Institution: Lancaster University

Unit of Assessment: 8 Chemistry

a. OVERVIEW

The Department of Chemistry was re-established in 2012, admitting its first undergraduate students in Oct 2013. It builds on, strengthens, and integrates the thriving chemical research in the Lancaster Environment Centre (LEC) (environmental chemistry), the departments of Physics (materials chemistry) and Engineering (nuclear chemistry), and within Biomedical Sciences (biophysical chemistry). Lancaster's ambition for Chemistry is for it to become a leading department in the UK and internationally, in both the quality of its research and teaching. This ambition is underpinned by appropriate resources that include year on year staff appointments, a fit-for-purpose chemistry space (with an initial £19 million+ refurbishment) followed by a new purpose-built extension building, and investment in state-of-the-art infrastructure for teaching and research. When fully established, the Department will have 28 academic staff, with 5 new members of staff appointed each year until we reach the target complement in 2016.

Given that Chemistry was established at a late stage of the REF 2014 period, it will be understood that there is no track record with respect to research doctoral degrees awarded (REF4a) and research income (REF4b; REF4c). It also follows that an evaluation of our research position relative to that described in RAE2008, and evidence of achievement of strategic aims during the assessment period, are also inappropriate. Therefore, the environment profile presented here is forward-looking, focussing on the strategy and processes in place and being developed in going forward. As an indication of the Department's stage of development, the staff appointment timings were: Smith (Jan 2012); Fielden (Oct 2012); Anwar, Danos, Coogan, Peach, Platel, and Franckevicius (Jan-Mar 2013); and Evans, Gortz, Middleton, & Trewin (Aug-Sept 2013).

Departmental Research is structured into three sub-discipline or capability-based teams: Synthetic Chemistry (comprising Coogan, Evans, Franckevicius, Gortz, & Platel); Chemical Theory & Computation (Anwar, Peach & Trewin); and Analytical Chemistry & Spectroscopy (Danos, Fielden, Middleton & Smith). Research in the Department is advancing the respective core subdisciplines but with a focus on the chemical complexity at the disciplinary interfaces, the so-called 'white spaces' or frontiers between chemistry and other disciplines. The latter define the application cross-themes which are (i) Energy, Sustainability, & Environment, (ii) Life Sciences & Health Care, and (iii) Functional Materials. There is also interaction between the core subdisciplines.

b. RESEARCH STRATEGY

b1. Vision, strategic plans

The research vision of the Department is summarised in our mission statement: 'To advance chemical research at disciplinary interfaces underpinned by excellence in the core discipline of chemistry'. The focus is on chemical complexity at the disciplinary interfaces, utilising core and creative chemistry to underpin challenging problems that are limiting scientific and technology advances. This is not applied chemistry in the conventional sense, where developed chemical tools may be simply employed to add value to other disciplines. Impact of all forms is an integral part of the research activity, and the ambition is to amalgamate the very best in chemical research with industrial partnerships to address real-world problems and solve societal grand challenges.

The primary strategic aims are

- To advance the core sub-disciplines of: synthetic chemistry; chemical theory & computation; and chemical measurement science & spectroscopy, in particular NMR;
- To advance chemical sciences at inter-disciplinary interfaces of chemistry and physical sciences, and chemistry and biology, with applications and impact in energy, sustainability and environment, life sciences, health care, and functional materials.
- To pursue all strategic aims within a framework of research sustainability
 The sustainability of the research is underpinned by substantial investment by the University,
 external grant income, integration with highly successful research groups within the Faculty and
 externally, Lancaster's membership of the N8 group of universities (N8 is a partnership of the 8
 research intensive universities in the North of England), and partnerships with industry. The
 University is funding the appointment of 5 staff year on year until 2016 inclusive. Infrastructure
 investments are detailed in Section (d). Our focus on chemistry at the disciplinary interfaces and
 working with well-funded research groups in other disciplines enhances our success. The inter





