Institution: University of Southampton
Unit of Assessment: 8 Chemistry

a. Overview

Chemistry at the University of Southampton (UoS) aims to change the world for the better through our research, education and entrepreneurial outlook. As an Academic Unit within the Faculty of Natural and Environmental Sciences (FNES), Chemistry is led by **Prof. P.A. Gale** supported by the Chemistry Policy and Resources Committee (*CPRC*), which includes the Deputy Heads of Chemistry (DHoC), **Prof. R.C.D. Brown** (Research) and **Prof. A.E. Russell** (Education) and senior administrative staff for finance and infrastructure.

Our research is organised into 5 groups: *Magnetic Resonance (MR)* (led by **Prof. M.H. Levitt, FRS**); *Electrochemistry* (led by **Prof. P.N. Bartlett, FRS**); *Molecular Assembly, Function & Structure (MAFS)* (led by **Prof. G. Reid**); *Molecular Diagnostics & Therapeutics (MDT)* (led by **Dr B. Linclau**); *Computational Systems Chemistry (CSC)* (led by **Prof. J.W. Essex**). Heads of Research Groups form the *Research & Enterprise Committee* (*R&EComm*) chaired by the DHoC (Research), reporting to *CPRC*. The *Education* group (led by **Dr D. Read**) and *Characterisation & Analytics* (led by **Dr G.J. Langley**) support activity across Chemistry, reporting through the DHoC (Education) and R&EComm. Through the multidisciplinary nature of our research, our staff interact with groups across the UoS, nationally and internationally. Chemistry is fully engaged with the new Institute for Life Sciences (IfLS), a strategic priority that integrates biosciences across the UoS. The IfLS evolved from the Life Sciences Interfaces Forum (Director: **Prof. G.S. Attard**, 2003-08). Outputs: 1250 ISI papers published, 42 patents granted and 47 patents filed since 2008.

b. Research Strategy

Following the feedback from RAE2008, a rigorous review of Chemistry's research strategy and structure was made during 2009-10 to determine our research priorities and raise ambition. Led by **Bartlett**, with input from all academic staff, and guidance from the Chemistry Advisory Board (providing both academic and industrial perspectives), the review resulted in the formation of 5 new research groupings. These groups are focused on areas in which Southampton has strong core competencies, thereby delivering distinctive, internationally leading research. Our research strategy was backed by significant capital and infrastructure investment (*c.* £9 M, including the proceeds of the Ilika IPO which floated on AIM in 2010). This gave opportunities to existing staff (providing PhD, 'PhD+', equipment, facilities and support for research sabbaticals) and for strategic new staff appointments, resulting in 12 new permanent Cat A staff appointments since 2008.

The Electrochemistry and Surface Science and Chemical Biology groups were highlighted as '*excellent*' in RAE2008: Electrochemistry was strengthened with a new appointment; Chemical Biology was strengthened and focussed by forming the Molecular Diagnostics and Therapeutics (MDT) group, with 3 new appointments, plus an IfLS Interdisciplinary Fellowship. This aligns with the strategy defined in RAE2008 '*to develop our distinctive position as an internationally leading centre for electrochemistry…'*, and '*to be an international centre for chemical biology research and to be major contributors at the Life Sciences Interface'*.

The Magnetic Resonance (MR), Computational Systems Chemistry (CSC) and Molecular Assembly, Function and Structure (MAFS) groups build on international excellence and bring a sharper focus on magnetic resonance, theoretical/computational chemistry and to challenges in molecular, supramolecular and structural chemistry. MR and CSC cut across the Electrochemistry, MAFS and MDT groups, strengthening them further *via* collaboration. A key component of our strategy was the renewal of the *EPSRC National Crystallographic Service* (**NCS**) in 2010. **Gale** and **Coles** led the successful NCS bid, which resulted in the Southampton Diffraction Centre – a truly world-leading facility (£3.6M EPSRC funding; £0.5M UoS investment).

Our 12 new Category A staff have been recruited strategically to strengthen the research groups, bring new research synergies and achieve a balanced age profile (median age of Cat. A staff = 43 years). We nurture research excellence through active mentoring by senior research leaders. Southampton's culture of multi-disciplinary research is a particular feature, with collaboration encouraged by strategic allocation of PGR funding and cross-faculty networks.

Chemistry is a central element of the IfLS with the establishment of the MDT, CSC and MR research groups in particular. The IfLS provides exciting UoS-wide bioscience-facing multidisciplinary research opportunities, bringing together expertise across science, medicine and engineering. Other University Strategic Research Groups (USRGs) create synergies between

disciplines towards understanding and addressing global societal challenges. Staff in Chemistry lead the *Energy* (**Raja**), *Computationally Intensive Imaging* (**Frey**) and *Complexity* (**Essex**) USRGs, and there is strong engagement from Chemistry in the *Digital Economy* and *Nanoscience* USRGs. A regular seminar programme from our staff encourages cross-fertilisation of research.

Our philosophy of embedding research groups from other disciplines within the Chemistry building complex to promote interdisciplinary research, highlighted as a strength in the RAE2008 feedback, has been maintained. Chemistry hosts Prof. F. Walsh's group (Electrochem. Engineering), Dr A. Kanaras' group (Physics) and the nCATS group (Tribology) led by Prof. R. Wood. Joint appointments have been made with other units in the UoS when opportunities arise (e.g. **Tavassoli** with Chemistry/Medicine; **Mahajan** and **Fischlechner** with Chemistry/IfLS).

