Institution: Queen's University, Belfast

Unit of Assessment: 8

a. Overview This is a combined submission from staff in the Schools of Chemistry & Chemical Engineering (CCE) and Mathematics & Physics (M+P). There has been extensive collaborative research between the Schools, particularly between the Atomistic Simulation Centre (ASC) in M+P and CCE with a significant number of joint grants and papers. Strategic investment in chemical engineering has provided a critical mass of staff to be submitted to UoA12 rather than to UoA8, as occurred in 2008. This investment has strengthened the already strong links between chemists and chemical engineers as well as between CCE and M+P. Over the REF period, we have further enhanced our reputation in catalysis, ionic liquids (ILs), sensors and in synthetic organic chemistry. We have also developed new research in chemical biology, materials chemistry and fuel cells. This research is conducted in four interdisciplinary groups: *the Centre for the Theory and Application of Catalysis (CenTACat); Innovative Molecular Materials (IMM); Synthetic and Bioorganic Chemistry (SynBIOC);* and *the ASC.* Staff from both Schools are also strongly involved in two industry-university research centres, the Queen's University Environmental Science and Technology Research Centre (QUESTOR) and the Queen's University Ionic Liquids Laboratory (QUILL).

b. Research strategy

Achievements since RAE2008

CenTACat **Atkins, Burch, Hardacre, Hu, James, Lin, Marr, Muldoon, Seddon, Thompson**: The aims within CenTACat from the RAE2008 were the development of new catalytic and ionic liquid (IL) processes based on fundamental developments of the underpinning chemistry. These aims have been achieved and highlights include **Hu's** use of DFT to understand multiphasic heterogeneous catalysis, including the development of a new formalism to correlate surface reaction kinetics with chemical potential. **Burch** has significantly increased the surface specificity and time resolution of SSITKA-DRIFTS-MS techniques for mechanistic studies of gas phase reactions, enabling, for the first time, intermediates and spectators to be distinguished under realistic reaction conditions. **Lin** has combined theory with *in-situ* ATR-IR and electrochemistry to develop new direct alcohol fuels cells to understand the CO_2 selectivity. **Thompson** has been instrumental in developing cutting edge heterogeneous catalysts designed by DFT for the selective hydrogenation of amides/acids, enabling reactions to proceed below 20 bar H_2 and 100 ^oC, for the first time. **James** has pioneered the use of mechanochemical synthesis for the formation of porous media, such as metal-organic frameworks. From an understanding of the industrially important methanol carbonylation reaction utilising gold based supported catalysts, **Hardacre** has established a method to manipulate the gold nanoparticle size and successfully reactivated supported gold catalysts. **Muldoon** has developed an exceptionally active catalyst for the challenging selective oxidation of aliphatic alcohols without deactivation due to oxidation of the ligands. **Marr's** use of chemoenzymatic catalysis has enabled the efficient conversion of waste glycerol to secondary amines as well as the dynamic kinetic resolution of alcohols via a hydrogen transfer process-mediated amination. Using theory and neutron scattering, the mechanism of how biomass dissolves in ILs has been elucidated (**Hardacre**) and the critical micelle concentrations for ILs in aqueous solutions has been determined using fluorescence quenching and NMR spectroscopy (**Seddon**). This understanding has led to their use in films which possess impressive, antimicrobial/antibiofilm activity against pathogens (**Seddon**), efficient separation processes in crude oil treatment, and catalytic processes in the petrochemical and biomass sectors (**Atkins**).

IMM **Bell, Doherty, Fletcher, Holbrey, Lagunas, Manesiotis, Mills, Nockemann, de Silva, Vyle, Xiao**: Specific aims from the RAE2008 for the IMM group included Surface Enhanced Raman Spectroscopy(SERS) based assays as novel theradiagnostics, the design/synthesis of increasingly complex "lab on a molecule" systems and of materials with tailored functionality. Biological assays based on SERS have been developed for nucleobases, nucleosides/nucleotides, pterins, and single nucleotide polymorphisms (**Bell**). Fluorescent DNA mismatch sensors and methods for detection of cytosine methylation have been developed by **Vyle**. New two-input AND and INH molecular logic gates have been constructed, and the design of molecular logic gates by associating easily available lumophores and receptors in detergent micelles has been demonstrated (**de Silva**). Complex fluorescent multiplexing sensors which probe the proton concentration maps near micelles have been designed (**de Silva**). Superhydrophobic metallic particles have been assembled to create mm sized objects including self-assembled elastic particle

rafts (**Bell**). **Xiao** has demonstrated metal organic frameworks with selectivity for NO and frameworks with switchable adsorption properties. **Manesiotis** has designed and tested molecularly imprinted polymers with affinities for targets ranging from ibuprofen to riboflavin. **Holbrey** has optimised ionic liquids for desulfurisation of oils while **Nockemann** has prepared luminescent lanthanide-doped $LaF_3:Ln^{3+}$ nanocrystals within IL hosts. Nanoelectrodes have been prepared by homogenising functionalised multi-walled carbon nanotubes in ILs on carbon or carbon film electrode substrates (**Doherty**)**.** Gold-silver luminescent honeycomb aggregates have been prepared (**Lagunas**). Nanoparticle modification to create sensors which signal analyte binding through their scattering signals has been achieved through covalent modification of metal nanoparticles with disulfide-tethered bipyridine ligands (**Fletcher**). **Mills** has pioneered photocatalyst activity indicator inks, which are being adopted as a European standard. His research in intelligent inks and plastics for food packaging is currently being commercialised.

