2012) and a Bronze Award in 2013. The gold award was only the second given to a UK department since the Charter was initiated in 2005. Our profile has been further enhanced by Arnold's 2012 Royal Society Rosalind Franklin prize for outstanding scientific achievement and work to promote women in science worldwide. We are active in promoting good practice within the community with over 30 invitations having been accepted to provide advice to University departments and policymakers both nationally and internationally since April 2012. We have also produced a film highlighting gender issues, which was produced as part of the Rosalind Franklin prize project. This has been viewed by over 6000 website visitors in 2 months and screened in six countries to date. Two of the major leadership positions in EaStCHEM are held by women (ECampbell and Arnold). Cazin and Ashbrook are elected members of the Royal Society of Edinburgh Young Academy and Slawin is the only female scientist in the list of top 50 authors in Angewandte Chemie. All staff members receive equality and diversity training, and our Equality and Diversity committee meets regularly to frame policies that ensure that we have an open, transparent and supportive environment for all our staff and students. A new nursery is being built in the grounds of the Edinburgh site with the goal of improving work/life balance for staff.

ii. Research students

EaStCHEM views its PhD students as its single most important investment for the future of chemistry. We place a very strong emphasis on supporting an inspirational Chemistry graduate school that exploits the state-of-the-art facilities for chemistry and related disciplines.

Year	EaStCHEM FTE PhDs
2008/09	236.2
2009/10	241.6
2010/11	252.8
2011/12	257.2
2012/13	270.4

Numbers, Recruitment and Interdisciplinarity The EaStCHEM Graduate School has increased by ca. 15% during the REF2014 period. This increase is in the context of a difficult funding climate for studentships coupled with an increase in standard PhD length to 3.5 years (average) from 3. EaStCHEM investment in PhD funding (£4 M in the period) is used to attract outstanding applicants with career development scholarships (involving enhanced training in outreach, teaching or entrepreneurship), prize studentships for international candidates and the availability of attractive training courses. Excellent PG research is rewarded with conference grants and the possibility for students to apply for small research grants. We reward academics who bring in matching external funding with prioritisation in the distribution of studentships. The resulting co-supervision with industrial partners, specialist research centres, national facilities and other academic disciplines adds value to the students' development. Industry involvement in PhD projects is highly valued, and specific industry-matching schemes have been run in some years. UK Industry funding to EaStCHEM totalled £6.6 M during the REF2014 period, with much of this funding directly supporting PhD students; 110 have been fully or partially funded by industry in the period. Recruitment activities that showcase the excellent facilities and expertise and success of the current and recent cohorts are coordinated by the PG recruitment group, led by Smith and Jones. We incorporate our cross-disciplinary research approach into our Graduate Training School, which now includes joint supervised PhDs with Engineering, Geosciences and Medicine.

Training and Cohort Experience The PhD training programme is fully integrated across the two Universities to ensure a single 'cohort' experience. All facilities are available to the entire PhD cohort, and both Universities amended their regulations to allow staff from either partner to act as internal examiners for PhDs. Students develop a range of skills in chemical techniques and theory, often going beyond their immediate specialism, and transferable skills such as oral and written presentation, business and innovation training, leadership and team working, public engagement, and health and safety. They also benefit from targeted courses delivered by world-leading scientists within the EaStCHEM visiting professor programme. Full use is made of communications technology to stream these courses, the weekly research colloquia, and specialist training courses across the site and to personal devices, with interactive capabilities. Students also take responsibility for USIC, the Scottish Chemistry Postgraduate Conference.