Research Groupings:

• **Magnetic Resonance (MR):** In RAE2008 we said we would build upon the world-renowned work of **Levitt** '*to create and apply novel NMR experiments for molecular structure determination for materials and biomolecules*'. Establishing the MR group has been central to this, enabling the group to employ quantum theory, numerical simulations, MR experiments and chemical insights to design new techniques and apply them to problems ranging from physical science to medicine. Distinctive and unique strengths are NMR at very low temperatures, and the exploitation of long-lived nuclear spin states - a phenomenon first discovered in the Levitt group - which are now being combined with nuclear hyperpolarisation techniques that enhance NMR signals by up to x 10^5, in order to develop new magnetic resonance imaging (MRI) methods. As well as confirming **Carravetta**'s position (previously RS URF), the group has been strengthened by 2 new senior appointments that interface with UoS strengths in theoretical chemistry (CSC) and high performance computation (**Kuprov**) and nanofabrication/microfluidics in Electronics and Computer Science (ECS) and Optoelectronics (**Utz**). Since 2008, considerable UoS investment (~£1M) linked to a Wolfson refurbishment grant, has enhanced the infrastructure for MR. The group is supported by large grants from EPSRC, ERC and the RS, coupled with significant international collaborations (Section e). Priorities include development of methodology and applications of long-lived nuclear spin states; cryogenic NMR, including quantum rotors and molecular endofullerenes; NMR of superconductors; biomolecular structure determination by NMR, especially in the solid state; new methods for enhancing MR signals and new agents and methods for MRI; computational methods for large coupled spin systems and for the calculation of EPR parameters; simulation of spectra and spin chemistry effects; microfluidic NMR devices ('NMR on a chip'). Strong synergies exist with MAFS (synthetic chemistry), CSC (simulations), as well as Physics and Engineering.
[Unique publications from staff in MR since 2008=99]
Future goals: (i) to develop and extend the concepts of hyperpolarised long-lived states, completing the translation into viable methods in medicine and the NMR of living matter; (ii) to realise new hyperpolarisation methods including the exploitation of molecular quantum rotors; (iii) to combine these methods with nanofabrication and microfluidics; (iv) to extend further the application and understanding of cryogenic magnetic resonance phenomena; (v) to develop and apply methods for biomolecular structure determination in the solid state.

• **Electrochemistry:** As stated in RAE2008, a significant focus has been in *Energy Conversion & Storage*, where the group provides distinctive and internationally leading expertise in the application of synchrotron methods (**Russell**) to *in situ* studies of fuel cell catalysts. The group has made major contributions to the development and application of high throughput methodology for new materials discovery (**Hayden** with Ilika), particularly for proton exchange membrane (PEM) fuel cells, solid-state Li-ion batteries and functional ceramics for energy harvesting. EPSRC, industrial and UoS investment (£3.9M) will establish new facilities for advanced composite materials from 2014 (PI=**Hayden**). A major EU project (**Russell**, **Pletcher**) is developing redox flow batteries for load levelling and storage applications on the grid. Significant effort in battery development (**Owen**, **Hector**) has been strengthened by the appointment of **Garcia-Araez** (Lecturer), studying new Li-air, Na-ion and 3-D battery architectures. In the field of supercapacitors, high surface area electrodes, new redox electrode materials and biofuel cells are being studied.

Electrodeposition of Nanomaterials was identified as a priority in RAE2008 and the group has internationally leading programmes on electrodeposition from non-conventional media and on templated electrodeposition (i) to prepare regular nanostructures, and (ii) to apply them in electrocatalysis. The group maintains a leading position in plasmonics and surface enhanced Raman spectroscopy, enabling the discrimination and detection of DNA (**Bartlett**). *Supercritical*

Fluid Electrodeposition, a new technology for the deposition of functional nanostructures (sub-10 nm), originally developed under a Basic Technology Grant, and identified as a strategic priority in RAE2008, has been advanced significantly under an EPSRC Programme Grant led by **Bartlett** (with **Hector**, **Reid**, Smith (Physics) and with Nottingham & Warwick). This is complemented by work on templated electrodeposition of phase change memory materials from non-aqueous solvents. Distinctive interdisciplinary activity in *Sonoelectrochemistry,* involving electrochemistry (**Birkin**) and acoustics (Leighton, Engineering) has led to major innovation in cavitation detection and surface cleaning, studies of bubble dynamics and mass transport effects at surfaces.
[Unique publications from staff in Electrochemistry since 2008=192]
Future goals: to exploit our internationally leading position in Electrochemistry with key priorities in energy storage and functional (nano)materials deposition, and to expand our links with staff in MDT and the IfLS to lead new developments in bioelectrochemistry, diagnostics and detection.

• **Molecular Assembly, Function & Structure (MAFS):** The MAFS group combines our significant expertise in organic, inorganic, supramolecular and structural chemistry. While rigorous PhD student training in the individual organic and inorganic sub-disciplines remains a very high priority, the group was established to also promote strong synergies and collaborations across these areas. Well-funded programmes are focussed on new synthetic methodologies and target synthesis of organic compounds. This theme has been strengthened by the appointments of **Rios** (Reader), with particular expertise in enantioselective organocatalysis, and **Bloodworth** (Lecturer) working on optimisation of small peptide analogues for cancer treatment (with Blaydes, Medicine & Kilburn, QMUL). The group has attracted significant EU funding to establish a Cross-Channel consortium to promote regional (Anglo-Norman) academic-industry partnerships (Section e). A significant focus is in the development of new methodologies and microfluidic reactors for automated flow synthesis and electrosynthesis (with Electrochemistry) for applications in organic chemistry. This aligns to a primary theme in the EPSRC *Dial-a-Molecule* Grand Challenge network (led by **Whitby** & **Harrowven**), with strong industrial and external collaborations.

A developing theme is in new organic and inorganic late-stage F-18 radiolabelling strategies for medical imaging (PET) (**R. Brown** with Perrio, Caen; **Reid**, **Levason** with GE Healthcare).

Gale's work on supramolecular chemistry and anion coordination, especially in the areas of lipid bilayer transport of anions and the detection of nerve agents, is a particular strength in Southampton (he is among the top 500 most cited Chemists world-wide – ESI 09/13). The appointments of **Bradshaw** (Reader), **Kitchen** (Lecturer) and **Keene** (Marie Curie IIF) have increased our effort in supramolecular chemistry significantly, bridging the development of organic, metal-organic and inorganic framework materials in separation, sensing, magnetism and catalysis; the latter linking strongly to **Raja**'s work on new multifunctional catalyst designs.