disciplinary research focus broadens funding opportunities enabling us to target almost all major funding research councils and foundations in the UK as well as European sources. A further strategic objective is to partner with industry, with respect to which we are well placed. The North West (NW) of England has the largest concentration of chemical manufacturers in the UK, with the chemical industry being the leading exporter, accounting for 27% of the UK's chemical exports and contributing £3 billion to the NW economy. Towards engaging industry, we are leveraging Lancaster University's N8 research partnership, and are creating the Reaction Centre at Lancaster which will provide small and medium enterprises (SMEs) access to research expertise, capabilities, and dedicated analytical equipment. We already have projects with Compact Instruments (Bolton), The REACH Centre (a Lancaster University start-up based in the Lancaster Environment Centre), and Process Instruments (Burnley). These interactions will open up industry-led research income opportunities, including industry-supported studentships, KTPs, and access to TSB funds. Finally we are developing strategic links with premier research institutions in China including institutes of the Chinese Academy of Sciences (CAS). These links will build on current collaborations in the Department and the Faculty: Anwar is CAS Visiting Professor of the CAS Shanghai Institute of Materia Medica; and the CAS-Lancaster International Research and Innovation Centre for the Environment. The links will leverage funding from China's MOST/NSFC to deliver research excellence through synergy.

We have a strong emphasis on recruiting, developing, and retaining exceptional research staff at all ranks, which we consider essential to achieving sustained excellence in research, and our procedures (detailed in Section (c)) have been developed to reflect this.

- To embed research in all aspects of our organisation and practice, and provide an enablingenvironment. The procedures are based on best practice to create a research-enabling environment unencumbered by unnecessary bureaucracy but supplemented by strong support. A key goal has been to embed a culture of strategic readiness built on horizon-scanning and responsiveness, to enable exploitation of new research-income opportunities and to identify exciting science where we could add value.
- To develop a culture of identifying and tackling research problems of significance and impact. High quality research is often characterised by the significance of the research question being tackled. We promote and encourage interdisciplinary interaction (via symposia, away-days, laboratory visits) both within Lancaster and externally, and industry engagement with a view to identifying significant research problems and opportunities. Being a new department, it essential to extend our reach to the research and wider community: we proactively pursue opportunities to host major chemical conferences and events at Lancaster, and to give leadership to agendasetting networks/forums and international collaborations.

Specific objectives for 2014-2020

- 1) To integrate and consolidate our research teams, maximise synergies within and between teams via joint projects and joint grant bids, and to develop inter-disciplinary collaborations.
- 2) To recruit new staff strategically to either address exciting emergent areas in chemistry, fill gaps, or add value to our core strengths (see staffing strategy (c1)).
- 3) To develop a strong profile of research funding (research councils, European, and industry).
- 4) To increase research student numbers and to partner/lead a Centre for Doctoral Training.
- 5) To develop long-term partnerships with industry and clinical centres. A particular objective is the creation of the **Reaction Centre**, which will provide large companies and SMEs in the North West access to research expertise, capabilities, and dedicated analytical equipment.
- 6) To develop an internationally-leading centre for solid state NMR spectroscopy that advances methods development with applications to materials and biomolecular interactions.
- 7) To develop and maintain strategic research partnerships with premier institutions in China including institutes of the Chinese Academy of Sciences.
- 8) To adopt Athena SWAN principles. This confirms the significant value we put on our staff and will consolidate our commitment to diversity and equal opportunities, and generate an ethos of collaboration, mutual support, and teamwork within the Department.

b2. An evaluation of our current research position

Whilst the Department has no track record with respect to PhD student numbers and grant



income, pooling of the individual staff research outputs, associated PhD students, and grant income (see Section (d1)) suggests exceptional vitality. Over the REF period our publications totalled 297, which equates to about 25/FTE. A number of these publications are in the highest impact factor journals including *Nature* (1 output), *Nature Chemistry* (2 outputs), *Nature Communications* (1 output), and *Nature Materials* (1 output), whilst a significant proportion are in the discipline's highest impact factor journals including *Angewandte Chemie Int Ed.* (10 outputs), *JACS* (12 outputs), and *Chemical Science* (3 outputs). Outstanding inter-disciplinary contributions include *PNAS* (1 output), *Physical Review Letters* (1 output), *ACS Nano* (2 outputs), *Advanced Materials* (1 output), *Advanced Functional Materials* (4 outputs), and *Biomaterials* (1 output). For the 5 experienced staff (i.e. not early career), the number of PhD completions over the REF period was 32 students, with 8 still current (3 at Lancaster and others elsewhere).

