Institution: University of Bristol

Unit of Assessment: Chemistry UoA 8

a. Overview

The School of Chemistry is one of the largest Chemistry departments in the UK, and its research is internationally recognised for quality, breadth and impact as exemplified by the number of staff recently elected Fellows of the Royal Society (**one** in ***each*** of the last ***five*** years). Moreover, the School's building and instrumentation infrastructure is either new or completely refurbished since 1999 as a result of >£50m investment.

The School of Chemistry (SoC) maintains a traditional managerial structure with three sections, namely Inorganic & Materials, Organic & Biological, and Physical & Theoretical, but the School's research profile is defined according to **nine** themes, each with a critical mass of reseachers, which inform future strategy in terms of both staffing and infrastructure investment. These themes are **Soft Matter, Colloids and Materials**; **Energy**; **Supramolecular and Mechanistic Chemistry**; **Catalysis**; **Synthesis**; **Biological and Archaeological Chemistry**; **Spectroscopy and Dynamics**; **Atmospheric and Global Change Chemistry**; **Computational and Theoretical Chemistry** which encompass the frontiers of research in the discipline and broadly follow those used in the RAE 2008 submission but with the addition of **Energy** to reflect new activity. These themes are not intellectual silos, however, and there is much intradisciplinary research which crosses these boundaries as well as inter- and multi-disciplinary activity involving other Departments both in Bristol (*eg* Physics, Biological Sciences, Biochemistry, Earth Sciences, Archaeology) and beyond. Many interactions are also facilitated by more formal SoC Centres, such as the *Centre for Computational Chemistry* and the *Centre for Organised Matter Chemistry*, as well as multi-departmental groupings such as the *Cabot Institute* and the *Centre for Nanoscience and Quantum Information*.

The quality of the SoC's research outputs since RAE 2008 in all research themes (REF 2 and Section **b** which highlights significant discoveries) is amply illustrated by the volume of publications in the highest impact journals. For example, since 1 January 2008, SoC staff have published a total of 10 papers in *Science*, 6 in *Nature*, 9 in *Nature Chemistry*, 4 in *Nature Materials*, 76 in *J Am Chem Soc*, 80 in *Angew Chem*, 14 in *Chemical Science,* 11 in *PNAS* and 13 in *Phys Rev Lett*. Moreover, two examples of signal successes beyond the expectations set out in the RAE 2008 RA5 document are the award of: (i) EPSRC Centres for Doctoral Training in *Chemical Synthesis* and in *Functional Nanomaterials* (both recently renewed) which have driven much new collaborative research and attracted PG students of the highest quality, and (ii) substantial EU research funding, as exemplified by the award of **seven** ERC Advanced Investigator Grants since 2008.

Research activity is supported through income raised externally from Research Councils (EPSRC, BBSRC, NERC, ERC), Government (*eg* The Royal Society, AWE, DECC, USAF), charities (*eg* Welcome, Leverhulme, Cancer Research UK) and industry (*eg* GSK, AstraZeneca, Syngenta, Novartis, Pfizer, Merck, BP, Shell, DSM, Sasol, Lucite, Element 6, GKN Aerospace, Infinium, EON AG, Hewlett Packard, Unilever, BASF) with significant additional University investment in building refurbishment and instrumentation. Full details are in REF 4b/c and a summary is in Section **d**.

All research is led by Category A staff (REF 1a) which comprise research leaders (42) and Early Career Researchers (7) supported by Research Assistants, either SoC staff (9) or employed as PDRAs (75 at 31 July 2013) on research grants or their own personal Fellowships, including 11 current EU Marie Curie PDFs (23 since the start of 2008). Research activity is also critically dependent on the large postgraduate (PGR) body (REF 4a and Section **c(ii)** below) most of whom are PhD students (~225 at 31 July 2013) funded by RCUK (primarily EPSRC but including BBSRC and NERC) either through the DTG, ICASE or one of the CDTs (*Chemical Synthesis*, *Bristol Centre for Functional Nanomaterials, Advanced Composites, BBSRC SWDTP*), industry or overseas funding sources (typically 17-20% of PGRs are non-UK/EU).

The HEFCE-funded Centre for Excellence in Teaching and Learning (CETL), Bristol ChemLabS established in 2005, offers many opportunities for PGs in outreach and public engagement activities (winner of **3** Business in the Community Big Tick Awards) nationally and internationally and all who take part (>400 since 2005) are trained as STEM Ambassadors. Furthermore, the highly innovative, web-based, interactive teaching laboratory software (the Dynamic Laboratory Manual or DLM; winner of the THE Outstanding ICT Initiative of the Year Award in 2010) has evolved from an undergraduate resource to support many aspects of PG research training.

Impact is detailed in REF 3 but one highlight to note here is the very significant commercial opportunity afforded by the School's spin-out, Revolymer Ltd which designs, develops and formulates novel polymers to revolutionise consumer products including **Rev7**, a non-stick, degradable chewing gum, launched in the USA in 2011.

b. Research Strategy

The School's strategy for research is to be internationally leading in the key themes identified in Section **a** by maintaining a critical mass of well-funded, world-class researchers in each theme. Future activity is informed by a view on how these themes will develop, and by being alert to new themes (*eg* **Energy** since RAE 2008) which capitalise on existing expertise and exploit emerging opportunities. The School appoints a Research Director who plays a leading role in strategy development and who chairs a Research Opportunities Group (ROG) comprising key research leaders the remit of which is to define and articulate areas of research excellence and to consider future directions in the short, medium and longer terms including both staffing and funding. Decision making is the responsibility of the Head of School, Section Heads and Research Director informed on specific issues both by ROG and through wider consultation which takes place within the SoC and also with a Faculty Research Director. The School maintains a Research Strategy document and a Departmental Plan which both articulate strategic research ambitions and inform a UoB led Departmental Review which takes place every 5 years (most recently in 2012).

Evidence of the success of the School's strategy and ambition to achieve excellence in each theme is set out below with, for each theme, a list of active staff (core funded and ECR) and a brief description which also highlights intradisciplinary work across themes. This is followed by a collection of selected, high impact research highlights for the period 1 January 2008 to 31 December 2013, the majority of which are also listed as individual staff outputs in REF 2; in some cases, a particular output is highlighted in more than one theme in order to demonstrate intradisciplinary activities referred to above and these publications are <u>underlined</u>. For each theme, **Future Directions** anticipates new developments, articulates the challenges which lie ahead and offers a realistic expectation of likely achievements. In all cases, research capability is critically dependent on people, grant income, infrastructure, and facilities, the strategies for the maintenance and development of which are addressed in Sections **c** and **d**.