SynBioc **Cook, Goldring, Hale, Sheldrake, Stevenson, Tchabanenko**: The synthesis of pharmacologically-active natural products was a major research aim of the group from RAE2008. The outcomes have included **Hale's** total syntheses of (+)-azinothricin and (+)-kettapeptin, which helped demonstrate that members of the A83586C family operate as antitumour agents by potently disrupting the oncogenic β-catenin/TCF4 protein-protein interaction (IC_{50} 3-5 nM) by inhibiting E2F-transcription factors, and by inducing dephosphorylation of oncogenic hyperphosphorylated retinoblastoma protein. **Hale's** fully stereocontrolled synthesis of (-)-echinosporin also deployed the Padwa allenylsulfone [3+2]-cycloadditive elimination in enantioselective total synthesis for the first time ever, and it introduced a powerful new method for ketone enolate C-alkoxycarbonylation. **Hale's** synthesis of (+)-pumiliotoxin B applied his O-directed free radical hydrostannation of alkylacetylenes for stereodefined olefin construction. **Stevenson's** chemoenzymatic syntheses of (+)-pericosenes A and C provided the shortest routes to these targets. His syntheses of (+)- and (-)-epibatidines, and his study of their vinylic halide substitution reactions, have shown the versatility and power of the bacterium *P.putida* UV4 in synthesis. **Goldring's** synthetic efforts on caryolanes have resulted in the strained bicyclo[4.3.1]decene core via RCM, and opened a potential new pathway to these natural products. **Tchabanenko's** pioneering use of chiral oxazolidinone enamides for oxidopyrilium ylide cycloaddition has led to *single cycloadducts being obtained* and demonstrated that such auxiliaries can be cleaved by catalytic hydrogenolysis. **Cook's** hydrosilylation methology and their use to form stereodefined chiral allylsilanes via Ir-catalysed isomerisation and tandem Claisen rearrangement are powerful new reaction advances. **Cook** has also introduced useful new palladium catalysed π-allyl rearrangements of alloc indoles and Cu-catalysed oxidation reactions for the synthesis of indoles and quinolines. **Sheldrake** has synthesised lignin mimics for use in biomass depolymerisation studies and has demonstrated efficient catalytic depolymerisation of both bark and lignosulfonate derivatives.

ASC **Dundas, Grüning**, **Huang, Kohanoff, Lane, McCann, Stella, Todorov, Tribello**: The strategic aims for the ASC from the RAE2008 were to develop theoretical and computational methods for atomic scale modelling and simulation of hard and soft condensed matter systems. **Todorov** and **Dundas** have modelled the advantages of nanoscale conductors in real-time using in-house methods for non-equilibrium, non-adiabatic molecular dynamics, including the discovery of directional cyclic current-driven motion as a further driving mechanism both for mechanical failure and for notional atomic-scale engine "designs". Three codes have been developed for the study of laser-matter interactions. EDAMAME is a real-space, time-dependent density functional code (**Dundas**) to study the interaction of molecules with intense, ultra-short laser pulses. YAMBO is a many-body code for the accurate calculation of optical spectra of solids and molecules (**Grüning**). PolyCEID is a code for non-adiabatic molecular dynamics used to study exciton dynamics in conjugated polymers (**Stella**). The ability to identify possible laser cooling targets was demonstrated by **Lane**. **McCann** has developed models of ultrafast laser-induced coherences in molecules. **Kohanoff** has shown that electrons in irradiated ILs can localise on either the cation or anion, thus leading to their degradation, e.g. in electrochemical devices. Using first-principles MD simulations, research in irradiation of materials and biological systems (**Kohanoff, Todorov**) has shown that DNA strand breaks can be produced by low-energy electrons. Irradiation of metals by protons and α-particles was shown to produce electronic excitations that induce structural damage. In protein structure-function relationships and enzymatic catalysis, the long-standing debate in the

mechanism of human galactokinase was solved by means of hybrid QM/MM simulations and has led to a way to develop mechanism-based GALK inhibitors (**Huang**). **Tribello** has developed the reconnaissance metadynamics technique to sample rare events and sketch-map to analyse complex free energy landscapes, applied to crystal growth and protein conformation.

Strategic aims of each cluster from 2014 onwards

Our vision is to expand our world class capability in multidisciplinary research at the interfaces between Chemistry, Physics, the Life Sciences and Engineering to address societal needs in healthcare, energy, and the sustainable environment.