A priority in RAE2008, reinforced by the strategic review, '*to be an internationally leading centre for research in materials chemistry both in solid state materials and in the rapidly developing field of nanomaterials and new materials chemistry'*, has stimulated the development of strong links to both Electronics and Computer Science (ECS) and Physics, benefiting from Southampton's superb nanofabrication and clean-room facilities**. Reid** leads research on non-aqueous electrodeposition of nanostructured phase change memory materials, with **Levason**, **Hector**, **Bartlett** and de Groot (ECS). This team has also developed systems for highly area-selective chemical vapour deposition (CVD) of thin film materials onto micro- and nano-patterned substrates, an important new capability for electronic and optical applications. This area has been further strengthened by the appointment of **Hyett** (Lecturer), working on controlled deposition of nanomaterials and solid-state chemistry. Structure determination using the outstanding facilities in the Southampton Diffraction Centre is crucial to our work in MAFS, and **Coles**' group also specialises in structural systematics, charge density distributions, structure-property relationships and crystal growth. Distinctive structural science projects in macromolecular crystallography (with Tews, Biological Sciences), X-ray laser spectroscopy and imaging (Brocklesby, Horak, ORC) and CT Imaging (Sinclair, Engineering) are complemented by well-funded (JISC) projects in Information Management, eResearch and eLearning (with **Frey**). Synchrotron-based structural science is the focus of **Evans**' ground-breaking work on development and applications of time-resolved (and freeze-quench) X-ray absorption spectroscopy - linked strongly to the *Catalysis Consortium* and EPSRC *Catalysis Hub*.
[Unique publications from staff in MAFS since 2008=505]
Future goals: (i) to develop a centre of excellence in flow chemistry for (electro)synthesis of industrially relevant targets; (ii) to lead in the development of (supra)molecular chemistry towards

applications in biology, medicine, sensing and catalysis; (iii) to expand our work in precursor chemistry for functional material deposition, exploiting distinctive synergies with ECS and Physics; (iv) to ensure renewal of the NCS contract (2015) and retain a leading role in structural science.

• **Molecular Diagnostics & Therapeutics (MDT):** MDT was formed as a result of refocusing on our distinctive strengths in nucleic acids, peptides and proteins, and to increase our footprint in glycobiology. Our strategic priority was the diagnostics and therapeutics aspect of these areas to enable us to accomplish our ambition *to be internationally leading in chemical biology and major contributors at the life science interface*. Under the leadership of **T. Brown** (until Oct. 2013) and **Linclau** these three priority areas have been strengthened *via* high profile publications, large grants and the appointment of outstanding early career academic staff.

Brown is an international leader in the development of molecular diagnostics based on nucleic acids chemistry. The development of click-DNA ligation at Southampton has led to several high-profile publications and a broader collaboration between **Brown**, **Tavassoli**, **Stulz**, Fox (Biological Sciences), and others at Oxford University, through a BBSRC sLoLa 'Extending the Boundaries of Nucleic Acid Chemistry'. The appointment of **Watts** (lecturer) has brought expertise in RNA chemistry, nucleic acid-based therapeutics and next-generation sequencing protocols. **Stulz**'s work on detection of cancer genes *via* electrochemical, optical and nano-ring resonator technologies further enhances our footprint in this area.

We collaborate closely with clinicians in Medicine, including **Tavassoli**'s joint appointment (Chemistry/Medicine), and **Linclau**'s work (with Essex and Skylaris) on the modulation of protein-lipid and -carbohydrate interactions *via* chemically modified ligands. **Tavassoli**'s work in the design and development of protein-protein interaction inhibitors has led to extensive collaborations with industry, and has resulted in important insights into several proteins in cancer biology. Mechanistic enzymology and crystallography (**Roach**) feature strongly, with **Lee**'s appointment (lecturer) further strengthening this area and linking to **Linclau**'s expertise in carbohydrate chemistry.

In diagnostics we have strengths in novel *in vitro* and *in vivo* molecular imaging techniques and the development of nanosensors for medical diagnostics (**Roach, Nandhakumar**), an area further strengthened by the joint appointment of **Mahajan** (Chemistry/IfLS), who is coupling advanced optical imaging with Raman spectroscopy.

We are also active in the emerging field of synthetic biology, with **Tavassoli**'s bacterial high-throughput screening platform, and **Attard**'s bottom-up approach to the construction of a synthetic nucleus. The appointment of **Fischlechner** (IfLS Fellowship) brings microfluidics-based high-throughput screening platforms into the group and further strengthens our bio-medical focus.

*[Unique publications from staff in MDT since 2008 (incl. **Brown**)=260]*

Future goals: In Oct. 2013 **Brown** took up a Chemistry/Medicine Chair in Oxford. We have therefore appointed **Gerrard** for 1 year (Lecturer) to cover the transition period; identifying a replacement for **Brown** at a senior level is our top priority in 2014, both to provide leadership for the younger staff in the group and to add further research strength in the area of glycobiology. We will remain at the forefront of international research in diagnostics and therapeutics.

• **Computational Systems Chemistry (CSC):** Formation of CSC as a primary research group led by **Essex**, coupled with the excellent new appointments of **Day** at Reader level and **Minns** (RS URF) and refurbishment of computational space and facilities, have allowed the group to exceed the strategic objective in RAE2008 '*to develop coarse-grained and multi-scale molecular modelling approaches to study large-scale functional biological assemblies*'. The CSC group is well-funded and broadly based, with research covering multiple lengths, time-scales, and methods, and founded on strong activity in the development of new theories and computational techniques. Its research is unified by the common theme of exploring interacting systems, where the larger scale system behaviour arises from a series of complex interactions of individual smaller components. The notion of linking methods with differing levels of approximation is a strong one. Through this ***multi-scale approach*** the CSC group is linking quantum and classical models, with atomistic, coarse-grained and continuum modelling approaches.