Soft Matter, Colloids and Materials

Allan, Ashfold, Bartlett, Briscoe, Davis(S), Eastoe, Faul, Fox, Hall, Mann, Manners, May, Royall, van Duijneveldt, Wass, Woolfson

Research under this heading comprises activity in several sub-themes much of which is focused through the SoC's *Centre for Organised Matter Chemistry*.

Highlights. In ***soft matter self-organisation*** the first direct experimental evidence for a long-sought structural mechanism for dynamical arrest was shown (**Royall**, *Nature Materials* 2008, *Phys Rev Lett* 2010 & 2012) and a new class of protein-based biomaterials based on α-helical peptide hydrogels for cell growth (**Woolfson**, *Nature Materials* 2009) and *de novo* design of gigadalton peptide-based structures (**Woolfson**, *PNAS* 2012, *Science* 2013) were pioneered. Solvent-less liquid proteins and viruses (**Mann,** <u>*Nature Chemistry* 2010</u>; *Angew Chem* 2009; *Adv Mater* 2012) were discovered and unprecedented hyper-thermophilic stability and folding dynamics in solvent-free liquid myoglobins were established (**Mann**, *J Am Chem Soc* 2012; *Chem Sci* 2012). For ***complex self-assembled nano- and microstructures***, new synthetic approaches to controlled structures over multiple length scales based on block copolymer self-assembly were demonstrated (**Manners**, *Science* 2012; *Nature Materials* 2009; *Nature Chemistry* 2010, **Faul**, *J Am Chem Soc* 2013), an overarching framework for the self-assembly and transformation of hybrid nano-objects and nanostructures was established (**Mann**, *Nature Materials* 2009) and a new model of protocell compartmentalisation based on membrane-free peptide/nucleotide microdroplet assembly was reported (**Mann**, <u>*Nature Chemistry* 2011</u>). In the field of ***functional materials and interfaces*** the structural properties of hierarchical sea-urchin spines were elucidated for the first time (**Davis(S)**, *PNAS* 2012) while the first ionic liquid-mediated synthesis of phase-pure functional oxides was reported (**Hall**, *Adv Mater* 2012). The development of novel CO_2-philic surfactant systems was described (**Eastoe**, *Angew Chem* 2009), along with addressable surfactants utilised for magnetic control over liquid surface properties (**Eastoe**, *Angew Chem* 2012; *Adv Mater* 2012), and photo-responsive hybrid structures (**Faul**, *Adv Mater* 2012). The first example of bio-based motifs for hierarchical porous polymeric constructs was reported (**Faul**, *Angew Chem* 2011) and the use of diamond as a substrate for biological cells for brain-computer interface implants was demonstrated (**May**, *IEEE* 2011). Fundamental insights into polymer brush lubrication under physiological conditions were reported (**Briscoe**, *Science* 2009) and nanoparticles were shown to cause DNA damage across a cellular barrier (**Davis(S)**, *Nature Nanotech* 2009).

Future Directions. The overarching aim in this theme is to maintain and advance our international leading status in pioneering chemical strategies for the design and controlled assembly of materials across multiple length scales, interfaces and functionalities with applications in energy, health and biology. More specifically, we will continue to explore the chemistry and synthetic biology of artificial cells and functional protein-polymer nanoconstructs, nano- and mesoscale structural and functional control for novel electroactive and supramicellar constructs, biotemplated high T_c superconductors, nanoparticle-biomembrane interactions, control of gelation behaviour and colloidal aggregation and absorption phenomena including self-assembly and phase separation processes, and novel diamond-neuronal interfaces. We will also aim to pioneer innovative analytical, imaging and scattering methodologies for advanced materials characterisation that will be underpinned by fundamental developments in theoretical modeling, simulation and calculations.

Energy

Faul, Fermin, Fox, Manners, Wass

This theme represents a new priority for the SoC since RAE 2008 and comprises research in both chemical energy and solar energy conversion.

Highlights. Research highlights in ***chemical energy conversion*** relevant to portable hydrogen-storage materials and high performance electrocatalysts for low temperature fuel cell systems include detailed mechanistic studies on hydrogen transfer in ammonia-borane systems (**Manners**, *J Am Chem Soc* 2012) and tuning electrocatalytic activity of ultrathin Pd-nanoshells by controlling their average lattice strain (**Fermin**, *J Phys Chem C* 2011). Recently, the current best homogeneous catalysts for the conversion of ethanol to butanol have been developed (**Wass**, *Angew Chem* 2013). With regard to ***solar energy conversion***, highlights include the development of materials with tuneable optical and electronic properties based on oligo(aniline)s (**Faul**, *Chem Eur J* 2011), as well as insight into charge transfer kinetics involving quantum dots self-assembled at electrode surfaces (**Fermin**, *J Am Chem Soc* 2010). Nanostructured and doped diamond films are providing new paradigms for photothermal solar energy harvesting (**Fox**, *Nano Energy* 2012; **Fox**, *Phys Rev B* 2010; **Fox** & **Fermin**, *Langmuir* 2011).

Future Directions. We will continue to focus on fundamental principles associated with active materials and catalysts in both chemical and solar energy conversion processes. Key areas will continue to include the development of catalysts for upgrading biomass derived alcohols to more advanced biofuels, low-temperature conversion of methane to methanol, molecular compounds for hydrogen storage, active layers for thin-film photovoltaic systems, and novel functional materials for photoinduced water-splitting and CO_2 conversion to fuels. Fundamental quantum mechanical aspects of light harvesting in nature and how they can inform efficient solar energy capture will be explored together with interdisciplinary research on the study of materials for electrocatalysis and solar energy conversion as well as nuclear-focused research such as neutron-irradiated graphite as beta-radiation sources for incorporation into diamond-based, beta-voltaic nuclear batteries and thermionic energy converters. Much of this multidisciplinary research will be facilitated through the *Cabot Institute* and *the Bristol-Oxford Nuclear Research Centre*.

Supramolecular and Mechanistic Chemistry

Aggarwal, Butts, Bedford, Davis(A), Harvey, Russell

This theme combines the disciplines of ***supramolecular chemistry*** with studies which probe ***mechanism*** across a range of reaction types particularly relevant to **Catalysis** and **Synthesis**.