DEVELOPMENT

c1. Staffing strategy in relation to the Department's research strategy and infrastructure

The Head of Department was appointed (Chair) from an analytical chemistry background, a capability of wide interest to Lancaster: environmental measurements (Lancaster Environment Centre), novel materials characterisation (Physics); process measurement (Nuclear chemistry and Chemical Engineering); and bioanalysis and diagnostics (Biomedical and Life Sciences).

Computational chemistry was a targeted theme given that computational modelling is a highlysuccessful research theme at Lancaster, resulting in appointments of Anwar (Chair), Peach and Trewin. This team strongly complements the solid state NMR capability in Chemistry (see below) where computational modelling is now increasingly used to model spectra and to extract structural information. There is also considerable synergy with the exceptionally-strong condensed matter theory/modelling groups in Physics led by Vladimir Falko and Colin Lambert. The computational needs of the team are provided by the substantial High-End Computing (HEC) facility at Lancaster and the N8 HPC cluster Polaris at Leeds, both of which are supported at University level. A strategic objective is to develop and consolidate world-class capability in solid state NMR research, based around two complementary Chair appointments in NMR, Smith and Middleton. Smith focuses on structure-function relationships of molecules and materials, whilst Middleton's focus is on biomolecules and bio-molecular interactions serving as a strategic link between Chemistry and Life Sciences. Chemistry has secured matched funding from the University in support of acquiring a 600 MHz solid-state NMR instrument.

The synthetic chemistry appointments (1xSL, 4xLecturers) complement the other two capability groups and have impact across all three application themes. There is also synergy and collaboration with Chemical Engineering and the Energy Lancaster research centre.

In terms of staff profile, we endeavour to have a good mix of experience and new blood as we recruit towards the full complement. The current profile (4 x Chair, 1 x Senior Lecturer, 7 x Lecturer:ECR) is dominated by early career researchers, which is by design. High-calibre early career researchers display ambition and drive coupled with fresh ideas and creativity, and boldness to try out new directions, giving the Department agility and responsiveness. The challenge is to harness this energy and to provide the environment (support and infrastructure) for them to excel – how we do this is detailed below. Planned new appointments will include: addressing remaining gaps (e.g. biophysical chemistry; spectroscopy), the introduction of exciting emergent areas of chemistry (e.g. synthetic biology); and enhancement of our core strengths (e.g. additional lectureships in computational chemistry and solid state NMR with a materials focus). **c2. Career development support for researchers**

A primary strategic objective is to recruit, develop and retain high-calibre research staff. The Departmental procedures are designed to support staff throughout their career through appropriate resources and support structure. Early career researchers receive enhanced opportunity to develop their research and to integrate within the Department and the Faculty. Support and training for career development are provided through mentoring by a senior colleague whilst working through a personal development plan designed to develop competencies and skills. Whilst early career researchers have special needs (which we address) and their development is integral to long term sustainability, the provision for development is not restricted to junior staff. Skills and competences for all staff are developed via workshops to disseminate best practices (e.g. grant writing) and training courses delivered by the University's Organisation and Educational Development (OED) department and the Faculty. Leadership and management skills training is delivered by OED. Performance management is through an annual Performance and Development



Review (PDR) to identify strategic goals (personal and institutional), new initiatives, and targets. Promotions follow University procedures, with transparent criteria. Fixed term staff are issued with a clearly defined contract and are mentored to promote their integration within the Department and enhance their employability elsewhere. Research assistants are mentored by senior colleagues. c3. Implementation of the Concordat to Support the Career Development of Researchers

Motivated staff are critical to delivering high guality research, and guality training and support are essential to realising potential and maximising output. Lancaster's commitment to the Concordat has received European recognition with an HR Excellence in Research award.