CenTACat will work on grand challenges in the areas of energy and the sustainable environment where catalysis is a key enabling technology. Staff will have a major role in the UK Catalysis Hub (where the UoA is leading the Energy area), in the new Competence Centre in Advanced Sustainable Energy (CASE) funded by Invest Northern Ireland, and in numerous industrially funded projects. We will address the challenge to develop the energy efficient conversion of dilute waste feedstreams into high value chemicals; investigate ground-breaking theoretical and *in-situ* spectroscopic and diffraction methods to probe catalysis at the gas-liquid-solid interface in order to understand heterogeneously catalysed and fuel cell systems; design novel anode material formulations for the selective oxidation of higher alcohols in acid/alkaline fuel cells; develop a suite of catalysts for the benign hydrogenation of carboxylic acids and amides in the presence of reducible functional groups; investigate innovative new low temperature plasma-catalysed activation of hydrocarbons for VOC and exhaust emission control. Within QUILL, we will also develop commercially viable new IL-catalytic technology for the activation/conversion of CO_2 to fuels and chemicals; utilise the ability of ILs to dissolve biomass to efficiently convert cellulose to sugars and then to produce olefins and diols; design the next generation ILs for the promotion of enhanced oil recovery and replacement lubricants under extreme temperatures and pressures.

IMM has grown significantly supplementing existing strong research in nanostructured materials, photocatalysts and advanced sensors with 6 new appointments in inorganic membranes, molecularly imprinted polymers and metal-organic frameworks since 2012. In the next 5 years we will exploit this critical mass by developing IMM as a centre of excellence in complex, intelligent multifunctional materials which address the key challenges in delivering healthcare to an aging population, ensuring energy supply and building a secure society. This centre will incorporate existing planned new developments such as the International Photocatalyst Testing Centre as well as developing highly collaborative programmes which will work on intelligent, multifunctional materials. Typically, this multifunctionality will come from a combination of chemical specificity combined with larger meso-scale structure to create macroscopic materials with tailored properties i.e. we will move “beyond the molecule”. These materials will range from molecular logic switches arrayed in polymer hosts for optical data processing to marine-derived microstructures for drug delivery, from molecularly imprinted polymers on plasmonic metal surfaces to nanostructured photocatalysts in water-splitting solar cells.

SynBioc’s research effort will continue to be focused on the total synthesis of complex pharmacologically-active natural products and their analogues, and in the novel applications of these molecules in deconvolutional chemical biology and medicinal chemistry. Target molecules whose synthesis will be attempted will include (+)-acutiphycin, (+)-monanchorin, aspergillin PZ, (+)-pancratistatin, coleophomone A, palau’amine, and diazonamide A. Much new organic reaction development will underpin these efforts, most especially the design and synthetic application of novel cascade and organometallic chemical reactions and unusual new biotransformations. Research into flow- and new-reactor chemistry will also be undertaken. In addition, major new research directions are being planned in the areas of high performance organic materials synthesis for applications in microelectronics and energy generation.

Staff in the *Atomistic Simulation Centre* work on the real-time dynamics of classical and quantum systems. This expertise in classical and first-principles molecular simulation, time-dependent DFT and tight-binding approaches, and non-adiabatic electron-nuclear simulation has been strengthened by 3 recent appointments. The ASC’s main goal for the next 5-10 years is to further

develop and integrate these modelling techniques in order to push the frontiers in areas where the ASC has already made world-leading advances including in electron transport in nanostructures, irradiation of materials and biological matter and ultra-fast laser-matter interactions. Equally important will be the development of integrated approaches that exploit theoretical understanding to rationally design processes and functional materials, which have the potential to generate disruptive technologies. This philosophy, which is already in place, will be actively pursued in collaboration with experimentalists in CCE and Nanomaterials and Plasmas (M+P), as well as elsewhere in the UK and worldwide. Target areas, some of which address key challenges such as Healthcare and Energy production, are: ILs, crystallization, mechanochemistry, biomolecular dynamics, laser-cooling of molecules, heterogeneous catalysis and photocatalysis, pharmaceutical drugs, nanoelectronic/photonic/plasmonic devices, and radiotherapies.

c. People, including:

i. Staffing strategy and staff development

The strategy for staffing is set out in the School's annual academic plan and is to provide a balance across the Schools to support teaching and research. For any new appointment, the School Management Board discusses the research areas of strategic importance with respect to funding councils, the local and UK economies and then reviews the balance between strengthening under-resourced areas and supporting areas which are already strong. Using this strategy, **Mills** was appointed to a Chair in Materials Chemistry; **Cook** and **Tchabanenko** replaced **Malone** and **Hamilton** to enhance synthetic organic chemistry and chemical biology; **Lin** was appointed to develop fuel cell and energy research; **Panesiotis** and **Xiao** were appointed in the area of analytical chemistry and functional polymers; **Holbrey** broadened our presence in physical organic chemistry and ILs; **Thompson** and **Muldoon** successfully transferred from RCUK fellowships to lectureships, and **Nockemann** was appointed as an additional RCUK academic fellow in nanoparticle synthesis; **Dundas** and **Grüning** have been appointed to strengthen links between CCE and M+P and to reinforce research in nanoconduction, electron dynamics and laser-matter interactions. **Tribello** has been appointed in the area of soft matter, liquids and biological systems and **Stella** in the area of non-equilibrium non-adiabatic dynamics. The latter is a joint appointment between the CCE and M+P. **Atkins** has been appointed from BP/Petronas as a Chair in Innovation. Strengthening the interface with Chemical Engineering is also key to our recruitment strategy, particularly where this overlaps with sustainable processing. CenTACat and IMM have almost equal representation from "chemists" and "chemical engineers", with significant research undertaken in multidisciplinary projects at this interface. Within the UoA, 10 staff are aged $\leq$40; 14 between 40-50, 9 between 50-60 and 3 >60. Six new members of staff are international with ~41% in total as well as 45% of PDRAs. Four academics and 44% PDRAs are female.