A particular strength is in modelling biologically relevant systems at increasing levels of organisation, from nucleic acids and proteins, to membranes and beyond to the whole cell. The group collaborates extensively with industry through consultancy, funded PhDs and PDRAs. Its activities are underpinned by the UoS's latest 12000-core supercomputer, the GPU cluster at Rutherford Appleton Laboratory and supercomputer at Southampton, funded by the e-Infrastructure South Consortium, of which Southampton is a founding partner, as well as the

EPSRC DTC in Complex Systems Simulation (PI=**Essex**). CSC is also a central component of the new EPSRC CDT, 'Theory & Modelling in Chemical Sciences', jointly with Oxford and Bristol, to be launched in 2014. Key synergies include **Essex/Day/Skylaris** on application of classical simulations and quantum mechanics to model small molecule interactions both in the solid state and in biological systems for drug discovery; **Essex/Khalid** on coarse-grained and dual-resolution simulation methods to study membrane systems and their interactions with proteins and small molecules; **Frey/Coles** on chem-informatics, pervasive computing, large data and electronic lab notebooks (ELNs). CSC collaborates extensively with experimental groups within Chemistry, the UoS and externally, providing the computational expertise that informs other research projects.
[Unique publications from staff in CSC since 2008=191]
Future goals: (i) to further develop our strength in method development and integration, at multiple length/time-scales, and detail of description (electronic structure, atomistic, coarse-grained), focussing on our strengths in biological (in silico synthetic biology) and materials simulation; (ii) to fully exploit the *application* of our computational methods through strong collaboration and with industry; (iii) to exploit our leading position in intelligent chem-informatics approaches for management, interrogation and exploitation of large-scale chemical data.

c. People, including:

I. Staffing strategy and staff development

The UoS is committed to delivering excellence in research, education, postgraduate training and early career development. We aim to sustain and improve performance by attracting, developing and retaining high-achieving staff, and by nurturing staff in the early stages of their careers.
Overall Strategy: Our research strategy informs staff recruitment. Since the last RAE census, we have appointed 12 new Category A staff to permanent contracts. Investments in physical infrastructure are made to support new and existing staff – as described in Section d. Research groups are expected to generate funding for technical support, but for each group a base level of support is provided to support UG and Masters projects and subject-specific PG skills training.
Career development - RAs: Throughout the REF period, on average *c.*50 Chemistry PDRAs, distributed across the research sections, have been in post. Several EPSRC PhD+/Doctoral Prizes have been awarded to exceptional individuals in Chemistry *via* the UoS selection panel. Induction of new RAs is provided in Chemistry upon arrival. Following a 12-month probationary period, all RAs are appraised annually. Workshops and resources tailored to support the career and professional development of individual RAs are provided by the UoS through the Professional Development Unit. Interviews with RAs prior to departure explore potential career opportunities.
Career development - ECRs: All new staff are supported by significant 'start-up' packages and reduced teaching and administration work-loads during the 3 year probationary period, to enable them to build successful independent research programmes. Essential requirements are met through the provision of laboratory space and equipment. ECRs are prioritised in the allocation of internal funding for studentships. Chemistry has a research and teaching fellow network to provide a cohesive identity for researchers and to ensure that the seven principles of the *Concordat to Support the Career Development of Researchers* are implemented. The Dean's Prize recognises excellence in research, enterprise and teaching, addressing the principle of recognition and reward. Within the Faculty we have consulted with researchers and developed an action plan, with a particular focus on induction, mentorship, and performance review and appraisal. The Faculty policy complements UoS policies that have been in place since 2009, focussing on disseminating the Concordat; raising awareness among all staff; seeking input from research staff; seeking appropriate implementation mechanisms; identifying lines of responsibility; institutional review of practice, and establishing professional development support for researchers. Two of the senior staff are female (**Reid**, **Russell**) and provide role models for younger colleagues. Mentoring by senior staff provides a strongly supportive framework for all ECRs and RAs.
Career development - established academic staff: Clear targets for research are set through an annual PPDR which reflects on past performance, sets goals for the coming period and defines development and training needs. Periods of study leave are encouraged every four years. Mechanisms are in place to accommodate experimental beamtime at the major research facilities.
Research fellows: RS URF: **Carravetta** (2007-15), **Minns** (2011-16), **Day** (2005-13), **Skylaris** (2004-12)**;** RCUK Fellow: **Khalid** (2007-10). ERC Fellowships: **Bradshaw** (2010-15), **Day** (2012-17). EPSRC Adv. Fellow: **Kuprov** (2007-12); RS Dorothy Hodgkin Fellow: **L. Brown** (2009-15); RS

Newton Fellow: **Gurnani** (2011-13); Marie Curie Fellows: **Keene** (2012-14), **Calvillo** (2011-13). Several of our independent fellows have already progressed to permanent positions in the UoS.

International recruitment: Academic posts are advertised widely in media such as *New Scientist*, *Chemistry World* as well as on-line. Of our 12 new staff, 9 have either come from non-UK institutions (US, Canada. Ireland, Spain) or have non-UK nationality. We host many international visitors, distinguished academics and young researchers, many with prestigious scholarships, including from India, US, Brazil, China, Japan, Singapore, Australia, Egypt, Iraq, and Europe.

Equality and diversity: The UoS recognises the importance of improving gender and diversity equality in STEM disciplines, which can otherwise both severely reduce the talent pipeline and negatively affect female and/or minority group career progression. We have a strong commitment to alleviating these issues as a founding signatory of the Athena SWAN Charter, to maximise the potential of all our available talents. Several initiatives have been implemented (e.g. Action Learning Sets, career guidance, peer mentoring, Diversity charter, well-being survey, changes to recruitment and selection policy, Equality Plan). These developments were formally recognised with a Bronze Athena Swan Award in 2006. Establishment of a self-assessment team (SAT) for Chemistry (led by **Russell**) facilitated a recent consultation with staff across all levels, including analysis of perceptions and culture across Chemistry, leading to the award of Athena Swan Bronze to Chemistry in 2013. The SAT, chaired by the Head of Chemistry, continues to meet and reflect on good practice. It has identified a set of priority actions and is working with *CPRC* to further improve our working environment to a level commensurate with Athena Swan Silver within 2 years.

c. II. Research students

The Graduate School in Chemistry coordinates training and monitors the progress of a very vibrant and talented cohort of PhD (and MSc) research students (Table). This cohort forms a large, diverse, international and truly multi-disciplinary research community. Over the REF period 159.35 FTE students have been awarded PhD degrees in Chemistry. The PhD research training and skills development within the Graduate School is highly valued by the large companies and SMEs who employ our graduates, such as BP, Johnson-Matthey, GSK, AZ, Merck, Novartis, Syngenta, Ilika.