Progress through and beyond the PhD Student progress is rigorously assessed by staff (9, 24 and 36 months) and they have a mentor who is external to the project, to ensure quality and transparency. The programme is monitored by the PG committee, headed by Buehl, Kilian and Robertson, and its effectiveness proven by the awards of international thesis prizes (2), PDRA fellowships, and research outputs (on average ca. 2.5 publications per annum per PhD student).

d. Income, infrastructure and facilities

Competitive research income (as reported in REF4) during the census period for EaStCHEM is currently over £73.8 M. Academics have also been particularly successful in winning competitive research awards during the REF2014 period with the total value of awards announced £118 M (up from a RAE08 value of £65 M). Research awards in the 2012/2013 academic year alone are £42 M, making the income per FTE in 2012/13 £0.51 M.

Fig. 3 Funding Awarded

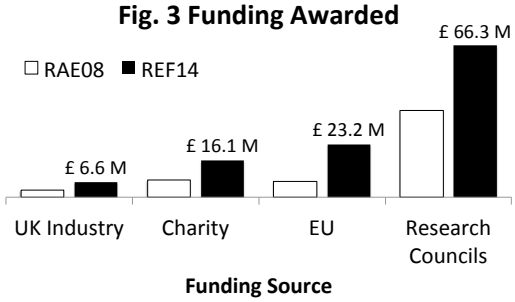

Figure 3 shows the competitively awarded grants for the main sources compared to the RAE08 period. The step change upwards in all areas is a clear indicator of improved quality since RAE08. In addition, "income in kind" over the REF2014 period, defined as Research Council facility time allocated through peer review amounts to > £9 M. In future, we will continue to diversify our income sources and, with specialist University administrative support, will target European funding schemes such as Horizon 2020. The appointment of an EaStCHEM Director of Internationalisation, who will be part of the senior management structure, will provide the strategic leadership for increasing EaStCHEM's role in major international consortia and we will continue to increase the value and strategic importance of industrial sponsorship through the support of our BDEs and an increasing network of collaboration partners.

Research Funding Highlights

- Research funding (by value) has increased by more than 80% and continues to show an upward trajectory. Research Awards announced for 2012/13 are > £42 M (for comparison, in 2007/08 research awards were £12 M).
- UK industrial award funding has doubled since RAE08 to £6.6 M.
- EU funding has tripled since RAE08 to £23 M. A major contributor to this is success in winning ERC grants. We have received seven ERC Advanced Investigator grants (£10 M), and four ERC Starter/Consolidator Grants (£5 M) in REF2014, plus two more announced in Nov 2013.
- The number of competitive grants of more than £1M has gone up from 6 in RAE08 to 38.
- Large competitive grants have been secured for specific infrastructure to develop leading science. These include £11.5 M (EPSRC at 100% FEC, PI: Bradley) for the EaStCHEM-led Interdisciplinary Research Collaboration (IRC) in Molecular Sensing and Imaging, and £6.2 M (Wellcome Trust, £5 M, Scottish Funding Council £1.2 M, PI: Naismith) for the Biological Sciences Research Centre.
- Provision of consulting and infrastructure use by industry generated ~£4.4 M income during

the REF2014 period, and generated some new industrial collaborations (e.g. with Dyson, worth £2.9M in research funding and Selex-Galileo).

Infrastructure and Facilities

EaStCHEM has high quality facilities across the breadth of Chemistry with ready access for all researchers. Our infrastructure also attracts significant use from external industry, generating ~£4.4 M income during the REF2014 period, as evidence of the success of our strategic investments detailed below. The provision of an excellent equipment base and service infrastructure underpins all of the research within EaStCHEM and our core strategy is to ensure the complementarity and synergy between the EaStCHEM partners. Each partner has a suite of analytical equipment that can be regarded as essential infrastructure for every top-class Chemistry Research School and dedicated scientific support. These are coupled with specialised units where cutting-edge characterisation work is led by appropriate world-leading scientists.