There is a vibrant and extensive seminar programme, with approximately 50 talks per annum. An annual Thomas Andrews research lecture, inaugurated in 2010, aims to appeal to all levels. Biannually there is also the QUILL lecture series (est. 1999). Visiting international speakers have included Sayer (NIDDK, USA), Desiraju (Hyderabad), Bao (Dalian Institute of Chemical Physics), Anastas (Yale), Kumar (Florida Atlantic U.), Davis (Temple U.), Smith (U. Pennsylvania), Marshall (U. Virginia), Cahill (George Washington U.), Sheldon (Delft University of Technology), Li (McGill U.), Yamamoto (Tohoku U.), Chan (Hong Kong U.), Sun and Tian (Xiamen U.), Alper (U. Ottawa), Sadoway (MIT), Zei (National Central U., Taiwan), Hashmi (U. Heidelberg), Basset (KAUST), Kappe (U. Graz), de Haan (Eindhoven U. Technology), MacFarlane (Monash U.), Friščić (McGill U.), Hoffmann (CalTech), Ollis (North Carolina), Lehn (Strasbourg U.), Fichthorn (Penn State U.), van Ruitenbeck (Leiden U.), van de Vondele (ETH-Zurich), Stefanucci (U. Rome).

<u>Career development</u>

Appraisal and Workload: all academic and postdoctoral research staff undergo annual appraisal. Academic staff are appraised by their Director of Research (DR) or Head of School (HoS), and PDRAs by their academic supervisor. For PDRA's, the focus is on identifying development needs and then mapping out a personalised career plan. Academic appraisal provides support and guidance for research strategies and opportunities in, for example, funding, multidisciplinary research, publication opportunities, and leadership/management training. It is a forum to discuss promotion criteria and examine workloads across research, teaching, and administration. An academic workload allocation model is used to ensure fair administrative and teaching loads which allows all research active staff to have broadly the same amount of time for research. The criteria

for sabbatical leave are set out in the School's Staff Handbook and academic staff are encouraged to take sabbatical leave to enhance their research profiles.

Training: staff and PDRAs can access an extensive training programme which is integrated between the Schools and the central University. Centrally-available opportunities include the Postgraduate Certificate in Higher Education Teaching (PGCHET) and a wide range of generic courses, including: supervising research students, report writing, grant/fellowship applications, leadership training, entrepreneurship, IP, and career development (CV preparation, academic interview advice, etc). The Schools provide subject specific training (either in house or via external bodies) in, for example, health and safety, instrumentation, analysis of data and technique specific courses (XPS, XRD, single crystal, NMR, MS, modelling, IT). Of particular note is the leadership development course aimed at SLs, Readers and Chairs.

PDRAs and PhDs: as well as formal training, they can contribute to tutorials, laboratory supervision, and outreach, thereby developing interpersonal and transferrable skills. PDRAs applying for fellowships have a mentor to help prepare the scientific case as well as the financial aspects and impact statements. QUB supports the concordat for training research staff through the staff training and development unit which won the European Commission's HR Excellence in Research Award for their work in this area.

Early career staff undergo a 3 year probation, with associated support. A senior academic acts as mentor, and a committee (the HoS, mentor, relevant DR, Director of Education) reviews their progress against an agreed development plan. The committee also provides advice and guidance, including reviewing grant applications and publications, recommending funding possibilities, teaching methods, research directions, and training and development opportunities. All grant applications are reviewed by at least two senior colleagues, and go through several iterations. Probationers have reduced teaching loads starting at 33% and reaching 100% after 3 years and no large administrative duties. Mandatory training, including PhD supervision and the PGCHET, is an integral part of probation. Early career staff receive a School studentship, and start-up funding of £16K. They also receive 50% of the FEC earned to support their research.

Financial support: All staff can bid for School equipment funding, and typically >£50K is distributed from the fund each year to support staff research. University equipment funding is also available with collaborative bids normally given priority. Most analytical services are provided free within the School using FEC contributions to support these activities. The School is well-supported with studentships from the studentship budget provided to QUB by the Department for Education and Learning (DEL). A proportion of DEL studentships are allocated to the research groupings on a pro-rata basis according to research income/applications, and then distributed within the cluster by the DR based on grant income and strategic priority, for example to support grant applications, to strengthen areas of research or to promote interdisciplinary research. Partial funding of studentships within the School (50%) is available to encourage interaction with industry. Other DEL studentships are available for all staff via a QUB wide competitive process, including some ring-fenced for interdisciplinary research. All studentships are provided with consumables funding. A university central conference fund encourages networking.