Year	2008/09	2009/10	2010/11	2011/12	2012/13
FTE PhDs*	128.89	120.00	120.90	137.83	130.64

* PhD students (excl. Nominal); a further 25 PhD students are co-supervised in Chemistry, but registered in other Faculties; 75.3 MSc students since 2008.

Recruitment: PGR (mainly PhD, MSc) student recruitment has continued to be very strong since 2008, averaging ~50 students per year. The cohorts have a large international contingent, with ~40% entering from the EU or overseas. PhD students are supported variously by EPSRC Doctoral Training Grants (DTG), Doctoral Training Centres (DTCs), Industrial Case awards, industrial sponsorships, competitively awarded UoS VC scholarships, Chemistry funds, and a range of European and international scholarships. An increasing number of (mostly international) research MSc. students have enrolled in Chemistry since 2008. Notable highlights are the large InterReg PG training consortia, 'Innovative Synthesis: Culture and Entrepreneurship' and "AI-CHEM Channel", both collaborative ventures bringing together >100 PhD/MSc students in joint Anglo-Norman research projects since 2008, including 13 PhD and 20 MSc studentships in Southampton. All PhD projects are advertised widely using national and international recruitment websites. The PG Admissions Officer, Head of Chemistry and DHoC (Research) are gatekeepers to ensure the best candidates receive DTG or internal funding, in line with Chemistry's Strategy.

Training and support: All PG students receive stipends at or above the RCUK levels and are treated equally with regards to supervision and training opportunities. They engage in subject-specific training and safety following a 'training needs analysis' performed jointly with their supervisory team, as well as generic skills training. There is a wide range of advanced skills and advanced knowledge courses that PG students are required to attend. Students are expected to attend relevant seminars and symposia selected from a vibrant programme including internal, UK and international speakers, as well as final year PhD students. They are also strongly encouraged to contribute (posters, orals) to national/international conferences (PhD student Busschaert was selected to present her work at the 63rd Lindau Nobel Laureate meeting in 2013) and other events, including SET for Britain (PhD student Treharne won both the Roscoe medal for best chemistry poster and Westminster medal for the best overall poster in 2011).

Monitoring: Each PGR student is assigned a second supervisor who provides additional support and guidance on progress throughout the PhD, both informally and through direct feedback on the student's quarterly progress reports. An independent academic performs the role as one of the

Examiners in the MPhil/PhD transfer viva, and as Internal Examiner for the PhD *viva voce*. ECRs supervising students for the first time are required to co-supervise with more senior staff, and an experienced academic provides oversight of the examination processes. The upgrade from MPhil to PhD registration occurs after 12 months and involves a formal report, inspection of experimental records, and a *viva voce*, with a 6 month checkpoint to identify any progression issues.

d. Income, infrastructure and facilities

Specialist infrastructure and facilities: Chemistry is housed in facilities that are either purpose-built or have undergone major refurbishment since 2000, providing excellent containment *via* ~170 fume cupboards, facilities for high pressure chemistry, a Cat 2 laboratory for biological samples. Research is supported by a comprehensive Characterisation & Analytics base with expert staff, including specialists in NMR, mass spectrometry, diffraction and microscopy (6 FTE), while computational support for CSC is provided centrally *via* the UoS iSolutions. Three FTE mechanical workshop staff interface with a specialist NMR engineer. We also have 3 FTE Chemistry stores staff and an exceptional scientific glass-blowing workshop (3 FTE). A dedicated Safety Officer leads researcher training in risk management, COSHH and chemical safety, while our Facilities Manager is responsible for the technical staff and infrastructure across Chemistry. **Coles**, recently appointed Sustainability Officer for Chemistry, is working towards reducing our carbon footprint.

Since 2008 a priority has been to ensure the availability and long-term sustainability of the key research facilities necessary for our work in Chemistry. We have actively pursued external funding and made successful bids to the UoS's annual Multi-User Large-Scale Equipment for Research (MULSER) scheme (£0.5M and £0.3M, respectively, for diffraction and high-field NMR), and matching funding from the Faculty where possible. Sustainability and maximum usage of the NMR, MS, electron microscopy and diffraction facilities is achieved through their operation as Small Research Facilities with access available across the UoS (and externally). As a result of this strategy, the majority of our research equipment has been renewed since 2010. Key facilities are:

- The *EPSRC NCS* and *Southampton Diffraction Centre* provide state-of-the-art ultra-high flux X-ray sources for single crystal structure determination with 2 Rigaku Superbright FR-E+, a Rigaku 007 and a Rigaku R-axis Spider diffractometers, a macromolecular crystallisation pipeline with robots and imaging facilities. Additions since 2012 include a Bruker D2 Phaser for PXD and a Rigaku SmartLab optimised for thin film and microfocus diffraction.
- Outstanding *Mass Spectrometry* facilities include high-throughput equipment for HPLC-MS/MS, UPC^2-MS/MS and GC-MS with several ionisation techniques. There is also specialised capability in oligonucleotide analysis, high resolution MS (EI, ESI), structural elucidation (MS/MS), petrochemical analysis and lipidomics (with Medicine). The ultra-performance convergence chromatography (UPC^2)-MS and tandem MS capability is unique in UK academia. Other specialist equipment is available in Biological Sciences, Medicine and Ocean & Earth Science.
- *NMR* facilities include open-access service instruments (3 x 400 MHz, 500 MHz, incl. multinuclear capabilities) and specialist instruments used mainly by the MR group (wide-bore 300, 400, 600 MHz instruments with specialist MAS solid-state probes; micro-imaging equipment; a 500 MHz instrument for hyperpolarised solution NMR equipped for imaging experiments; superwide-bore magnet for DNP hyperpolarisation). Specialist equipment for cryogenic NMR (to 1 K), a unique cryogenic high resolution MAS NMR probe for solid-state NMR experiments down to 9 K; a home-built dissolution-DNP polariser (94 GHz) with a dissolution wand capable of generating NMR signal enhancements by factors of up to 10^5 at room temperature.
- Computational work is underpinned by the UoS's 12000-core supercomputer, *Iridis*, currently the largest in any UK university, the GPU cluster at Rutherford Appleton Laboratory and HECToR.
- Materials deposition and characterisation capabilities in Chemistry include UHV PVD equipment and data processing systems for high throughput thin film materials discovery, CVD rigs for thin film and nanoparticle growth, environmental SEM with EDS/WDS detectors. Photo- and e-beam lithography, sputtering, fabrication, FEGSEM, AFM, Raman and electrical characterisation are available in the Zepler Institute (ECS) and TEM *via* the Southampton General Hospital.
- Electrochemical equipment, multichannel potentiostats, high-pressure equipment and glove boxes for experiments associated with nanomaterial electrodeposition and Li battery research.
- Dedicated glove boxes for synthesis/materials chemistry.
- A suite of flow reactors and in-line analytical tools for synthesis, electrosynthesis and catalysis.
- IR, Raman and UV-visible and fluorescence spectrometers are available across Chemistry.

• DNA synthesisers for oligonucleotide work primarily in the MDT group.

Current & planned investments: The UoS has made significant investments over the REF period to enhance the research infrastructure and facilities in Chemistry, directly supporting our research strategy, in addition to the appointment of new staff. Staff are encouraged to raise external funding towards major equipment and facilities, with mechanisms in place both at UoS and Faculty level to provide matching funds. A new laboratory to house equipment for enhanced MRI, and expansion of the mechanical workshop, will be completed in late 2013, as part of a major enhancement (£1.4M) of the research environment to support Magnetic Resonance. The provision of advanced cryogenic NMR, hyperpolarisation and MRI equipment and the implementation of helium recycling will ensure that the group will continue to lead international developments in NMR and MRI through the next REF period. Refurbishment of CSC space was also undertaken in 2011/12.

New equipment for single crystal and powder XRD will be installed in 2013/14 in the initial phase of developing a dedicated advanced training facility to support a new MSc in *Characterisation and Analytical Chemistry*. Further MSc programmes are under construction, include *Electrochemistry and Electrochemical Engineering*, in response to requests from industry.

EPSRC Capital Funding (£3.3M and £0.6M from Ilika) will establish an Advanced Composite Materials Facility in Chemistry from 2014, allowing the scale-up of materials on wafers using MBE-based methodologies developed in Chemistry. This will allow their incorporation in advanced thin film devices in the energy, electronics, optoelectronics sectors, and compatibility with the clean-room fabrication facilities in the UoS's Zepler Institute. Capital equipment investment required over the next 5 years to develop and enhance the research infrastructure and strategy include, small angle scattering (SAXS) for (bio)molecular structures; high resolution PXRD for structure solution from powders; increased solid-state NMR capability to augment structure determination capability across the full range of solids; high resolution MALDI-TOF mass spectrometry.

Research funding portfolio and plans: ***Research income*** from 2008-2013 was £30.2 M, increasing significantly since 2011. Funding from RCUK sources has grown from ~£3.7 M (08/09) to ~£4.6 M (12/13), with a total income of £19.3 M since 2008. EPSRC is the main funding agency, together with BBSRC. EU sources have contributed ~£5.7 M. Industry sources total £2.3 M from 2008-13, with a further £1.4 M from charities. Non-research external income from RCUK, industry *etc.* totals £5.7 M, with a further £1 M income from JISC and £0.5 M from short courses, summer schools and donations. We have been successful in securing an EPSRC DTC (Complex Systems Simulation), a large EPSRC Programme Grant (Supercritical Fluid Electrodeposition, > £5 M), a BBSRC SLoLa award (Extending the boundaries of nucleic acid chemistry - total £4 M; £2.3 M to UoS), Platform Grants and many Standard Grants. The annual value of new research awards has been very substantial: £5.5 M (2008/09), £5.7 M (09/10), £9.4 M (10/11; including EPSRC NCS award), £11.9 M (11/12) and £9.1 M (12/13). We received considerable funding (total ~€11 M) *via* 2 EU InterReg Programmes for innovative organic synthesis. Our staff are involved in several UoS-led and multi-centre final stage CDT bids. We expect our research strategy will enable our continued success in securing funding from a range of sources, maintaining a diverse research income portfolio, as well as strong UG and PG cohorts.

Professional services & facilities access: Staff consult for biotechs, large pharma, fine chemicals industries and Government agencies. We operate a successful professional service, ***Southampton Chemistry Analytical Solutions*** (led by **Langley**), providing commercial access to specialist spectroscopic, diffraction and scientific glass-blowing facilities. This provides support for the instrumentation base in Chemistry and resources future investments. The total external commercial income from these activities since 2008 = £2.5 M.

e. Collaboration and contribution to the discipline or research base

Chemistry's strategic links with institutions around the world are supported through EU networks, programmes such as the EPSRC/NSF collaboration in chemistry, Erasmus programmes, the World University Network and others. Key examples include A*STAR (Singapore, 14 joint PhD students currently), La Sabana (Colombia) and Xiamen (China), leading to a significant research portfolio involving academics at each institution and supported at the UoS level through bilateral 2+2 PhD programmes, institutional research visits, and also by delivery of the Electrochemistry Summer School to *ca.* 600 students in Xiamen (2009, 2012). Targeted partnerships with Sao Paolo, Brazil (including Electrochemistry School, Sao Paolo, 2013) and key institutions in India are being developed. Visiting Professorships help to foster links with specific individuals (e.g. Tian, Xiamen).