Recognising that **strategic investment** is vital to the growth in quality we have targeted competitive external funding where internal investment can be leveraged to add significant value. Areas selected during the census period are:

- **New build** such as the 3000 m^2 £16 M EaStCHEM-led Biomedical Sciences Research Centre, built with a University investment of £10 M plus £6.2 M of external research funding.
- **Laboratory refurbishment** investment of £7 M has updated 2500 m^2 of existing laboratory space. The synthesis laboratories, facilities for catalyst evaluation and biomolecule preparation, the ultrafast spectroscopy laboratory, and materials characterisation have all benefitted from investment. EaStCHEM received first prize in 2013 in the Laboratory Environmental Improvement category under the S-Lab Award Scheme, which recognises excellence in laboratory design, safety and sustainability.
- The **equipment base** has received substantial investment, with all the major facilities being upgraded to the state-of-the-art. NMR (both solution and solid-state), XRD, electron microscopy, mass spectrometry, EPR, research computing facilities, micro-Raman spectroscopy, atomic force microscopy and ultrafast spectroscopy have all been upgraded.
- Employment and training of highly skilled **scientific support staff** has been a priority, with eight new scientific support staff having been employed and trained to deliver the highest standard of research facility, resulting in enhanced levels of industrial use of our facilities.

State-of-the-art **specialist infrastructure and facilities** include 800 MHz solution state NMR, together with more than ten 400-700 MHz magnets, several equipped with cryoprobes. REF2014 investment in solid-state NMR includes 600 and 400 MHz wide-bore magnets and funding is secured for a 400 MHz solid-state pulsed field gradient instrument.

Complementing the Walker Press and other high-pressure materials synthesis capabilities are high-pressure-enabled and high-intensity X-ray crystallography. Diffractometers with robotic sample changers have been developed in EaStCHEM, together with rotating anode Cu and Mo sources, and microsources. Powder X-ray diffraction equipment has been completely renewed during REF2014, with a suite of four new Panalytical goniometers.

Mass spectrometry (MS) has received significant investment from both BBSRC and EPSRC Advanced Materials and Core Capability funding, focussing on proteomics applications, ultra-high resolution FTICR-MS of biomolecules, MALDI imaging and ion-mobility MS.

Cutting-edge computational facilities and theoretical/modelling support staff are available for all EaStCHEM researchers within the EaStCHEM research computing facility (RCF), contributing to >200 EaStCHEM publications in the period by providing access to major computational chemistry packages (e.g. Gaussian, Amber, CASTEP) to cover a broad spectrum of modelling techniques and applications as well as providing training in the use of these packages. Additional facilities include the Edinburgh Parallel Computing Centre (EPCC) (including the national high performance computing service HECToR).

Biomacromolecular sciences are supported by excellent core facilities for microbial cell growth, protein purification and characterisation. A suite of computer-controlled fermentors are available in a facility that also houses instruments for circular dichroism, light scattering, isothermal titration calorimetry and surface-plasmon resonance.

EPR spectroscopy now includes advanced capabilities for both materials and catalysis characterisation, and biomacromolecular structure determination including 3 pulsed EPR spectrometers and 2 CW spectrometers.

An extensive array of equipment is available for surface characterisation: scanning probe microscopes including variable temperature UHV-STM, electrochemical STM and liquid phase AFM/STM, several specialised FTIR instruments one linked to a liquid cell for *in situ* studies of molecular adsorption in liquids, micro-Raman spectroscopy combined with AFM and FTIR, UHV-based HREELS, SFG facilities and two XPS instruments.

Scanning and transmission electron microscopy instruments are available in an EPSRC-funded facility, which will be expanded in early 2014 after a new £2 M investment from the EPSRC. Other materials characterisation facilities include: ToF-SIMS, porosimetry, BET measurement, TGA, DTA, DSC, Solid State NMR, QCM, EQCM, SQUID magnetometry x2, and conductivity.

The laser spectroscopy facility within the Collaborative Optical Spectroscopy, Micromanipulation and Imaging Centre (COSMIC) has high repetition rate Ti:Sapph lasers available for fluorescence lifetime spectroscopy/imaging. In addition, an amplified system is available for gas phase chemical physics studies. A variety of ns laser systems are used for high-resolution spectroscopy and laser-induced crystallisation research.