Visiting Scholars (incoming and outgoing)

Over the REF period >50 academic visitors have been hosted including: Yuan (Hainan U.), Zei (National Central U., Taiwan), Korneichuk (Lomonosov Moscow State U.), Ma (ZJUT, China), Margulis (U. Iowa), Correa (Livermore National Laboratory), Gu (NUIST, China), Frederiksen (UPV, Spain), Stella (U. Basque Country), Sadoway (MIT), Delgado (U. Cadiz), Triolo (Istituto per i Processi Chimico-Fisici, Italy), Gunaseelan (U. Malaya). In addition, visiting Professorships are held by **Burch** (ECUST, China), **Hardacre** (ZJUT, China), **Hu** (Fudan U., DICP, ECUST, China), **Lin** (Xiamen U., Shangdon U., ZJUT, BUCT, China), **Nockemann** (Ghent U.), **Seddon** (ITQB, Portugal; Chinese Academy of Sciences), **de Silva** (Chulalongkorn U., Thailand; ECUST, China).

Equality and Diversity

Retention of all staff is important, and the retention and promotion of female academics and

researchers is critical. We promote flexible working patterns, and all the female academics have taken advantage of this opportunity: currently, 50% of our female academics work part-time. Our workload allocation model ensures that their research is not swamped by an uneven balance with respect to administration/teaching. We introduced a returner's policy in 2009, whereby academics taking maternity or adoption leave are free from administration and teaching for six months on their return. A part time teaching fellow was appointed in 2010 to support the returners' policy and flexible working. The flexible working policies have led to an increased number of male academics and staff taking paternity and other leave, which has enhanced morale and the working climate for all in the school. We make significant efforts to accommodate all working patterns when arranging meetings etc. Equality and diversity activities are now classed within the workload allocation model to recognise the importance and influence that these have on all aspects of school life. All staff are required to take the online training "DiversityNow" which raises staff awareness on equality and diversity issues. Women at all levels are visible in all promotional material. Career development information is widely distributed to staff, and promotion panels have representation from across the Schools as well as the University to ensure fairness. A PDRA (**Srinivasan**) was awarded a Unesco L'Oreal Women in Science Fellowship in 2012. CCE has a SWAN silver award and M+P has a SWAN bronze award. QUB has an institutional SWAN Silver Award.

ii. Research students

Approximately 40% of our PGR students are from outside the UK including China, Malaysia, Poland, Jordan, Canada, Bulgaria, Colombia, Spain, France, Ghana, Hungary, India, Italy, Nigeria, Romania, Russia, Saudi Arabia, USA, Taiwan and there is an almost equal split of male and female students. Specialist support for international students is available in the International and Postgraduate Centre as well as from the international academic staff. We regularly recruit students funded by, for example, MARA, Malaysia, who only allow the top students within the country to participate, and the Chinese Scholarship Council (CSC) through which QUB has a minimum quota of 20 students each year. All studentships are advertised widely and are appointed via a competitive process whereby the students are interviewed by the supervisors as well as references obtained. Websites such as FindaPhD are used regularly to attract high quality candidates.

PhD Students (FTE)	**2008-09**	**2009-10**	**2010-11**	**2011-12**	**2012-13**
	84	76	81	75	70

Research students receive support on many levels and all have two supervisors with specific training in PhD supervision. A senior member of staff acts as Postgraduate Tutor who oversees PhD administration, ensures compliance with regulations and acts as a point of contact for students. Student progress is reviewed on an ongoing basis, starting with a review after the first three months to confirm the feasibility of the project and the availability of the necessary resources. Differentiation, a significant exercise involving a 30+ page written report and an interview, normally takes place at the end of first year. There is a requirement to have ≥6 formal supervisory meetings per annum (in addition to the normal day-to-day contact between students and supervisors). At the end of the year, second and third year research students give a presentation to the research group and the School, respectively. In addition to School and project-specific training, the University-wide training programme, funded by the N.I. Assembly/RCUK provides access to a wide range of training courses and skills development co-ordinated by the QUB Postgraduate Training Team.

d. Income, infrastructure and facilities

Infrastructure and facilities: Since 2008 there has been substantial strategic investment in building new state-of-the-art research laboratories for synthetic chemistry and catalysis research (SRIF £6.7M) with accommodation for > 50 researchers. This is in addition to the £6M investment in new laboratory infrastructure just prior to the RAE2008. Excellent new UG chemistry teaching laboratories were completed in 2011. Further investment in research and teaching laboratory space of ~£1M is planned for 2014. There has been substantial investment in key new equipment including a 400 MHz NMR spectrometer, environmental SEM, Biotage automatic chromatographic purification system, LC-MS and £1M of strategic small equipment investment via SRIF and EPSRC. These supplement the existing equipment base (4 NMR spectrometers, 3 mass spectrometers, SMART single crystal XRD, monochromated powder XRD and XPS, ICP-AES, BET and Hg porosimetry, 2 Raman microscopes, CD spectrometer, nanosecond pulsed laser

systems as well as standard spectrometers, reactors, chromatography and computational facilities). 15 technicians provide support for NMR, high-resolution mass spectrometry, microanalysis, glass-blowing, mechanical engineering, electronics, computer management and laboratory safety. Central QUB facilities include transmission and scanning electron microscopy as well as access to shared equipment through a database (including specialist mass spectrometry, chromatography and particle size analysis). We have a Class II biological laboratory and a radiochemical laboratory. Access to high performance computing is provided both through central QUB facilities and smaller clusters in the ASC and CenTACat. The University's new £44M library provides on and off-site access to electronic journals for all researchers.