International, national and industrial research collaborations: We have a wide range of collaborations where the team brings together the appropriate combination of expertise and skills pertinent to the scientific challenge. In addition to those in Section b, important *examples* include:

- **Magnetic Resonance** with Horsewill (Nott.): neutron scattering, mK NMR; Köckenberger (Nott.), Bodenhausen (Paris): hyperpolarisation; Morton (UCL), Smith (St Andrews): pulsed EPR; Madhu (Mumbai), Sebald (York): solid-state NMR; Murata (Kyoto), Turro† (Columbia), Bacic (NY): endofullerenes; Rõõm (Estonia): THz and IR spectroscopy; Rakitzis (Iraklion): pulsed IR; Johnson (ILL): neutron scattering; Brindle (Camb.): *in vivo* NMR/MRI.
- A large EU InterReg programme (€6.5M), 'Innovative Synthesis: Culture & Entrepreneurship', (Co-PIs=**Harrowven**, **R. Brown**), supports research in clean synthesis, healthcare, the ageing population and organic materials; follow-up project, AI:Chem (€4.5M), is building closer links with industry in catalysis, reagentless and automated synthesis (with **Harrowven**, **R. Brown, Linclau**, **Whitby**, **Rios-Torres**, **Raja, Gale, L. Brown, Read** & collaborators in Caen, Rouen, LeHavre & UEA, and research centres: IRCOF, ENSICAEN, INSA Rouen & CNRS-Délégation Normandie).
- **Whitby** on a large EU InterReg 'Materials for Energy Efficiency in Transport' project with 10 institutions and companies in France and the UK.
- **Gale** with Davis (Maryland) and Quesada (Burgos), EPSRC/NSF-funded, on bicarbonate transport by small molecules; with Perez-Tomas (Barcelona) on the anti-cancer properties of transporters; with A.P. Davis and Sheppard (Bristol) towards treatments for cystic fibrosis (EPSRC); on sulfate transport with Jolliffe (Sydney) and Plavec (Ljubljana) (WUN & COST).
- **Essex** with industrial partners (including Novartis, Syngenta, Merck, GSK, Unilever) on molecular simulations to study proteins and intermolecular interactions, and *via* the Complex Systems Simulation DTC; with Bureau (Caen), Clark (Erlangen), Verma (A*Star Singapore), Acquavia (Turin); UK collaborations include Mulholland (Bristol), Sansom (Oxford), Bond (Cambridge), Michel (Edinburgh), Todorov, Sherwood (STFC).
- **Bartlett** and **T. Brown** with DSTL, developing electrochemical approaches for DNA discrimination and detection; with Kilburn (QMUL) on high-throughput bioelectrochemistry, supported by EU funding involving ~14 European universities and 6 companies.
- **Day** with Sanders (Cambridge) on mechanochemical synthesis, and Cooper (Liverpool) on microporous molecular crystals (both EPSRC funded); with Sirringhaus (Cambridge) on charge transport in organic semiconductors; with Pfizer Global R&D predicting formation and stability of crystalline pharmaceuticals; with Emsley (Lyon) solid-state NMR for crystal structure solution.
- **Reid** and **Levason** with Bhalla (Brisbane) and GE Healthcare, developing new metal fluoride complexes as scaffolds for rapid, late-stage F-18 radiolabelling.
- With the Research Complex at Harwell through 2 EPSRC consortia: (i) Dynamics Group- **Evans**, (ii) Catalysis Consortium, and also as co-Is on the EPSRC Catalysis Hub - **Evans**, **Russell**, **Raja.**
- **Raja** with Honeywell and SiGNa using framework catalysts for sustainable processes.
- **Frey** works with Brocklesby, Horak & Richardson (ORC) developing desktop laser-based X-ray systems, and with Rutland (KTH Stockholm) on interfacial chemistry. He also has strong links with Oxford e-Research Centre (de Roure), Penn State, PNNL/EMSL (Mueller), with **Coles** and colleagues in Maths and Statistics (UoS) on cheminformatics, large data and electronic lab notebooks (LabTrove - JISC, Lonza Biologics plc, Microsoft Research).
- **Skylaris** with Cambridge and Imperial College developing the ONETEP program for *ab initio* quantum chemistry simulations (EPSRC Platform Grant, commercialised by Accelrys); with the UK Car-Parrinello Consortium, Johnson Matthey and Boehringer-Ingelheim**; Skylaris** and **Essex** with Head-Gordon (Berkeley), Case (Rutgers), Tuckerman (NYU), Ponder (Washington) & Neremberg (Claremont, US) on the development and implementation of polarisable force fields into a range of advanced classical and QM molecular simulation programs (EPSRC/NSF-funded).
- **Russell** with Johnson Matthey plc to advance development and understanding of the cathode & anode components in electrocatalysts and fuel cells for the automotive industry (EPSRC & EU).
- **Roach** with DSTL on novel protein targets and their inhibitors – potential antibiotics that could provide protection against bacterial biological warfare agents and have wide significance for public health in tackling antibiotic resistant pathogens (DTRA-funded).
- **Dyke** with Percival (Manchester), Shallcross (Bristol) on reactive intermediates in atmospheric chemistry (NERC); with Mok, Chau (Hong Kong), La Sapienza and Lisbon.
- **Attard** with Nylander (Lund) on structural studies of cell-free biosynthesis (EU).

