Institution: University of Liverpool

Unit of Assessment: 8

a. Overview

The Chemistry Department has been part of the School of Physical Sciences (SPS) since 2010. The School comprises the Departments of Mathematics, Physics and Chemistry and sits within the Faculty of Science & Engineering (PVC **Holloway**, Chemistry). The Head of School (**Cooper** to 2011, McGrath, Physics) is supported by a leadership group, with Chemistry representation from the Head of Department (**Hodgson**), **Cosstick**, **Aspinall** and **Raval**.

In recognition of the interdisciplinary nature of our research, Chemistry is organised into five closely interlinked research clusters, based around the themes of **Materials Chemistry, Medicinal and Bio-nano Chemistry, Energy and Catalysis, Functional Interfaces,** and **Theoretical and Computational Chemistry**, each led by a cluster leader (**Rosseinsky, O'Neill, Xiao, Raval** and **Persson** respectively). Our clusters offer a flexible organisational structure, able to accommodate and manage changes in research interests and funding patterns whilst ensuring a coherent research direction. Research strategy is led by the Department's Research Committee (chaired by **Rosseinsky**), while interdisciplinary collaboration is encouraged by a School Research Committee (chaired by Lucas, Physics) and the Faculty Research Strategy group (chaired by **Hofer**). Several Chemistry staff were joint appointments with other Departments; **Hofer** (Physics) and **O'Neill** (Pharmacology) are returned in Chemistry, but **Levy** is returned in Biological Sciences).

b. Research strategy

The Department's vision is to deliver internationally excellent research and knowledge exchange through our core capabilities in synthetic control, materials discovery, assembly and organisation of molecules, and theory. Our strategy is both to focus on existing research strengths and to identify new research opportunities in areas considered to be of future societal importance. We achieve this by:

- identifying and developing new research themes, including energy storage, nanomedicine, drug discovery, photocatalysis and biotechnology, with the potential for future economic, environmental and health impact in the UK,
- appointing high calibre staff with international research profiles to initiate new research themes, particularly at the interface between scientific disciplines (e.g. Health and Life Sciences, Pharmacology), and to encourage local, national and international collaborations,
- targeting investment in equipment and startup for new staff, including capital startup, direct PDRA support and PhD studentships to new staff in the REF period,
- engaging directly with industry, e.g., through the Centre for Materials Discovery (CMD), promoting contacts that have led to Regional Growth Fund (RGF), UK Research Partnership Infrastructure Fund project (the £68M Materials Innovation Factory, MIF), TSB and other collaborative grants,
- investing in core research infrastructure by leveraging University support to target external capital funding, e.g., recently in EPSRC Chemistry Equipment call, RGF bid for the Micro Biorefinery (MBR), and European Research Development Fund (ERDF) bids.

Research strategy is led by the Department's Research Committee, which comprises the research cluster leads (above), PGR Director (**Kozhevnikov**) and four other staff, including early career research (ECR) representatives. The Committee allocates resources, such as EPSRC and University studentships, on a competitive basis, in alignment with our research strategy, while giving priority to ECR staff. The committee is supported by School Research Cluster leaders meetings, with strategy disseminated and discussed via regular staff meetings. Our research clusters provide a flexible structure, which can be adapted to reflect new funding opportunities and changes to our research themes, for example in response to RCUK Challenge areas and EU policy, while maintaining a coherent direction. Most staff contribute to several themes, reflecting the cross-disciplinary nature of the Department's research. The Theoretical and Computational Chemistry theme is unique in being an umbrella grouping whose members' core research interests are based in the other research themes. Chemistry contributes to three of the University's seven Research Themes (Materials for the Future, Sustainable Energy and Global Health).

Achievement of strategic aims: In RAE2008, the Department identified energy, bionano-

technology and medicinal chemistry as areas for future growth, building on our existing research strengths in materials discovery, catalysis, interface science and theory. Ten new appointments have been made to build activity in Energy and Catalysis, Materials and Nanomedicine. In response to these appointments, and the consequent change in the Department's research profile, our research themes were modified in 2011/12. The Energy and Catalysis theme has been developed by establishing a new interdisciplinary research institute, the Stephenson Institute for Renewable Energy (SIRE). SIRE is a cross-Faculty initiative, based around a new Chair (**Shchukin**) and six new Chemistry lectureships, with six equivalent appointments in Physics, housed in new £4.9M state-of-the-art laboratories. The Institute links fundamental research in Chemistry to applications in energy and renewable feedstocks. Following the departure of Evans to Queen's, Ontario, we have refocused organic research by developing the Medicinal and Bio-nano Chemistry theme, reflecting the strong functional links with Health and Life Sciences at Liverpool. The new Functional Interfaces theme brings together expertise in nanoscale science, electrochemistry and surface science to enable molecular design of interfaces, so mapping our research more closely towards the different groups of end users.