Research funding portfolio and consultancy

The grant spend (£21.2M) is equivalent to ~£123K per fte per annum for the staff submitted (including 6 members of staff on probation (5 appointed in 2013)). This is split 57% from government/charitable sources and 43% from industry showing strong support for both fundamental and applied research. In addition, £1.3M of funding from central facilities has been awarded including time on ISIS, Diamond Light Source and HECToR. Of significant note are two EPSRC programme grants (CASTech and 4CU) worth >£4M, successive contracts with Petronas since 2008 of >£9M, fuel cell research funded by the TSB/EPSRC (£1M) and research into cancer research and hit drug candidates from Almac Sciences through the Almac-QUB Centre for Small Molecule Drug Discovery (£3M). In addition, grants including the EPSRC Catalysis Hub, the IKC in synthetic biology, the CASE competence centre and a new 5 year programme with Petronas as well as many other small grants totalling >£10M have been awarded in 2013 which provides sustainability for the future. We aim to obtain follow on EPSRC funding in the area of catalysis with Cardiff and Cambridge Universities, central facilities and industry to develop both the fundamentals and applications of liquid phase heterogeneous catalysis. Moreover, our proposed research feeds directly into the EPSRC's Grand Challenges on Systems Chemistry and on Directed Assembly of Extended Structures with Targeted Properties and proposals will be targeted at these calls. We will target Horizon 2020 by building on existing networks in, for example, the Secure Societies theme to developing sensor materials to combat terrorism (nanostructured, optical, electrochemical, IL based, functionalised polymer sensing materials) as well as working with European partners developing materials/catalysts for use in healthcare, manufacturing, diagnostics, high value biomaterials derived from sustainable sources and materials for energy production and storage. Green chemistry and cancer research are areas of strategic priority for QUB and are also being supported by donations to the QUB fund raising campaign. We will continue to develop projects in medicinal chemistry, catalysis, ILs and SMART materials through key industrial partnerships, e.g. Petronas, Johnson Matthey, Almac Sciences. International academic partnerships are also a key part of the future funding plans. Specific links are being developed with Stanford U., Shanghai Institute of Organic Chemistry, Dalian Institute of Chemical Physics, Xiamen U. and East China U. of Science and Technology as well as with collaborators in the Middle East and Brazil for joint research through initiatives such as the Qatar National Research Foundation and the US-Ireland initiative in ILs, total synthesis, materials and fuel cells. For example, substantial grant applications are being prepared to support future research activities in non-viral transfected gene therapy and monoclonal-antibody-conjugated natural product synthesis for non-toxic cancer cell receptor-targeted chemotherapy and photocatalysis.

Industrial consultancy is managed through the Research and Enterprise Directorate with clear guidelines in terms of time and responsibilities. Staff are encouraged to undertake relevant consultancies. These include: Almac Sciences (**Huang**), Warner Chilcot (**Fletcher**, **Hardacre**); GSK, Pfizer, AZ, Mitsubishi Tanabe (**Hale**) and Unilever, Johnson Matthey, Sun Chemical, Pilkington Glass, Crown Holdings, St. Gobain, Tata Steel, Millennium Inorganics, Croda (**Mills**).

e. Collaboration or contribution to the discipline or research base

Interdisciplinary research and research strategy

Much of our research is multidisciplinary, particularly at the interfaces between chemistry, engineering, physics, biology, medicine and pharmacy. A number of large consortia have been established involving academia, industry and government. CASE is an industry led initiative within QUB to develop sustainable energy technology. Two industry-university research centres provide focus in environmental research (QUESTOR, 20 industrial partners) and ILs (QUILL, 15 industrial partners). The industry-academic links are driven through discussion with their industrial advisory

boards supporting both fundamental and applied projects. Strong research across the academic boundaries has been developed, e.g. in the EPSRC funded project to develop IL chemistry for medical research involving chemistry, pharmacy and medicine. Interschool collaboration is supported by QUB funding for green chemistry, clean energy and medicinal chemistry.

The School has extensive links and major grants involving >35 industrial partners including Johnson Matthey, Merck, Eastman Chemicals, Toyota, GE, Invista, Eli-Lilly, GSK, Unilever, Solvay, BP, ExxonMobil, Umicore, Tata Steel, Proctor & Gamble, Astra Zeneca. These collaborations have been crucial in identifying challenging scientific problems that have the potential to lead to commercial outputs and have resulted in >40 patents. Staff also hold major collaborative grants with other universities and industry in catalysis and ionic liquids, including the EPSRC UK Catalysis Hub, CASTech (U. Birmingham, U. Virginia, USA, U. Cambridge + industrial partners), 4CU (UCL, U. Sheffield, U. Manchester). The ILs group has had major contracts with Petronas since 2008. Fuel cell research has been undertaken with Johnson Matthey and DICP, China. A strategic alliance has also been formed with Almac Sciences. 5 Proof of Concept grants from INI and an EU Transfer of Knowledge grant with Celtic Catalysts have been awarded.