Specialist facilities for catalytic testing include continuous flow autoclaves (fluorous supercritical fluid/ionic liquid, supercritical fluid/supported catalyst), high pressure IR and NMR, reactIR, the only solution microcalorimeters in the UK for homogeneous catalysis, automated and parallel batch autoclaves with liquid sampling capacity, high throughput and fully-automated 16-parallel reactors, advanced thermal cycling equipment and continuously operated reactors with integrated membrane filtration for catalyst separation (from 10 mL to 1.5 L).

We are also heavy users and developers of national facilities. In the UK (Diamond, RAL, etc) and abroad; in Europe (ESRF, ILL, etc), the USA (ALS, APS, Oak Ridge, NIST etc) and further afield (e.g. ANSTO, Spring-8) EaStCHEM staff have collaborated on instrument development and taken on advisory board and facility directorship roles (see part e).

e. Collaboration and contribution to the discipline or research base

Interdisciplinary research: EaStCHEM takes a central role in interdisciplinary research with Biology, Physics, Engineering, the Earth Sciences and Medicine, and uses its strengths and skills achieved through pooling to form both direct links and collaborative centres. Appointments (e.g. CCampbell, Coleman-Zysman, Nudelman, Shaver) have been made specifically to drive interdisciplinary research and we have made key contributions to the following large (> £1 M) interdisciplinary centres with the aim of making an impact on other disciplines; The Biomedical Sciences Research Centre (BSRC), the Joseph Black Laboratory for Carbon Dioxide Chemistry (JoBLab), Scottish Centre for Interdisciplinary Surface Spectroscopy (SCISS), Collaborative Optical Spectroscopy, Micromanipulation and Imaging Centre (COSMIC), Centre for Translational and Chemical Biology (CTCB); Centre for Magnetic Resonance (CMR); Edinburgh Materials and Micro-Analysis Centre (EMMAC) and the Centre for Science at Extreme Conditions (CSEC). Examples of instrument development with National Facilities include high-pressure inserts for neutron beamline cryostats and cryomagnets (Attfield, with ISIS and STFC funding).

Collaborative Research Funding with academia, industry, and other: We are active members of many research consortia worldwide (e.g. EU consortia, UK consortia such as Supergen, CO_2 network, etc). We make contributions to research projects with a combined value of > £300 M.

Our strategy to increase industrial collaboration has led to the doubling of industrial research income (see above) including one major project worth £2.9 M with Dyson Ltd. We have significantly increased the exploitation of our own research through early development of KT initiatives, such as increased engagement with industrial users of our facilities, was enhanced through engagement with schemes such as the Royal Society Industry Fellowships (Morris, Clarke) and other enterprise initiatives, such as Scottish Enterprise Proof of Concept (8 PIs, £2 M total). Additional milestone driven translational projects include RCUK follow on funds exceeding £4 M. Close interaction with industrialists and the EaStCHEM advisory board helps to inform our research strategy, ensuring relevance to industrial needs. This is done via consultancies,

committee memberships and regular contact with Chemical Sciences Scotland (a Scottish Enterprise supported partnership between the chemical industry, academia and government agencies) now mediated by Tasker. Our success in developing closeties with industry is particularly apparent in the close involvement of industry in the EaStCHEM catalysis hub.

Extending International Reach: We see the formation of strategic international collaborative alliances with preferred academic and industrial partners to be of prime importance. Joint PhD training programmes exist for example with the TU Munich's Institute for Advanced Study, the University of Melbourne, Australia, and McGill University, Canada and negotiations have started with Ewha Univ., South Korea and Nagoya University in Japan. Kamer leads several initiatives in catalysis, in particular with the Netherlands and Finland while Attfield and Robertson lead a Global Initiative with Pacific rim countries. EaStCHEM members have been active as visiting professors in Lille, Rennes, Lyon, Aachen, Munich, Copenhagen, Cagliari, Compiègne, Milan, Tarragona, Wroclaw, Ekaterinburg, Nagoya, Seoul, Changzhou, and Fudan. The imminent appointment of a Director of Internationalisation will provide strategic leadership for our internationalisation activities with the aim of increased worldwide collaboration and impact.