Highlights. Research in ***supramolecular chemistry*** has led to a series of "synthetic lectins" able to bind carbohydrates in water with high selectivities (**Davis(A)**, *Angew Chem* 2009; *Nature*

Chem 2012) and steroid-based nanoporous crystals have been exploited to create CNT-like environments (**Davis(A)**, *Angew Chem* 2010) and organic alloys (**Davis(A)**, *Angew Chem* 2011). ***Mechanistic*** studies have been employed to develop an oxidative synthesis of biaryls from arenes and silylarenes (**Russell**, *Science* 2012), and to provide insight into lithiation-borylation methodology for the enantiosynthesis of tertiary alcohols (**Aggarwal**, *Nature* 2008; *Angew Chem* 2010). Combined mechanistic and theoretical studies have thrown light on iron-catalysed Negishi cross-couplings (**Bedford** & **Harvey**, *J Am Chem Soc* 2012) and boron-zinc transmetallation (**Bedford** & **Harvey**, *Angew Chem* 2012), and in NMR, a widely applicable new protocol for 3D structural determination from nOe data has been demonstrated (**Butts**, *Org Biol Chem* 2011).

Future Directions. In terms of supramolecular chemistry, a major aim for the future will be the development of systems which can be applied in biomedical contexts, especially carbohydrate receptors (synthetic lectins), anion transporters (with potential for treating channelopathies such as cystic fibrosis) and steroid-based nanoporous alloys (for drug delivery). Mechanistic studies will focus on determining the mechanisms involved in cutting-edge catalysis (in particular with paramagnetic iron catalysts) and synthesis (particularly with complex transmetallation processes using main-group nucleophiles) by employing combined structural, kinetic and computational approaches. In NMR spectroscopy, we will focus on the application of accurate internuclear distance measurements to elucidate the structural and dynamic nature of small molecules in solution which will be complemented by the development of new experimental NMR methods in the solution state, and in confined media such as liquid crystals, through new Residual Dipolar Coupling matrices.

Catalysis

Bedford, Booker-Milburn, Bower, Fey, Harvey, Manners, Orpen, Pringle, Russell, Wass

The catalysis theme is wide-ranging both in terms of the systems studied and the methods used and covers areas as disparate as fine chemicals, biofuels and composites. There is considerable synergy with the themes **Energy**, **Synthesis**, **Computational and Theoretical Chemistry** and **Supramolecular and Mechanistic Chemistry**.

Highlights. Research highlights include advances in new catalytic reactions and methodology including gold-catalysed direct arylation (**Russell**, *Science* 2012), iron-catalyzed C-C bond formation (**Bedford** & **Harvey**, *J Am Chem Soc* 2012), mild C-H bond activation (**Bedford**, *Angew Chem* 2011; **Booker-Milburn**, *Angew Chem* 2009) and intra- and intermolecular Pd(II)-catalyzed heterocycle generation (**Booker-Milburn**, *J Am Chem Soc* 2008; **Bower**, *Angew Chem* 2012). Materials catalysis highlights include the dehydrocoupling of amine-boranes (**Manners**, *J Am Chem Soc* 2010 and 2012, *Angew Chem* 2013) and the self-healing of composite materials (**Wass**, *Adv Func Mat* 2011) while ligand design and organometallic chemistry highlights include transition metal frustrated Lewis pairs (**Wass**, *J Am Chem Soc* 2011), predictive tools for catalysis (**Fey** & **Pringle**, *Angew Chem* 2012), mechanistic understanding and defining structure-activity relationships (**Pringle**, *J Am Chem Soc* 2008), and the structure and reactivity of Tsuji-Trost allylation intermediates (**Fey**, *J Am Chem Soc* 2008).

Future Directions. Homogenous catalysis will remain a major focus of our activity in all of the areas highlighted above but also increasingly as part of collaborative research with other catalysis disciplines (biological, heterogeneous, chemical engineering) via local partner universities and the UK Catalysis Hub. A key strength will be the synergy between experimental and computational studies with overarching objectives being the catalytic valorisation of existing and sustainable feedstocks, discovery of new catalysts led by fundamental organometallic/ligand chemistry, and improving catalyst performance by mechanistic understanding. We will continue to respond to and pre-empt the needs of the potential end-user community for pharmaceutical and fine chemical synthesis, bulk petrochemicals and materials, and energy and fuels.

Synthesis

Aggarwal, Booker-Milburn, Bower, Davis(A), Galan, Gallagher, Gates, Manners, Norman, Pringle, Russell, Willis, Woolfson

Chemical synthesis underpins a multitude of research encompassing organic, inorganic, materials and biological and is significantly augmented by the presence of the *Chemical Synthesis* CDT.

Highlights. Total syntheses highlights include a 7-step synthesis of prostaglandin $PGF_{2\alpha}$ (**Aggarwal**, *Nature* 2012), Californian red scale beetle pheromone (**Aggarwal** & **Willis**, *Angew Chem* 2012), (+)-faranal (**Aggarwal**, *Angew Chem* 2009) and cytisine (**Gallagher**, *Angew*

Chem 2011) while new methods and applications have included a fundamental new approach to quaternary stereogenic centres by boronic ester homologation (**Aggarwal**, Nature 2008; *Angew* 2011), the first room temperature Pd(II) catalysed C-H activation of anilides for heterocycle synthesis (**Booker-Milburn**, *J Am Chem Soc* 2008; *Angew Chem* 2009), reaction control by photon flux (**Booker-Milburn** & **Orr-Ewing**, *Angew Chem* 2008), room temperature, neutral solvolysis and substitution of hindered amides (**Booker-Milburn**, *Angew Chem* 2012), facile access to complex *N*-heterobicyclic scaffolds by $Pd/P\{C_6H_3(CF_3)_2\}_3$ catalysis (**Bower**, *Angew Chem* 2012), simple synthetic lectins for glucose recognition and sensing (**Davis(A)**, Nature Chem 2012), α-selective synthesis of 2-deoxygalactosides by organocatalysis (**Galan**, *Angew Chem* 2012), a new synthetic method for the rational creation of non-centrosymmetric, high aspect ratio, colloidally stable core-shell nanoparticles (**Manners**, *Science* 2012), new routes to diastereomerically pure phosphacyclic ligands for catalysis (**Pringle**, *J Am Chem Soc* 2009, *Angew Chem* 2012), new Prins cascades for the rapid stereocontrolled construction of bicyclic oxygen heterocycles (**Willis**, *Angew Chem* 2012) and *de novo* peptide assembly of fibres and discrete nanostructures (**Woolfson**, *J Am Chem Soc* 2012).