• **Owen** with EU partners on the 'Labohr' consortium (FP-7) on Li ion batteries and with Qinetic.
Major Facility Use: Chemistry makes considerable use of large facilities (synchrotron, neutron, lasers etc.); value of access to UK facilities = £4.4 M since 2008 (**Evans**, **Russell**, **Hector**, **Stulz**, **Frey**, **Coles**, **Light**, **Nandhakumar, Reid**), with a further 23 days at Daresbury (Jan. 08-July 08). Staff have also been awarded 278 days at European (e.g. ESRF, ILL, SLS, HASYLAB, MAX Lab, Elettra) and US (Brookhaven, Stanford, Berkeley) national facilities since 2008. Access to HPC facilities (HECToR) is essential for CSC (**Essex**, **Skylaris**, **Day**), receiving > 90 M AUs since 2008.
IP & Patents: 42 patents have been granted and a further 47 filed since 2008.
Academic Leadership and Prizes and Awards – examples are provided in each category.
Fellowship of Learned Societies: **Bartlett:** FRS (2012); **Levitt:** FRS (2007); 13 FRSCs.
Prizes and Awards: **Bartlett**: RSC Tilden Lecturer (2011); J. Calvin Giddings Lecturer, Utah, US (2008); Electrochimica Acta Gold Medal of the Int. Soc. of Electrochem. (2008); **Levitt:** Fellow Nat. Acad. Sci., India; Craig Lecturer, ANU, Canberra (2010); John Francis Vigani Lecturer, Italian Chem. Soc. (2008); Günther Laukien Prize (2008); Wolfson Research Merit Awards: **Levitt** (2012), **Gale**, **Essex** (2013): **Day**: Mol. Graphics & Modelling Soc. Silver Jubilee Award (2008). **T. Brown** (Oxford from Oct. 2013): RSC Interdisciplinary Prize (2009). **Mahajan**: RSC Ronald Belcher Memorial Award (2008). **Pletcher**: Vittorio de Nora Award, US Electrochem. Soc. (2010); Castner Medal of the SCI (2013). **Attard**: Rhodia Prize, Eur. Colloids & Interfaces Soc. (2009); **Watts**: Leibert Young Investigator Award, Oligonucleotide Therapeutics Soc. (2013). **Read**: RSC HE Teaching Award (2010); **Birkin** (& Leighton): RS Brian Mercer Award for Innovation (2011); IChemE Innovation Award (2012); **Tavassoli**: Silver Medal European Young Chemist (2008).
Leadership in Industry: **Hayden**: CSO, Ilika; **Bartlett**: Director, Southampton Asset Management; Southampton Innovations plc; Photonic Innovations Ltd.
Major External Advisory Roles: **Bartlett**: Blackett Review on Biodetection (Gov. Office for Science, 2012); External Assessor for Environmental Protection Agency, Eire; **Gale**: Reviewer Monash Chemistry (2011); Kyushu Univ. Center for Molecular Systems Int. Board; **Evans**: Chair Scientific Advisory Comm., Research Complex at Harwell; 20% secondment to Diamond Light Source.
External Committee Roles: **Bartlett**: Bioelectrochem. Soc. Council; **Gale**: Chair RSC Macrocycles & Supramol. Chem. Group (2012); ISMSC Int. Comm. (2008); RSC Sci., Ed. & Ind. Board (2009-12); HCUK Standing Comm.; Management COST CM1005 Supramol. Chem. in Water; **Reid**: Elected Member of RSC Council (2011-15); **Whitby**: RSC Organic Division Council; **Dyke**: Chair of the NSCCS (2009-15); **Frey**: RSC Faraday Council (2011-14). **Tavassoli**: President RSC Chem. Biol. & Bioorg. Group (2012-15); **Russell**: Titular Member of Division 1 of IUPAC (2011-15); Chair-elect of the Int. Soc. Electrochem. (2013); **Read**: Chair of *Ed. in Chem.* (2010-); **Levitt**: Sectional Comm. of the Royal Society (2013); Physical Science Awards Comm. of the Royal Society (2013).
Visiting Fellowships: **Raja**, **Gale**: Erskine Visiting Fellows, Canterbury, NZ; **Gale**, **Rios**: Japan Soc. for the Promotion of Science Fellowships; **Denuault**: Hanse-Wissenshaftskolleg Fellowship.
Visiting Professorships: **Levitt**: Adj. Prof. Tata Institute, Mumbai; **Russell**: Adjunct Prof. Case Western Reserve Univ.; **Gale:** Guest Prof. Xiamen; **Dyke**: Hong Kong Polytechnic Univ., La Sapienza University, Lisbon, Univ. Manchester; **Raja**: Turin; **Linclau**: Univ. Ghent.
Conference Organisation, International Plenary/Keynote Lectures: Examples: **Gale**: organiser & chair ISMSC, Brighton 2011; **Bartlett**: organiser & chair Zing Electrochem. Conf., Lanzarote 2012; **Levitt**: organizer & chair of Theo Murphy Discussion Meeting on endofullerenes, 2012; **Raja:** BZA 2010; **Linclau**: RSC Fluorine & Carbohydrate Chem. 2013. Over 50% of our Category A staff have delivered plenary/keynote lectures since 2008, in addition to numerous invited presentations.
External Panels: Academy of Finland Review Panel Chairs (**Dyke**, **Reid**); ERC Consolidator Grant Panels, ANR Laboratories of Excellence Jury, France, FCT-Portugal (**Gale**); Evaluation Committee for Chemistry Research in the Netherlands (**Levitt**). EPSRC Panels: **Attard**, **Bartlett**, **Evans**, **Frey**, **Gale**, **Harrowven**, **Levitt**, **Owen**, **Reid**, **Russell**, **Skylaris**, **Whitby**; STFC Science Board: **Russell**; Royal Society: **Bartlett** – URF; **Reid**, **Skylaris** – Newton; **Carravetta** - Rosalind Franklin; Research Council of Norway (**Owen**); Diamond Beamline Panels: **Stulz**, **Hector**, **Coles**.
Journal Editorial/Advisory Boards: **Gale**: *Chem. Soc. Rev.* Ed. Board Chair (2013-), *Chem. Commun.* (2005-13), *Chem. Sci.* (2013-); **Gale**, **Levason**: *Coord. Chem. Rev.*; **Bartlett**: *PCCP, ChemElectroChem, Bioelectrochem.*; **Essex**: *J. Comp. Aided Molec. Design, Chem. Central*; **Levitt**: *J. Chem. Phys., J. Mag. Res.*, and author of 'Spin Dynamics' (Wiley, 2008; >15000 copies sold); **Owen**: *J. Power Sources*; **Day**: *Front. Theor. Chem,*; **Russell**: *Electrocatalysis*; **Rios**: *Asym. Organocatal.*, and author of 'Stereoselective Organocatalysis' (Wiley, 2013).