Leadership in the academic community: EaStCHEM makes a significant contribution to the Royal Society of Chemistry's work in advocacy through the leadership of Yellowlees: President of the RSC; ECampbell: Chair of Heads of Chemistry UK (from 2013); Tasker: head of Dalton Division (to 2013), and Cole-Hamilton: head of Dalton Division and President of EuCHeMS from 2013. EaStCHEM staff members are heavily involved in refereeing for all the major journals and for grant awarding bodies across the world, and sit on national and international facility steering committees, e.g. Slawin is deputy Chair for the Belgian Hercules Commission, 29 academics are EPSRC college members and 1 is an NERC college member.

Staff members contribute as Editorial board members, with especially strong representation on RSC and ACS journals (Editor in Chief, Green Mater.; Co/Associate-editor, Dalton Trans., Catal. Sci. Tech., J. Comb. Sci., Acta Cryst. B.; Board membership includes Mol. Phys., Chem. Phys. Lett, Dalton Trans., J. Biol. Chem., Combin. Sci., Biomat. Sci. Biochem. J., J. Mol. Biol. Advisory board membership includes Chem. Sci., Chem. Commun., CrystEngComm, Organometallics, Biophys. Chem., Mag. Reson. Chem., Surface Sci., J. Biol. Chem, Front. Condens. Mater. Phys., and Phil. Trans. Royal Soc. A/B.

Members of EaStCHEM have delivered more than 350 plenary/keynote and more than 600 invited international talks within the REF2014 period. We have hosted several major conferences, including the 3rd International MOF meeting 2012, 20th EuCheMS Conference on Organometallic Chemistry 2013 and the International Neutron Scattering Conference 2013.

Staff expertise is actively sought out by the international community for reviewing government labs and University centres of excellence, e.g. CEA labs in France (Arnold), CSIC Institutes in Spain (ECampbell), Max-Planck laboratories (Bruce) and the DFG Excellence Initiative in Germany (Vogt), Berzelius Centres in Sweden (Morris), DoE labs in the US (Arnold, Love) and other countries' strategic research evaluations (e.g. Hong Kong, Richardson). Mount provides strategic advice to the National Nuclear Laboratory as an Academic Associate. Academics are also in demand for high-level reviewing activities, serving on panels for prestigious international funding schemes such as ERC (ECampbell) and international prize committees (e.g. Leverhulme Prize, Attfield; the IZA Donald W. Breck Award, Morris).

The high esteem in which our staff are held and our record of developing ECRs into scientific leaders is reflected in the recruitment of younger staff members to prestigious appointments elsewhere (Margadonna: Chair, Oslo University; Barran: Waters Chair, Manchester University; Lam: GSK-endowed Chair, Nottingham University; Greaney: Chair, Manchester University).

Our contribution to society is also through advice to Government via advisory/policy group membership, such as membership of the Department for Environment, Food and Rural Affairs Air Quality Expert Group (Heal), of the ESRF Council and STFC (Donovan), and through the Royal Society MP pairing scheme (Alexander). Robertson directs the Scottish Institute for Solar Energy Research, advising on the 2020 Government Routemap for Renewable Energy (Scotland).

Prizes, Awards, Other Recognition from the Community:
In addition to the 39 fellowships and 13 ERC grants, described above, junior and senior academic staff members regularly win national and international prizes (63 in total). During the REF2014 period, 11 PhD students and PDRAs from EaStCHEM have won early career/postdoctoral fellowships, including Fulbright and Presidential fellowships in the US, JSPS, and Marie Curie IEFs, while 52 former PhD and PDRAs have entered academia worldwide as fellows or lecturers.