Future Directions. Future directions will include exploring a fundamentally new approach to molecular complexity in which boronic esters will be reacted iteratively with enantiopure carbenoids to give natural and non-natural products with complete stereocontrol (ultimately automated) and we will study applications of photochemical flow technologies with the objective of discovering new reactions and the construction of complex new-molecular space inaccessible *via* ground state chemistry. New stereoselective metal-catalysed ring expansion, cyclisation, C-H activation and C-C bond-forming processes will be explored to target complex natural and non-natural products and new asymmetric reactions will be examined in relation to efficient synthesis of oxygenated polycyclic compounds, unusual deoxy sugars to give scaffolds for bioactive targets, and to allow access to novel "drug like" scaffolds to understand the impact of chirality on biological interactions. Sustainable routes to organophosphorus chemicals will be developed and we will also study hindered amides/ureas as 'Trojan Horse' ketenes/isocyanates in relation to labile enzyme inhibitors and genetic mutation and synthetic isotopic labeling techniques will target new metabolites and *O*-glycan probes to establish natural product structure, biological pathways and provide biomedical diagnostics. *De novo* protein design will focus on synthetic enzymes for stereo and regioselective organic transformations and new peptide-carbohydrate hybrid materials for applications in tissue engineering and regenerative medicine. Novel molecules with amphiphilic cores will be targeted as biomimetic receptors and synthetic methods for the preparation of self-assembled materials with hierarchical structures on the 10nm-10μm scale with bio-inspired precision and function will be examined.

Biological and Archaeological Chemistry

Briscoe, Bull, Cox, Crosby, Crump, Davis (A), Evershed, Galan, Gallagher, Gates, Haddrell, Harvey, Mann, Mulholland, Simpson, Willis, Woolfson

This theme combines two cognate disciplines of Biological (the larger, including biomaterials, chemical biology and synthetic biology) and Archaeological Chemistry (focusing on bio-organic compounds of archaeological significance).

Highlights. Regarding ***biomaterials*** and fundamental aspects of ***protein structure and function***, a simple multi-conformation model which accounts for the unusual temperature dependence of kinetic isotope effects in enzyme reactions has been developed (**Harvey** & **Mulholland**, Nature Chem 2012) and improvements in the modelling of enzyme reaction mechanisms in general have been made (**Harvey** & **Mulholland**, *J Am Chem Soc* 2012). The synthesis and properities of solvent-free liquid proteins have been described (**Mann**, Nature Chem 2010) as well as new insights into protein structure, stability and function (**Woolfson**, *Nature Chem Biol* 2010) whilst the structure of a hitherto unobserved protein fold has been designed and determined (**Woolfson**, *Nature Chem Biol* 2011). The structural and functional evolution of the IGF2 receptor interaction has been defined (**Crump**, *Science* 2012) and the solution structure of a photoswitchable peptide complexed to the pro-survival protein Bcl-xL has been determined (**Crump**, *J Am Chem Soc* 2012). In ***synthetic biology***, the foundations for a new modular approach to protein design and engineering has been developed (**Woolfson**, *J Am Chem Soc* 2009; *Synth Biol* 2012) and a new model of protocell construction and function has been reported (**Mann**, Nature Chem 2011). In carbohydrate ***chemical biology***, high-affinity, high-specificity interactions of natural carbohydrates to synthetic lectins have been defined (**Crump** & **Davis(A)**, *Angew Chem* 2009 & 2012), a stereoselective synthesis of 2-deoxygalactosides has been reported (**Galan**, *Angew Chem* 2012) and non-covalent interactions using a synthetic peptide model have been measured (**Gallagher** & **Woolfson** *Angew Chem* 2011). In ***polyketide research***, the question of how fungi make tropolone has been resolved (**Cox**, *PNAS* 2012) and novel metabolites from cultures providing insight into thiomarinol biosynthesis have been identified (**Simpson** & **Willis**, *Angew Chem* 2011). In ***archaeological chemistry***, the application of new lipid-based isotope proxies has provided the earliest evidence of milk use 8,500 years ago (**Evershed**, *Nature* 2008), revealed that milking of cattle began at least 6500 years ago (**Evershed**, *Nature* 2012), demonstrated the earliest evidence of cheese making in prehistoric Europe (**Evershed**, *Nature* 2012) and shed light on horse domestication in Europe 7000 years ago (**Evershed**, *Science* 2009).

Future Directions. The focus of new work will be in understanding the fundamental principles of biological processes such as biomolecular folding, interactions, assembly and function specifically regarding carbohydrates, peptides, proteins and membranes. In ***biomaterials*** we will work with cell biologists and clinicians to design new materials for 3D cell growth in cell culture and *in situ* moving towards applications in tissue engineering. In ***chemical biology***, we will study NMR and mass-spectrometry methods to screen and characterise small-molecule-protein interactions, and apply these to generate leads for new pharmaceuticals coupled with improved theoretical understanding of small-molecule binding and catalysis by enzymes together with probing sequence-to-structure relationships in protein folding and structure prediction. In ***synthetic biology***, we will continue to expand the toolkit of standard protein-folding components, and apply it to the *de novo* design of protein-based materials and encapsulation systems. We will also seek to develop systems for capturing and controlling the activity of enzymes, and the polyketide group will aim to manipulate multi-enzyme pathways in bacteria and fungi to generate new pathways to produce bioactive compounds. Related to this, and also to **Synthesis**, we will study synthetic methods for expediting the making of bioactive compounds through chemical synthesis and combine synthetic chemistry and computer-aided design to attempt to engineer new peptide-and protein-based catalysts. We will also look to design, construct and characterise supramolecular probes for the detection and analysis of sugars and ions in biology and develop automated methods for carbohydrate synthesis. In ***archaeological chemistry***, future research into human prehistory will continue to use innovative analytical chemical approaches to provide hitherto unattainable levels of molecular and isotopic information from complex organic residues associated with aged bioorganic materials, including pottery and skeletal remains, recovered from sites across the world.

Spectroscopy and Dynamics

Ashfold, Butts, Crump, Orr-Ewing, Reid, Roberts, Shallcross, Western

Laser spectroscopy is used to study molecular dynamics on fs to μs timescales and aerosols at the single-particle level. The SoC also engages in important new work in NMR spectroscopy.

Highlights. Photodissociation dynamics have been probed by high-resolution velocity imaging and translational spectroscopy to explore non-adiabatic dynamics, *eg* at conical intersections between potential energy surfaces (**Ashfold**, *PNAS* 2008; *J Chem Phys* 2011). Pioneering studies have been carried out using femtosecond lasers contrasting chemical reaction dynamics in bulk liquids with those of isolated molecules (**Orr-Ewing**, *Science* 2011; *Chem Sci* 2012) and extended to aromatic molecule photochemistry in solution (**Ashfold**, *Faraday Discuss* 2011). The PGOPHER program (**Western**) is now internationally established as *the* spectral simulation software of choice for gas-phase spectroscopy and dynamics studies. The first ever direct detection of carbonyl oxide (Criegee) intermediates, crucial in atmospheric oxidation pathways, is enabling kinetic studies of their reactions (**Shallcross**, *J Am Chem Soc* 2008; *Science* 2012 & 2013) and particle manipulation with light beams has permitted ground-breaking studies of single aerosol particle optical properties and condensation, evaporation and coalescence dynamics (**Reid**, *PNAS* 2012; *Phys Rev Lett* 2010) allowing the viscosity of particles to be retrieved over a range of 12 orders of magnitude. New NMR methods aimed at solution-state structure determination (**Butts**) and biological high-field NMR spectroscopic work on IGF-2 (**Crump**) are noted above in **Supramolecular and Mechanistic Chemistry** and **Biological and Archaeological Chemistry** respectively.