c4. Research opportunity

To ensure and maintain vitality, the Department is committed to creating opportunities for staff. Thus, early career staff have a restricted teaching load for the first two years to enable them to develop and establish their research. The University has an Early Career Small Grant Scheme with a maximum allocation of £7k (total sum allocated: £96k in 2012/13). The Faculty offers PhD studentships, some reserved for early career staff. In 2013 the Faculty offered 14 PhD studentships, of which 6 were reserved for early career staff. Chemistry secured one of the early career studentships. The Faculty has a Business Partnerships & Enterprise team (13 FTEs) which is highly effective in linking individual academics to industrial partners. As a result, Chemistry recently picked up 5 (Pilot) Impact Acceleration Account (IAA) awards of average value of £5k, 4 of which went to early career researchers. Industrial partners included Sharp and GSK. The Department values sabbaticals in infusing vitality into an individual's research, with a policy of one term after seven terms and shorter-term leaves on an *ad hoc* basis of up to a month to visit collaborating laboratories, e.g. Danos spent a month at Southampton. Opportunity is also created by means of an incentive fund, which is allocated by the Department to all staff to enable them to present results at conferences, develop collaborations, and/or purchase consumables or software. This support is particularly useful to early career researchers as they attempt to secure grants and other colleagues seeking pump-priming support. The Faculty and Departmental seminar programmes expose staff to exciting research being carried out by leading researchers (both internal to Lancaster and external), and provide opportunity to build collaborations. A particular feature of the Department is a culture of inclusiveness, based on giving opportunity to staff, in particular early career staff, to lead on initiatives, take up positions of responsibility, and involvement in important decisions, all demonstrating trust in an individual's ability.

c5. Personal research fellowships

Despite its recent inception, the Department has successfully attracted two University Research Fellows. Trewin and Gortz, confirming the attractiveness of the Lancaster Chemistry environment. Trewin has a Royal Society University Research Fellowship (2009-2013) and is currently seeking an extension, whilst Gortz has a Royal Society Dorothy Hodgkin Fellowship (2009-2013). Internally, within Lancaster, the Department has secured a Lancaster-supported University Fellowship (Danos) which serves as Chemistry's interface with the Energy Lancaster initiative. c6. International staff appointments, recruitment and visiting scholars

Internationalisation is an important element of Lancaster's strategy and we recognise that highcalibre international staff would strengthen our interactions with international partners and align us with global research priorities. All our appointments attracted a global field. International visiting scholars have included Jonas Fagerberg (Uppsala, Sweden) for 6 months, and Philipp Ectors (Erlangen-Nürnberg, Germany) for 1 week. Visiting scholars from India (Manipal University's College of Pharmaceutical Sciences) and China (Chinese Academy of Sciences Shanghai Institute of Materia Medica) are already scheduled for 2014.

c7. Support for equalities and diversity

The University holds Athena SWAN Bronze status, and has a central committee to oversee, promote, and encourage equality and diversity. The Department has an Equalities Officer to ensure effective implementation and embedding of equalities policies in all functions of the Department. The appointment provides a supportive environment to encourage staff and research students to raise and/or disclose any issues. All staff are required to undergo online diversity and equality training. Statistics are regularly reviewed to ensure that policies are being adhered to both in terms of equality/diversity as well as harassment. Our commitment to equal opportunities is expressed in our strategy that the department should strive for an Athena SWAN Gold. **QUALITY OF TRAINING AND SUPERVISION OF RESEARCH STUDENTS**

c8. Approaches to research student recruitment



As of Oct 2013, there were 5 research students in the Department, which we expect will increase quickly, particularly of overseas self- or government-supported students, as we raise our profile. The establishment of the Reaction Centre (see Strategy section) and resulting interaction with industry will give us impetus to increase research students via industry-supported studentships. Strategic Department and University links that include the Lancaster-Guangzhou campus initiative, Lancaster-Chinese Academy of Sciences collaboration, and proposed Lancaster-Sao Paolo collaboration will also lead to increased student numbers. The objective is to increase the applicant pool, making selection competitive to maintain quality, and not to increase student numbers *per se*. **c9. Research student training and support mechanisms**