International, competitively awarded prizes:
Junior staff highlights include prizes to Michel; ACS COMP Outstanding Junior Faculty award (2013), ACS Emerging Technology Prize (2009), Moggach; CCDC crystallography prize for young scientists (2010) and the European High Pressure Research Society award (2012); Shaver the CNC-IUPAC award (2010), Canada Foundation for Innovation Leaders Award, (2008, 2012), Schneider the GCOE Chemistry Innovation award (2009) and the Thieme Chemistry Journal award (2011), and Cazin the ACS Organometallic Prize (2011).

Senior staff highlights include prizes to Bruce; the Galileo Galilei Award (Italy, 2012), the Arfvedson Schlenk award (Germany GdCH, 2011), the Carl Wagner Memorial Award (US Electrochemical Society, 2011), and the Akzo Nobel Science Award (UK, 2012) for '*outstanding contributions*' to electrochemistry and lithium battery technology. ACS and NSF prize recipients include O'Hagan (Fluorine Chemistry, 2011), and Morris (ADVANCE Distinguished Lecturer Award, 2009). Arnold received the Hans Fischer Senior Fellowship (Germany, 2012), Bradley, the Society of Combinatorial Sciences Award (2009), and Yellowlees the IUPAC Distinguished Woman in Chemistry award (2011). Irvine was awarded the Chinese Academy of Science Lee Hsun Award in 2010. Naismith has been awarded a BIC Fellowship at Christchurch New Zealand (2011). Attfield, Lloyd-Jones, Nolan, O'Hagan and Morris all received Royal Society Merit Awards.

National, competitively awarded prizes: EaStCHEM staff members have received multidisciplinary awards such as the Royal Society Brian Mercer Award for Innovation (Morris, 2012), the Royal Society of Edinburgh Makdougall Brisbane Award for the Physical Sciences (Ashbrook, 2012), and the RS Rosalind Franklin award (Arnold, 2012). In addition, staff members have been awarded 18 RSC and a total of 26 other UK awards and prizes between 2008-13. Included in these are several of the flagship awards, such as the Corday-Morgan Medal (Brechin, Arnold), Tilden Awards (Nolan, ECampbell, Bruce), the Jeremy Knowles award (Naismith), and the Physical Organic Chemistry Award (Lloyd-Jones).

Elections to learned society fellowships: During the REF2014 period ECampbell and Lloyd-Jones have been elected as Fellows of the Royal Society. Woollins and Nolan were elected to the European Academy of Science, and Nolan to the Royal Society of Canada. Nine new Fellows of the Royal Society of Edinburgh were elected during the census period, and two younger members of staff (Ashbrook, Cazin) were elected to the Young Academy of Scotland. Morris was elected to the Learned Society of Wales, and Naismith a Fellow of the Academy of Medical Sciences.

Public Science: We share our knowledge and skills with public audiences both within and beyond the academic community and have a willingness to learn from the communities with whom we engage. Academics, three dedicated outreach officers, and our Public Engagement Career Development Scholars (EaStCHEM funded PhD studentships) have made our research accessible to more than 110,000 members of the public (see REF3a for full details). Our teachers' conference brings our research to over 150 teachers annually through lectures and discussions. Robertson started 'the Solar Spark', a public science initiative that is intimately intertwined with Supergen-funded solar cell work and now energy policy advisory work (see above). Pulham won an STFC Science in Society Fellowship (2009-11) to promote research in CSEC and STFC to the public, through lectures as far afield as Hong Kong. Total audience numbers exceeded 7000, with virtual audiences estimated at ~200,000.

Our research regularly generates international press interest: academics have had results highlighted by national TV programmes (including UK, Canada, and Russia), national radio (including BBC Radio 4 and North American public radio), newspapers (including the Times, Telegraph, Frankfurter Allgemeine Zeitung), the internet (including BBC, Guardian, and international press websites), and specialist press (including C&ENews, Chemistry World, and many highlight articles in Science and Nature journals).