Future Directions. We will continue to build on world-leading strengths in fundamental spectroscopy and dynamics on timescales from fs upwards and in applications of spectroscopy to atmospheric, aerosol, structural and biological chemistry. New advances will be underpinned by innovative developments in instrumentation and through collaborations with computational chemistry colleagues. Contrasting studies in molecular beams and in liquids will explore how solvents modify potential energy surfaces, non-adiabatic couplings between electronic states, and nuclear dynamics on ultrafast timescales, and will be extended to study biological chromophores. Unimolecular and bimolecular rates of reactions of key atmospheric intermediates will be measured using newly discovered absorption bands. Cutting-edge optical and electrodynamic trapping techniques will be employed to investigate the response of a wide range of aerosol particles to humidity and temperature, *eg* to explore the fabrication of microparticles and the dynamic process and consequent health impacts following aerosol particle inhalation into the respiratory tract. Improved NMR measurement of solution-state structural parameters will allow detailed determination of molecular conformations in complex dynamical systems and solution state NMR spectroscopy will be used to drive the optimisation of protein based therapeutics ('biologics') as demonstrated with the development of the IGF-2 ligand trap. New high-throughput cryoflow NMR screening and computational studies of molecular docking to proteins will also be combined to improve the hit-to-lead phase of drug development.

Atmospheric and Global Change Chemistry
Bull, Glowacki, Evershed, Haddrell, O'Doherty, Orr-Ewing, Pancost, Reid, Rigby, Shallcross
Research in this theme ranges from fundamental gas phase kinetic studies through state-of-the-art monitoring and modelling of greenhouse gases to mechanistic evaluation of past climate change and human impact on the environment.

Highlights. Highlights have been underpinned by advances in analytical chemistry, which encompass diatomic to macromolecular scales, and their application to laboratory studies and field measurements, in parallel with computer modelling on local to global scales. Branching between atmospheric oxidation pathways of acetylene has been shown to be controlled by non-thermalised vibrational excitation of intermediate adducts (**Glowacki**, *Science* 2012), challenging assumptions of local thermal equilibrium in atmospheric chemistry. Beyond the atmospheric impact of the Criegee intermediate and aerosol studies highlighted in the **Spectrocopy and Dynamics** section, applications of new analytical techniques included innovative cavity ring-down spectroscopy methods for trace gas sensing (**Orr-Ewing**, *Appl Phys B* 2011), and optical tweezer studies fundamental to aerosol-cloud interactions (**Reid**, *Atmospheric Chem Phys* 2011). GC-MS measurement of trace atmospheric constituents has culminated in the first high-resolution record of atmospheric HFC concentration (**O'Doherty**, *Atmospheric Chem Phys* 2010) making major contributions to international campaigns, *eg* AGAGE (NASA) and SOGE (EU). These developments have also led to new understanding of climate change (**Rigby**, *Geophys Res Lett* 2008), evidence that climate sensitivity is higher than models predict (**Pancost**, *Geology* 2009, *Earth and Planetary Sci Lett* 2010), and documentation of major agricultural advances during human prehistory (**Evershed**, *Nature* 2008; *Science* 2009).

Future Directions. With world-leading expertise in the development and application of state-of-the-art molecular and isotope ratio mass spectrometry we aim to characterise the global environment through the rigorous analytical and process-based examination of the atmosphere, biosphere and geosphere, and their interactions via biogeochemical cycles. This ambition is embedded in the wider University of Bristol strategy to address fundamental future societal challenges in global environmental change via the *Cabot Institute* with themes including interrogating the biogeochemical 'tipping elements' that govern whether soil is a greenhouse gas sink or source, using laboratory measurements to achieve a step change in our understanding of aerosol-cloud interactions, applying reactive tracer technology to probe Criegee chemistry in urban and forest environments, and linking our recent advances in the biomolecular understanding of the carbon cycle to macronutrient cycling across a range of temporal and spatial scales. Collectively, this will allow us to understand and model feedback responses to climate change, from geological timescales to predictions for the next century. Engagements with other disciplines to impact UK and international policy will continue (AGAGE) along with authorship and research contributions to the IPCC, and UK partnerships with DECC, the MET Office, NOC, BAS, IGER, CEH and many other RCUK Institutes.

Computational and Theoretical Chemistry

Allan, Fey, Glowacki, Harvey, Manby, Mulholland, Rigby, Royall, Shallcross, Tew

Computational and Theoretical Chemistry impacts on many aspects of research activity in the SoC both in its own right but also through numerous collaborative interactions much of which is highlighted for the other themes.

Highlights. Research highlights include development of local and explicitly correlated approaches to describe molecular electronic structure (**Manby**, *J Chem Phys* 2009; **Tew**, *J Chem Phys* 2010) as well as novel approaches to treating the correlation problem (**Manby**, *J Chem Phys* 2010 & 2011; *J Chem Theo Chem* 2012). A new theoretical approach for modelling atmospheric kinetics in a tractable yet rigorous way has been developed (**Shallcross**, *Atmos Environ* 2008) and computation has been used to predict the properties of materials (**Allan**, *Phys Rev B* 2009), to explore non-adiabatic reaction mechanisms in organometallic chemistry (**Harvey**, *J Am Chem Soc* 2009) and to design new ligands for organometallic catalysis (**Fey** & **Pringle**, <u>*Angew Chem* 2012</u>). The quantum dynamics of hydrogen tunnelling have been computed to high accuracy from first principles for a system of unprecedented complexity (**Tew**, *J Chem Phys* 2008) and new insight into the reaction mechanism of several enzymes related to human health has come from molecular dynamics and electronic structure calculations (**Mulholland**, *J Am Chem Soc* 2012; **Harvey** & **Mulholland**, *PNAS* 2011). Furthermore, a new general model has been proposed to account for the relation between protein structure and reactivity (**Mulholland** & **Harvey**, <u>*Nature Chem* 2012</u>) and in statistical mechanics of condensed phases, computation has been used to provide a new understanding of liquid-glass phase transitions (**Royall**, *Nature Mater* 2008; *Phys Rev Lett* 2012) and of reaction dynamics in liquids (**Glowacki**, **Harvey** & **Orr-Ewing**, *Nature Chem* 2011).