We fully subscribe to RCUK's Statement of Expectations for Doctoral Training, the principles and precepts of the QAA Code of Practice for Postgraduate Research Programmes, and the Researcher Development Programme (RDP) endorsed by RCUK. Thus students are given generic training to enable them to be more effective in their research, to manage their careers, and to be more competitive in the careers market place. This includes careers advice throughout the training period, development of professional and transferable skills, public engagement skills, and engagement with professional accreditation bodies (e.g. Royal Society of Chemistry), and research ethics and how to comply with ethical and legal frameworks governing research. Additionally, students receive training on intellectual property and knowledge transfer and to optimise the broader impact of their research. Subject-specific training includes in-depth development of the relevant technical knowledge and skill, as well as an understanding of the broader area of the research project. Student needs for training and development are identified at the outset and throughout the doctoral training period. Broader training, delivered by the Faculty's Graduate School, is based on the Researcher Development Programme (RDP) and covers the four domains: knowledge and intellectual abilities (e.g. research methods); personal effectiveness; research governance & organisation (e.g. writing grant proposals); and engagement, influence and impact.

Students are supported by two supervisors (sometimes three for industrially-support students) with early career staff being coupled with experienced colleagues. Research students are fully integrated into the research culture of the Department, being expected to attend and present results at Department/group research seminars, and have representation on the Department Research Committee. Students also benefit from being part of a college system, with all research students being part of the Graduate College which serves as peer support and a social centre. **c10. Research student progress monitoring**

Student progression is managed by formal monthly meetings with supervisors to review progress, and to identify support or training needs, and any other issues. The resulting reports are reviewed by the Department Research Committee to help identify any problems at the earliest stage. The monthly reports are supplemented with annual checkpoints, involving submission of a research report, oral presentation of results, followed by a *viva voce* examination by a panel.

d. INCOME, INFRASTRUCTURE AND FACILITIES

d1. Research funding portfolio and future plans

Given that the Department was established at a late stage of the REF2014 cycle, there is little or no income or spend associated with it. The research income secured by submitted staff at their previous institutions over the REF period totalled £12 million, averaging £168k per academic per year. Of this £8,341k was from research councils, £891k from UK-based charities, £1,633k from UK Central Government, and health and hospital authorities, and £400k from the EU. This individual-based track record gives us confidence that we have the potential to secure the level of grant income required to underpin our research ambition. The aspirational research funding portfolio (based on our track record and plans) in broad terms is about 40% EPSRC, 10% BBSRC, 20% other (NERC, British Heart Foundation, Wellcome Trust), 15% EU, and 15% Industry. We anticipate the industry funding to increase substantially once the Reaction Centre is in place. The target grant income is at least £150k per academic per year (the corresponding figure for the top 12 institutions in RAE2008 was £110-180k, with Cambridge being an outlier at £238k).

d2. Provision and operation of specialist infrastructure and facilities

The Faculty has extensive infrastructure and facilities for chemical research which are available for Chemistry, including: high resolution X-ray diffraction, range of atomic force microscopes, field emission SEM, and a helium recovery system for NMRs, all housed in Physics; and a Biorad multiphoton confocal microscope, HCT ultra ion trap LC mass spectrometer system, CCL GM400 3 squid cryogenic magnetometer, Isoprime Ltd isotope ratio mass spectrometer with elemental



analyser, and a radiochemical laboratory, all housed in LEC. Lancaster's high performance computing facility comprises 2200 CPU cores and is to be refreshed in 2014, adding another 1000 cores. Complementing this is the N8 HPC cluster at Leeds (>5000 cpu cores).

d3. Investments (current and planned) in infrastructure and facilities

Chemistry has a capital equipment budget of £3 million to resource its research and teaching laboratories to the highest international standards. Major items purchased/being purchased include: NMR (300MHz for mostly teaching; 400MHz – multinuclear for research); mass spectrometry (MALDI-MS-MS to support polymer and materials characterisation, and tissue imaging; Q-TOF for accurate mass measurement in support of synthetic chemistry); HPLC and GPC that is also linked to MS to support materials characterisation; X-ray diffraction (single crystal) for structure determination; time-resolved spectrofluorimetry to support our fluorescent reagent synthesis and photovoltaic research; electroanalytical instruments for sensor development and general diagnostics; and glove boxes for air and moisture sensitive synthesis. In addition, Lancaster is investing £19M+ in the complete re-development of the chemistry space, to include a state-of-the-art synthetic chemistry laboratory kitted with 27 full-sized fumehoods designed to facilitate efficient and safe synthetic work of all types, and an NMR suite. The University is also committed to acquiring a 600 MHz solid-state NMR instrument using matched funding.