Significant collaborations exist with groups in the UK (Liverpool, UCL, St Andrews, Aberdeen, Robert Gordon, Sheffield, Nottingham, Cambridge, Cardiff, Southampton) and internationally (Arvinte (U. Geneva), Zhou (State Key Laboratory Lanzhou), McCabe and Kelly (TCD), Forrest (U. Houston), Rebelo (Lisbon), Laschat (U. Stuttgart), Krysa (ICT, Prague) Rathousky (Heyrovsky Institute), Neurock (U. Virginia), Padua and Costa Gomes (U. Blaise Pascal), Parvulescu (U. Bucharest), Woodward (State U. New Jersey), Burke (UCal. Irvine), Frederiksen (DIPC, San Sebastian), Sun (State Key Lab, Xiamen); Elsaesser and Winzer (IWM, Freiburg), Correa (Livermore), Caro (Los Alamos), Daly (NIH)). Staff are involved in the following EU networks: **Bell** QSAFFE project, HOMER; **Dundas** XLIC, COST CM 1204; **Grüning** ETSF Research Theme Leader; **Hardacre, Seddon** EXIL COST CM1206; **Kohanoff** Nano-IBCT, COST MP1002; **Mills** European Photocatalysis Federation; **Seddon** Capita ERA-NET.

Research Council Staff act as assessors for research centres and grants: **Bell** Enterprise Ireland, Russian Skolkovo Fdn, NASA/EPSCo; **Burch** Swedish Competence Centre; **Hale** Science Foundation Ireland, JSPS; **Hardacre** Austrian RC, US NSF, Australian RC; **Kohanoff** US NSF, Argentina ANPCyT, Chile CONACyT, Finland Academy, ANR, France; **Lin** EPSRC panel member; **Marr** Israeli NSF, US NSF; **Mills** DFG, Germany; **de Silva** Sri Lankan government. **Burch**, **Doherty**, **Hale**, **Hardacre**, **James**, **Kohanoff** and **de Silva** are EPSRC college members.

Prizes and fellowships **Burch** OBE for services to science (2009); **Hale** JSPS Invitation Research Fellowship (2010), National Science Council of Taiwan Visiting Lectureship (2011), RSC Bader Award and Silver Medal (2011), RSC All-Ireland Symposium Lectureship (2012); **Hardacre** USA R&D 100 award (2008), IChemE Andrew Medal (2013); **Seddon**(#46) and **Holbrey**(#59) THES ranking of highest citation scores since Jan. 2000; **de Silva** RSC Sensor Award (2008), Intl Award for Molecular Sensors and Molecular Logic Gates (2012); **QUILL** IChemE Awards for Outstanding Achievement in Chemical and Process Engineering, Sustainable Technology and Chemical Engineering Project of the Year (2013). **Bell, Doherty, Hale, Hardacre, James, Mills, Seddon, de Silva** and **Stevenson** are Fellows of the RSC. **Burch, Hardacre, Hu** and **de Silva** are elected Members of the Royal Irish Academy; **Hardacre** Fellow of the IChemE; **Hale** Fellow of the Institute of Chemistry of Ireland & Council Member (2009-10); **Burch** Member of *Academia Europaea*.

Plenary, keynote and invited lectures Staff in the UoA have given >250 invited talks at universities and industry over the REF period. Over 100 invited, plenaries and keynote lectures have also been given including: **Bell** Smart Coatings Intl Conf., Florida, (2011); Federation Analytical Chem. & Spectroscopy Soc., USA (2010); 23rd Intl. Conf. Raman Spectroscopy, India (2010); **Burch** 21st Canadian Symposium Catalysis (2010); 6th Intl Conf. Environmental Catalysis, China (2010); 22nd North American Catalysis Soc. Meeting (2011); **Cook** Gordon Research Conf. Heterocyclic Compounds, USA, (2010); Zing Conf. Natural Products (2012); **Grüning** CCP9/CECAM Workshop, Oxford (2013); **Hale** RSC 21st Intl Symposium Organic Synthesis (2009); Gordon Research Conf. Heterocyclic Chemistry, USA (2013); OL/JOC Symposium Shanghai, China (2013); **Hardacre** 3rd Intl Conf. Ionic Liquids, Australia (2009), 6th TOCAT/5th APCAT, Japan (2010), 6th Intl Conf. Environmental Catalysis, China (2010); **Hu** ACS March meeting, USA (2009),