Future Directions. World-leading expertise in this area spans fundamental theory and algorithm development to applications across chemistry and beyond leading to many collaborations within the *Centre for Computational Chemistry* and with other colleagues in Bristol and elsewhere. A key current and future strength is and will be the development of accurate and innovative methodologies for treating molecular electronic structure in extended systems. Theory and software development for modelling reaction dynamics, atmospheric kinetics, and biomolecular chemistry will also be targeted and we will continue to develop our significant expertise in applying electronic structure and simulation methods to understanding the properties of minerals and materials, organometallic compounds, and proteins. In the coming years, there will be a focus on using our expertise on reaction mechanisms relevant to biological and organometallic catalysis to provide insights for designing new catalysts. Theory will also seek to expand still further from its traditional strongholds of small molecules, and simple liquids and solids to model the structure and dynamics of new materials, biomolecules, nanoparticles and colloids, and other complex systems.

c. People, including:

i. Staffing strategy and staff development

Currently, the School has an academic complement of 63 staff comprising 32 Professors, 6 Readers, 5 Senior Lecturers and 2 Lecturers plus another two proleptic lectureship appointments (**Glowacki**, **Royall**) with only one staff member over the age of 60. Included in the 63 staff are 9 Research Associates and 3 Teaching Laboratory Fellows who support research and teaching activities respectively. **Six** current staff are Fellows of the Royal Society, **five** staff having been elected in the last **five** years. There are also 10 University Senior Research Fellows, formally retired, 4 of whom are FRSs, who remain research active through collaborations with current staff and/or act as mentors to younger colleagues.

Academic staff (and postdoctoral staff and postgraduates) have an exceptionally strong track record of winning highly prestigious national and international research-based awards, *eg* since 1 January 2008, **eight** staff have either been awarded or continue on RS Wolfson Research Merit Awards (**Aggarwal**, **Evershed**, **Lloyd-Jones** (recently left), **Mann**, **Manby**, **Manners**, **Orr-Ewing**, **Pancost**), **seven** have secured ERC Advanced Investigator Grants (**Aggarwal**, **Evershed**, **Mann**, **Manners**, **Orr-Ewing**, and most recently **Pancost**, **Woolfson**), and several hold, or have recently held, externally funded Fellowships including EPSRC Senior Research Fellowships (**Aggarwal**), Leadership Fellowships (**Mulholland** & **Reid**) and Career Acceleration Fellowships (**Galan**) as well as Early Career Fellowships listed below.

The SoC currently hosts 7 Early Career Researchers (ECRs) all on competitively awarded, independent Fellowships, including the RS URFs **Bower**, **Glowacki**, **Royall** and **Tew**, the NERC ARF **Rigby** and Ramsay Fellow **Roberts**. Since 1 January 2008, several previous Fellowship holders have moved on to take up academic positions here or elsewhere including **Greaves** (EPSRC CAF to lectureship at Heriott-Watt, 2012), **Habershon** (Leverhulme Trust Fellow to lectureship at Warwick, 2012), **Hall** (RS URF to Bristol SoC lectureship, 2012), **Hart** (Ramsay Fellow to lectureship at UNSW, Sydney), **Hudson** (EPSRC ARF to lectureship at Leicester, 2008), **Owen** (RS Dorothy Hodgkin Fellow to lectureship at University of South Wales, 2013) and **Walker** (RS URF to lectureship at Newcastle, 2012). The School expects to appoint 1-2 new Fellows each year.

The SoC attracts a large number of academic research visitors both from the UK (~60-80 per annum) and overseas (~40 per annum) as well as PGs visiting for periods of up to one year (~30).

New staff appointments are made strategically in line with the School's key research strengths as defined in Sections **a** and **b** as replacements for staff who have left/retired or on the basis of exceptional talent appointments. With regard to the latter, since 1 January 2008, **Hall**, **Galan** (from Spain) **Glowacki** (from the USA) and **Royall** (joint with Physics) (all independent Fellowship holders) have been appointed proleptically to lectureships which took (or will take) effect upon completion of their Fellowships; such proleptic appointments are used to secure long-term employment of outstanding Research Fellows. Two new staff in biological organic chemistry are currently being recruited in order to maintain and further enhance critical mass in this research theme.

The School makes full use of the three academic career Pathways available to staff at the UoB and while the majority of academic staff are associated with Pathway 1 (Research and Teaching), high level research support is provided via Pathway 2 (Research), and Pathway 3 (Teaching and Learning) provides a career pathway for specialist teaching staff. Staff promotions since 1 January 2008 include 12 to Professor, 6 to Reader and 4 to Senior Lecturer which point to both staff quality and an infrastructure conducive to supporting world-class research. Academic staff management is provided at a Sectional level by the Section Heads and an annual Staff Review and Development process is carried out for staff on all Pathways. Staff are encouraged to take research sabbaticals of up to one year to develop and explore new research opportunities, *eg* most recently **Evershed** (Stanford), **Harvey** (Montpellier), **Mann** (Harvard) and **Manby** (Cornell, Caltech), and/or apply for UoB Research Fellowships (since 1 January 2008: **Gallagher**, **Manby**).

The SoC, as part of the UoB and therefore as a member of UUK, is committed to the Concordat to Support the Career Development of Researchers by working towards its associated principles and addressing such matters as Recruitment and Selection, Recognition and Value, Support and Career Development, Researcher's Responsibilities, and Diversity and Equality (see below) all of which are considered and monitored by an Implementation Group comprising HR staff and the PVC Research in accordance with expectations associated with holding the HR Excellence in Research badge. Training and development programmes include events for ECRs, a website and e-mail bulletin with information about career development opportunities, and a fixed term contract policy which goes beyond the legal requirement. Moreover, the SoC is committed to providing a working environment with excellent employment practices for all staff which includes positive action in equality, diversity and flexible working. In recognition of these policies the School submitted a successful application for a bronze Athena SWAN Award in 2012 led by Professor Christine Willis who provides the School with advice on equality and diversity issues as a member of the University SWAN Committee. Support for women at key career transition points is of vital importance and is fully recognised by the School which has established the Women-in-Science Mentoring Scheme particularly targeted at PGs, PDRAs and ECRs with the aim of providing a supportive environment for individuals and to encourage women to pursue careers in science.

ii. Research students

There are currently around 225 postgraduates in the School (mostly PhD; see REF 4a) carrying out a wide range of research activities, many involving collaboration with academic or industry groups in the UK and abroad. The graduates benefit from working in first class laboratories with access to state-of-the-art facilities and instrumentation and the School also hosts the EPSRC-funded Centres for Doctoral Training in *Chemical Synthesis* and *Functional Nanomaterials* (the BCFN, joint with Physics) which were launched in 2009 (both recently renewed).