d4. Organisational infrastructure

The research activity of the Department is guided by the Department Research Committee (DRC) with input from the Department's Advisory Board. The DRC is chaired by the Director of Research and identifies strategic opportunities and initiatives including pathways to impact for the Department's research, oversees their implementation, monitors PhD studentship progression, and continually evaluates key performance indicators including grant success and outputs. The DRC includes a representative from each of the research teams, the Postgraduate Research Tutor, and a representative from the Department's Impact Strategy Group for knowledge translation issues. It meets monthly and reports to the Department Executive. The Department Executive is chaired by the Head of Department and also includes the Director of Research and the Director of Board of Studies and amongst other things manages the division of time for staff between research, teaching and administration. The research activities of the Department are reported to the Faculty by the Director of Research through the Faculty Research Committee, which then reports to the University Research Committee and serves as a conduit for exchange of information and for development and implementation of University's research strategy. The Advisory Board meets 6-monthly and has representatives from industry, academia and Government laboratories.

d5. Consultancies and professional services

The Reaction Centre will serve as our focal point for consultancy and contract professional services to the research user community, extending both the reach and impact of our research. e. COLLABORATION AND CONTRIBUTION TO THE DISCIPLINE OR RESEARCH BASE

e1. Exemplars of research collaborations

Industry collaborations: AstraZeneca (crystal growth; high throughput formulation platforms), GSK (drug synthesis), Unilever (skin lipids), British Petroleum (oil well surfactants), Johnson Matthey (Materials), Sharp (solar cells), DSTL (bacterial detection), Carbon Trust (algal biofuels).

Pl or Cl on multi-partner funded projects: (i) Anwar with Chinese Academy of Sciences Shanghai Institute of Materia Medica, EPSRC Science Bridges: *Bradford-China programme for pharmaceutical sciences and medical technology*, PI: P. Coates, £1.27M, 2009-2011; (ii) Anwar with Unilever Port Sunlight, Yorkshire Forward/Unilever Industrial Research and Development Award, *Natural oils for deodorant technologies*, PI: M. Noro, £2.0M, 2010-2012; (iii) Fielden with the UK Home Office, *A SERS-based biological agent detector*, PI: R. Goodacre, £1.74M, 2006-2009; (iv) Fielden with Warwick University, *Studying stochasticity in eukaryotic gene expression*, PI: J. McCarthy, BBSRC, £1.12M, 2010-2015; (v) Smith with UK NMR and materials community, (a) with Johnson Matthey resulting in solid state NMR being a key internal capability for them; (b) *Creation of a state of the art 850 MHz and supporting NMR infrastructure*, source AWM, PI: M.E. Smith, £1.0M, 2008-2012; (c) *Solid-state NMR at 850 MHz: A world-leading UK facility to deliver advances in materials science, chemistry, biology, Earth science and physics*, EPSRC, PI: S.P. Brown, £3.7M, 2008-2013; (vi) Trewin, multi-institutional collaboration involving Lancaster, Liverpool, and York, and industrial partners Croda and Unilever, *Renewable chemicals from sustainable feedstocks via high throughput methods*, PI: J. Lopez-Sanchez, £1.86M, 2013-17.

Collaboration on publications: Extensive international collaborators. Institutions represented



include Lawrence Berkeley National Laboratory (USA), NTU (Singapore), CAS-SIMM (Shanghai, China), BHU Varanasi (India), Karolinska (Sweden), Victoria (New Zealand), Deakin (Australia), Erlangen-Nuremberg (Germany), Merck Advanced Labs (S. Korea), Paris VI (France), Syracuse (USA), Aarus (Denmark), Oslo and Tromsoe (Norway), and Piemonte Orientale (Italy).

e2. Support for and exemplars of interdisciplinary research

Interdisciplinary research is part of our vision (see Chemistry's mission statement (c1)), hence support for it is embedded in our strategy. A significant number of our submitted outputs and others are inter-disciplinary, with applications in the domains of energy, sustainability & environment, life sciences and health care, and materials. The submitted impact case study on the drug galantamine resulted from interdisciplinary research between chemistry and biomedical sciences.