ACS March meeting, USA (2010), 14th Intl Conf. Theoretical Aspects of Catalysis, Netherlands (2012); **Kohanoff** APS March Meeting, USA (2012), CPMD2013, Leipzig (2013), SLAFES, Colombia (2013); **James** Symposium Inorganic Chemistry in Ireland (2012), Intl Symposium Mechanochemistry in Synthesis & Nanoscience (2013); 96th Canadian Chemistry Conf. (2013); **Lin** UK-China Energy Conf., Beijing (2011), ACS Symposium Materials and Catalysis in Fuel Cells, San Diego (2012), ISE Satellite Meeting, Dresden (2012); **Marr** Gordon Conf., USA - 'Rising Stars of Green Chemistry & Green Engineering' (2010); **Mills** 19th Intl Conf. Photochemical Conversion & Storage of Solar Energy, USA (2012), 2nd European Symposium Photocatalysis, France (2011), 6th European meeting Solar Chemistry & Photocatalysis, Prague (2010); **Nockemann** 16th Conf. Materials Chemistry for Energy and Resource Utilization, Darmstadt (2012); **Seddon** 3rd Intl IUPAC Conf. Green Chemistry, Canada (2010), 3rd Asian-Pacific Conf. Ionic Liquids & Green Processes, China (2012); **de Silva** New Zealand Institute for Chemistry/Royal Australian Chemical Institute Conf., New Zealand (2008), 11th Research Institute for Electronic Science - Hokudai Symp., Japan (2010), Foundations of Nanoscience Conf., USA (2011), 3rd Intl Conf. Molecular Sensors and Molecular Logic Gates, Korea (2012); **Stevenson** Mona Conf. (2012); 2nd Sino-Ireland Synthetic Chemistry Symp., Shanghai (2011); **Tribello** CPMD2013, Leipzig (2013).

Conferences We have hosted a range of conferences including 5th Intl. Conf. Environmental Catalysis (2008), RSC Faraday Discussion on Ionic Liquids (2011), Intl Conf. on Mechanochemistry & Solvent-free Synthesis (2010, 2011), RSC Dalton Awards Symp. (2011), All Ireland RSC Awards Lecture (2012), UK-Semiconductor Photochemistry Network Mtg (2012); XIth Martin & Willis Spectroscopy Mtg (2011), CCP5 Summer School (2010, 2011), Electron Dynamics in the Life Sciences (2010). Staff also contributed significantly to the direct organisation of many international conferences held outside QUB including Europacat X (2011), EuChem (2008, 2010, 2012); 3rd Intl Conf. Semiconductor Photocatalysis (2009), Intl. Conf. Series on ILs (2007-13), ACS Symp. Fuel Cells (2012), 2nd RSC-CSJ Conf. Green Chemistry and Sustainability (2008); Biodegradability & Toxicity of ILs (2009, 2011); ACS Symp. ILs (2008); Gordon Green Chemistry Research Conf. (2012); 3rd Intl Conf. Semiconductor Photochemistry (2010), Structure & Dynamics of Hydrogen-bonded systems (2009), CECAM Workshop Density Functional Theory (2011), DIPC Workshop Dynamical Processes in Irradiated Systems (2010), ICTP Workshop Radiation Damage in Nuclear Materials (2011), CECAM Yambo tutorial on electronic & optical excitations (2013).

Journals
Editorial Advisory Boards: **Hale** Org. Lett. (2002-), Future Medicinal Chemistry (2008-), Wiley Postgraduate Chemistry Series (2009-2012), J. Chemical Engineering & Process Technology (2010-); **Hardacre** ACS Catal. (2010-), Catal. Sci. Tech. (2010-), RSC catalysis book series (2011-), Chemistry Central J. (2009-); **James** CrystEngComm (2006-2012), Nature Scientific Reports (2010-); **Kohanoff** ISRN Thermodynamics; **Lin** J. Chemical Engineering & Process Technology (2011-); **Mills** J. Photochemistry & Photobiology Chemistry A, J. Fluorescence, Open Chemical Engineering J. (2007-), Advances in Chemical Engineering & Science (2010-); **de Silva** J. Fluorescence (2002-); J. National Science Foundation, Sri Lanka, (2005-); J. Chinese Universities - E (2005-); **Seddon** Green Chem.; Crystal Growth & Design.
Journal Editorships: **Hale** Associate Editor Org. Lett. (2003-); **Hu** Science China: Chemistry (2013-); **Marr** PLoS one (2011-); **Seddon** Australian J. Chem. (2010-).
Guest Editorships: **Hale** Org. Lett./JOC/JACS Virtual Issue (2013); **Hardacre** J. Mol. Catal. A (2008), Faraday Discussion - Ionic Liquids (2011); **James** Chem. Comm. (2013), Chem. Soc. Rev. (2013); **Lagunas, Muldoon, Nockemann** CrystEngComm (2012); **Mills** Intl. J. Photoenergy (2008); J. Photochemistry Photobiology A (2010); **Seddon** Wiley book series on ILs (2011).

Others Indicators: **Dundas** Steering committee EPSRC Service Level Agreement with CSED (member); **Hardacre** FAP2 ISIS Panel Chair (2009-); I20 working group Chair Diamond Light Source (2008-); STFC Photon Advisory Panel (Member, 2009-2011), Faraday Council (elected member, 2013-); **Kohanoff** Gordon Research Conf. Radiation Chemistry (Discussion Leader, 2012); **Lagunas** Dalton Council (elected member, 2007-10); **Lin** Hydrogen & Fuel Cells Supergen Science Board (member); **Mills** EPSRC Network Semiconductor Photochemistry (Founder/Chairman); European Photocatalysis Fed. (secretary); British Standards Organisation (expert member); **de Silva** John van Geuns Fdn Lecturer, Van't Hoff Inst. Molecular Sciences.