A Table of the total FTE number of PGRs enrolled on doctoral programmes by academic year from 1 August 2008 to 31 July 2013 is presented below. Recruitment to all Graduate Programmes is handled by a Director of Graduate Recruitment and the SoC aims to recruit >60 high quality postgraduates each year. In the period 1 October 2003 to 30 September 2008, the PhD completion rate was 95% and the current ratio of PGRs to research leaders in the SoC is about 5.

Academic Year	Total FTE PGR
2008/9	228
2009/10	195
2010/11	191
2011/12	210
2012/13	222

The School of Chemistry recognises that postgraduate training should take place in a well-planned, structured setting which is achieved through a Graduate School under the leadership of a Director of Graduate Studies who chairs a Graduate School Committee and interacts closely with the Faculty Graduate Studies Committee. Within the graduate programmes, students are given scope to develop transferable skills including presentation skills, time-management, leadership, entrepreneurship and a knowledge of wider professional issues as well as being given opportunities to teach (after tailored training sessions) and to take part in outreach and public engagement activities (many are trained through Bristol ChemLabS as STEM Ambassadors; >400 since 2008). Dissemination of best practice developed in the School, particularly in the CDTs, is facilitated through the Graduate School and also through the newly established Bristol Doctoral College which aims to develop and share best practice more widely across the UoB.

All postgraduates are assigned an Assessor, who with the Supervisor, monitors progress annually throughout their studies. Progress monitoring requires preparation of an annual report which is discussed during an interview with the student. Detailed feedback is given to the student both orally and *via* an online report and students have the opportunity to comment about all aspects of their research degree programme. All staff and student comments are read by the Director of the Graduate School and any concerns acted upon. The forms are then forwarded to the Graduate Dean of the Faculty of Science. Analysis of the PG feedback shows a very positive attitude from the PG students towards their research, training and supervision.

d. Income, Infrastructure and Facilities

Income

Research income expenditure (REF 4b/c) to the School was £11.1m in 2012/13, and since 2008, **7** major ERC Advanced Investigator Grants (**Aggarwal**, **Evershed**, **Mann**, **Manners**, **Orr-Ewing**, and recently **Pancost**, **Woolfson**) worth €15.2m have been secured and Bristol (**Orr-Ewing** & **Ashfold**) is the lead institution on an EPSRC Programme Grant in Chemical Dynamics (£5.9m). Research income is mainly from Research Councils both in the UK (EPSRC, BBSRC, NERC, STFC) and increasingly exploiting EU opportunities (ERC), but charity/industry funding is also an important income stream. Total research awards during the period include: EPSRC £17.8m, BBSRC £3.8m, NERC £5.7m, other Research Councils £2.5m, UK Government £2.7m, ERC £14.4m, charities £1.8m, industry £2.8m and other funders £1.9m which totals £53.4m and equates to about £1m per staff (research leader) FTE.

Research Infrastructure and Facilities

The School offers a world-class research infrastructure. Major investment (>£50m since 1997) has provided a total available laboratory area of 6860m^2 (370 fume cupboards) accommodating around 300 postdoctoral and postgraduate researchers, plus (in 2012/13) 180 undergraduates engaged in final year research projects, all within space which is either new or completely refurbished since 1999. This has been further enhanced by the opening of the UoB's world-leading £12m Centre for Nanoscience and Quantum Information building in 2009, which houses some of the School instrumentation base in collaborative, ultra-low noise laboratory space. A further enhancement will come with completion of the £56m UoB Life Sciences Building in early 2014 which will offer state-of-the-art infrastructure to support collaborative research in biological chemistry/synthetic biology.

The School has an internationally competitive equipment and instrumentation base that is much enhanced since 2008. Investment of £9.1m since 1 January 2008 (from UoB, EPSRC, BBSRC, NERC, Wellcome Trust, RS Wolfson, Industry) has provided substantially upgraded laboratory space and new or upgraded instrumentation which comprises, for NMR [3 x 300, 2 x 400, 3 x 500 and 2 x 600 MHz spectrometers, 6 with multinuclear capability, 6 automated and 2 with cryoprobes], X-ray Crystallography [1 powder and 3 single crystal diffractometers, 1 with rotating anode], Mass Spectrometry [UPLC Ion-trap HR-MS/MS, Quadrupole LC-MS, 2 x Ion-trap LC-MS, 2 x MALDI-TOF, FT-ICR, MicroQTOF, automated EI/CI/FAB] and Electron/Force Microscopy [3 x TEM, 2 x SEM, 2 x AFM]. The School hosts additional 500 and 600 MHz NMR spectrometers associated with the new UoB MRC Unit in Integrative Epidemiology Unit and and also houses the NERC National Life Science Mass Spectrometry Facility (Director, **Evershed**) enhanced with £570k of investment in MS instrumentation since January 2008 providing a total of 10 spectrometers with capabilities including: GC/MS, HPLC/MS, thermal desorption GC/MS, pyrolysis GC/MS, LC/IRMS, GC-combustion-isotope ratio MS (C & N) and GC-thermal conversion-isotope ratio MS (H & O). EPSRC Programme grant, NERC and ERC investment has supported major investment in laser technologies (*eg* a 35-fs amplified, wavelength tunable ultrafast laser system with mid-IR to deep-UV capabilities) facilitating diverse studies across dynamics, aerosols and organic photochemistry including new dedicated laboratory space for ultra-fast laser spectroscopy and aerosol science, plus new and equipped chemical and synthetic biology laboratory space, and instrumentation for diamond-based materials analysis. Investments in TEM, AFM, micromachining, surface force, light scattering and confocal microscopy underpin growth in materials chemistry and soft matter science, while automated peptide synthesis and biophysics instrumentation, chromatography and mass spectrometry supports chemical biology, materials chemistry and synthesis. Computing facilities have expanded by over 100-fold since 2008, with two chemistry-dedicated HPC clusters comprising over 500 Opteron and Xeon processor cores, enhanced by the University High Performance Computing facility (Blue Crystal with >9000 cores; 3rd in UK academia based on top 500 benchmarking) of which Chemistry is one of the principal users and supported by a £2m investment in the petabyte Research Data Storage Facility. Investment in new equipment and instrumentation exploits RCUK initiatives (*eg* EPSRC and BBSRC Strategic Equipment Initiatives, EPSRC Core Capability for Chemistry Research and Advanced Materials calls) and is informed by continually updated equipment strategy documents looking five years ahead to identify both replacement needs and opportunities for instrumentation which enable new science. Access to and training for all instrumentation is provided for all staff and students according to need.