e3. Research interactions with users informing research activity and strategy An example here is the strategic intended decision to appoint staff in the area of chemistry underpinning synthetic biology, which resulted from discussions with industry (that included GSK, Pfizer, Croda, Unilever, Dr Reddys, Lucite, amongst others) as a part of N8 universities initiative culminating in the N8 Industry Innovation forum on Industrial Biotechnology (2013).

e4. Exemplars of leadership in academic community and esteem

Advisory groups: (i) Fielden: Member of the Home Office Science and Technology Reference Group; Chair of Home Office CBRN Advisory Group; Chair of CBRN Sub-Committee of the Scientific Advisory Panel for Emergency Response (SAPER); (ii) Smith: Member of National Management Committee for Ultrahigh Solid State NMR Facility; Chair, National CDT in Interdisciplinary Magnetic Resonance; EPSRC's Strategic Advisory Team for Infrastructure and also Strategic Advisory Network; author of EPSRC strategic review on NMR infrastructure; Member of the Prize Committee of the Ampère Society; (iii) Trewin: Royal Society round table discussion on Irreproducibility in Science.

Learned societies: (i) Anwar: Chinese Academy of Sciences (CAS) Visiting Professorship for Senior International Scientists; Fellow of the RSC, Royal Pharmaceutical Society, and the Academy of Pharmaceutical Sciences (APS); Elected Board Member of the APS; Committee Member and Lecturer on CCP5 Summer School; (ii) Fielden: Chair of RSC's Chemistry Electroanalytical Sensing Systems Group (Analytical Division); member of organising committee for Electrochemistry 200X series of meetings; RSC Faraday Discussion 2013 "Electroanalysis at the Nanoscale", and RSC's Analytical Research Forum; (iii) Danos: committee member, International Solar Energy Society (UK).

International invited/plenary lectures: (i) Anwar: Molecular Modelling Workshop 2013 (Erlangen-Nuremberg); China-Israel Bi-National Symposium on Drug Design, Changzhou, China,2010; Svedberg Seminar, Uppsala, Sweden, 2010; PSWC 2010, New Orleans, USA; APGI, Versailles, France, 2009; Gordon Conference, Waterville Valley, USA, 2009; TOP Institute Meeting, Utrecht, Netherlands, 2008; Helsinki Drug Research, Helsinki, 2008; (ii) Coogan: International Symp. on Organometallic Chemistry VIII, Camerino, Italy, 2011; Institute of Inorganic Chemistry, Zurich, 2012; (iii) Middleton: SHR North American section meeting, Alberta, Canada, 2012; Amyloids, Prions and Precursors, Halle, Germany, 2011; Sandbjerg Meeting on Ion Transport in Health and Disease, Denmark, 2008 (Speaker and Chair); (iv) Smith: Int. Congress on Glass Science, Brazil, 2010; Int. Symposia on DNP, Koenigstein 2009 & Lausanne 2011; Brazilian Summer School on Solid State NMR, Rio de Janeiro, Brazil, 2010.

Visiting fellowships/appointments: (i) Anwar: CAS Shanghai Institute of Materia Medica.

Journal editorship/editorial boards: (i) Coogan: Guest Editor, Organometallics, 2012; (ii) Peach: Guest editor, PCCP "Frontiers of Density Functional Theory, 2013; (ii) Middleton: Associated Editor, Molecular Membrane Biology; (iii) Smith: Editorial Board for Solid State NMR; Advisory Board for Journal of Applied Magnetic Resonance.

Grant review panels: (i) Fielden: Chair & Member of EPSRC Chemistry, BBSRC Synthetic Biology Panel; EPSRC's CDT Panel; Expert advisor – Norwegian Research Council; (ii)Middleton: National Solid-State NMR Facility Time Allocation Panel; BBSRC Committee C Pool; (iii) Smith: EPSRC(see advisory groups above); DFG (Germany) and NSERC (Canada) panels.

Organisation of conferences: Peach: Conference Chair, DFTM 2012, Ghent, Belgium; Coorganiser, DFT2013, Durham.