The School provides an in-house library plus a joint Faculty Mechanical workshop, Electronic and Glass workshops and a Microanalytical laboratory. There are 4 research officers supporting the instrument facilities and a further 4 supporting general research activities with a total of 31 FTE technical staff supporting workshop, research and teaching activity.

e. Collaboration or contribution to the discipline or research base

Many intradisciplinary collaborations are maintained between staff in the SoC across the research themes described in Section **b** some of which are evident in the highlighted (underlined) outputs and in the theme summaries. Several collaborations have been specifically developed as a result of the ethos within the *Chemical Synthesis* CDT, *eg* between traditional inorganic and organic groups (*eg* **Bedford**/**Gallagher**, iron cross-coupling), the development of photochemical synthetic methods (**Booker-Milburn**/**Orr-Ewing**) and computationally assisted ligand design (**Pringle**/**Fey**/**Harvey**). Extensive collaborations exist also across disciplines within the UoB, notably with Physics (facilitated in large part by the BCFN CDT), Engineering (*eg* through the *Advanced Composites* CDT) and with Biochemistry and other Schools in the Faculty of Medical and Veterinary Sciences all of which are driven by and enhance the strategically important SoC research themes. In some cases, these collaborations are facilitated by joint staff appointments with Physics (**Fox** & **Royall**) and with Biochemistry (**Woolfson**). Examples of successful collaborations which have resulted in significant outputs and grant income include research into bio-nanomaterials (**Mann**/**Manners**/**Woolfson** with Biochemistry), self-healing advanced composite materials (**Wass** with Aerospace Engineering), brain biotracers (**Galan** with

Neuroscience), agonists and antagonists for pain treatment (**Willis** & **Crump** with Biochemistry and Pharmacology), polyketide chemistry (**Cox**, **Crump**, **Crosby**, **Simpson** & **Willis** with Biological Sciences and Biochemistry), climate science (**Pancost** with Geographical Sciences and Earth Sciences), archaeological chemistry (**Evershed** with Archaeology), biological anion transport (**Davis(A)** with Physiology), nanoporous crystals (**Davis(A)** with Physics), ZnO nanofibre characterisation (**Ashfold** with Physics), solar cell nanostructures (**Fermin** with Physics), electrocatalytic conversion of liquid fuels (**Fermin** with Biochemistry), biocompatible diamond (**May** with Neuroscience), diamond supercapacitors (**May** with Electrical Engineering), photonic crystal cavities (**Orr-Ewing** with Electrical Engineering) and theoretical modeling of photosynthesis (**Harvey** & **Manby** with Maths).

Collaborations with groups (for both chemistry and other disciplines) in other UK institutions which are externally funded (EPSRC, BBSRC, NERC, CRUK, see REF 4b) and/or have resulted in publications include those with Bath, Birmingham, Cambridge, Cardiff, Durham, Edinburgh, Exeter, Glasgow, Imperial College, Leeds, Liverpool, Manchester, Newcastle, Nottingham, Oxford, Sheffield, Southampton, Strathclyde, UCL, Warwick, York and Rothamsted, while many industrial collaborations exist as is evident from the list of companies given in Section **a** (GSK, AstraZeneca, Syngenta, Novartis, Pfizer, Merck, BP, Shell, DSM, Sasol, Lucite, Element 6, GKN Aerospace, Infinium, EON AG, Hewlett Packard, Unilever, BASF) which includes many overseas companies. Much of the work carried out with industrial support has resulted in patent outputs which are discussed under Impact in REF 3a.

Many staff make frequent use of major UK and overseas facilities including HECToR, the Central Laser Facility, ISIS and Diamond (at RAL, UK), ESRF, ILL, Maxlab, Elettra (Europe), and the ALS at Berkeley (USA) overseas (in-kind income associated with these activities is in REF 4c).

International collaborations which have resulted in joint publications include those with institutions in *Europe* (*eg* Amsterdam, Bochum, Bonn, Budapest, Carlsberg, Dublin, ETH Zurich, Gothenburg, Grenoble, Helsinki, Karlsruhe, Leiden, Leuven, Lisbon, Lyon, Madrid, Marburg, Moscow, Nijmegen, Oslo, Paris, Regensburg, Salerno, Seville, Stockholm, Stuttgart, Utrecht, Venice), *USA/Canada* (*eg* Brown, Caltech, Chapel Hill, Harvard, Illinois, Madison, MIT, Michigan, Naval Research Laboratory, Notre Dame, Penn State, Pittsburgh, Princeton, Purdue, Sandia Labs, Stanford, Toronto, Tufts, USC, Yale), and *Asia/Africa* (*eg* Beijing, Cape Town, Bangkok, Hokkaido, HKBU, Kyoto, Nagaoka, Rhodes SA, Tokyo, Wuhan. Visiting Professorships have been/are held at institutions including Beijing IoT, Berlin (TU), Caltech, Cornell, Harvard, Helsinki, Stanford, Utrecht and Wuhan.

In terms of Academic Leadership many staff are members of RCUK Colleges and serve on or chair funding panels (>30), are members of journal editorial boards (>30), provide leadership in the academic community [*eg* president of the RSC Faraday Divison (**Ashfold**), Chair of the Science, Education and Industry Board of the Royal Society of Chemistry (**Ashfold**)], have organised high profile international conferences [*eg* the *Bristol Synthesis Meeting* (**Aggarwal**) held annually since 2001], or act as advisors on international committees [*eg* the Physical, Chemical & Mathematical Sciences Scientific Committee of Science in Europe (**Mann**)].

Research leaders at the forefront of their science are frequently invited to international meetings to inspire the next generation of scientists. Since 1 January 2008, >485 invited, keynote or plenary lectures at international conferences and/or lectures associated with prizes have been given by our staff, a total of ~50 prizes or prestigious awards/named lectures have been received [*eg* an Alexander von Humboldt Research Award (**Manners**, 2011), the RSC de Gennes Prize and Medal (**Mann**, 2011), the David A Shirley Award for Outstanding Scientific Achievement awarded by the ALS, Berkeley, (**Shallcross**, 2012), the Dirac Medal awarded by The World Association of Theoretical and Computational Chemists (**Harvey**, 2009)]. Three staff have been awarded RSC Tilden Awards (**Aggarwal**, **Manners**, **Orr-Ewing**), two staff have been awarded Corday-Morgan Awards (**Manby**, **Reid**) and **5** staff have been elected to the Royal Society, one in each of the last **5** years (**Evershed**, **Ashfold**, **Manners**, **Aggarwal**, **Lloyd-Jones**).