The Department has a strategy of strong engagement with industry, for example through the CMD, an open access facility for academic-industry collaboration and knowledge transfer in Chemistry, equipped with state-of-the-art robotics and informatics for automated synthesis and high-throughput characterisation of materials. In addition, the Knowledge Centre for Materials Chemistry (KCMC) has engaged with over 120 companies and set up Knowledge Exchange partnerships enabling a total of £9M revenue, including £1.5M industrial funding, during the REF period. KCMC is now supported by TSB as the national materials chemistry KE activity for its Materials Chemistry Special Interest Group. The Department currently has active research links with >30 companies, including AstraZeneca, BP, Johnson Matthey and Unilever, and SMEs such as ACAL Energy Ltd.

Industrial links are being further developed by creation of the new Materials Innovation Factory (MIF), which will co-locate academic research in Materials with industrial research partners by adding a new 11,000 m^2 wing to the Chemistry building. This £68M project, part funded by the award of one of the first UK Research Partnership Infrastructure Fund projects, is based around six core research themes (Sustainability, Inorganic Materials, Nanomedicine, High-Throughput Formulation, OMICS/ Biotechnology, and Organic Materials) that have been identified for their future scientific and industrial impact. The project includes nine new academic posts (2013-16), as well as £2M 'in kind' Unilever equipment and £5.5M University investment in the equipment base. This project builds on an RGF grant (£2.6M with Unilever) for the Micro-Biorefinery, and recent University and EPSRC investment in our core instrumentation (£1.8M), to create a dedicated analytical facility for the Department and our industrial partners.

In RAE2008, the number of Chemistry PhD students was identified as a weakness and this has been addressed by supporting University Research Studentships, and by establishing research agreements with international partners, including RIKEN, NTHU, BiomaGUNE, A-STAR and Dalian Institute of Chemical Physics (DICP), to fund joint PhD studentships and to expand our international student numbers. As a result, the number of PhD students has grown from 63 FTEs in 2007 (RAE2008) to 94 in 2012/13.

The vitality and success of the Department's research strategy is evidenced by £33M of research income in the REF period and an increased number of high impact papers (staff have published >800 papers, with >12,000 citations (WoS Nov13), in peer-reviewed journals since 2008, including four Science, 27 Nature group, and >236 in journals with IF≥8). £43M new research grants have been started in the period (a rate 100% greater than RAE2008), which, with £6.1M capital investment in buildings and research infrastructure, place the Department on a sustainable and upward trajectory. Ten staff are inventors on a total of 59 unique WO, European, US or GB patents (published since 2008). Of these 25 were published in collaboration with Unilever, Bayer, Johnson Matthey and Thermo Electron.

Achievement of research aims over the last five years

Research in the Department is highly interdisciplinary in nature. The research clusters work interactively to tackle multidisciplinary challenges with the aim of creating new scientific concepts. An example is the discovery and understanding of adaptable peptide-based porous materials (*Rosseinsky, Science #1*) through engagement of researchers in the Materials, Medicinal and Bio-

nano Chemistry, and Computational clusters: the combination of biological perspectives on guest response with materials chemistry concepts of porous materials was a major feature of this work. Similarly, integration of the skills and research perspectives of the Energy, Materials and Computational clusters allowed the computationally-assisted isolation of a new solid oxide fuel cathode (*Rosseinsky, Science #4*), demonstrating a new and generic working method for the identification of functional materials.

This working-level engagement across research areas has led to new national-scale research activities. For example, the Materials cluster worked with **Levy** (joint Biology) to establish an EPSRC-funded activity, including Manchester Imaging Science, in stem cell imaging. Building on the close interactions between Chemistry and Pharmacology in drug discovery and nanomedicine, this programme was integrated with the University's MRC Centre for Drug Safety Science in Pharmacology to permit Liverpool to lead the (£4.5M) Safety Hub of the UK Regenerative Medicine Platform from October 2013. Similarly, the Open Innovation Centre in Antimicrobial Surfaces (Q4 2013) is a new collaboration between the Functional Interfaces cluster and Health and Life Sciences, funded (£3.7M) by ERDF and TSB, to target a new area of impact for Liverpool.

Specific research achievements in this period include the following:

Materials Chemistry: The appointment of **Adams** (peptide-based assembly and porous materials), **Boulatov** (mechanochemistry) and **Blanc** (solid state NMR) strengthen Liverpool Materials research. Materials Chemistry links closely to SIRE and the Energy theme, and to the nanomedicine theme of the Medicinal and Bio-nano cluster. We have made core fundamental advances with the discovery of high-surface area porous molecules (*Cooper, Nature #1; Nature Mat. #2*) with unique, perfect selectivity for C9 aromatic isomers (*Cooper*, *Nature Chem. #4*), the discovery of the highest transition temperature molecular superconductors and their demonstration as correlated electron systems of generic importance (*Rosseinsky, Science #3; Darling, Nature #1*) and the discovery of new classes of oxide ion conductor (*Claridge, Nature Mat. #2*).

Medicinal and Bio-nano Chemistry: Strategic investment in the nanomedicine area includes the appointment of **McDonald** (Q3 2013), a joint appointment with the Department of Molecular and Clinical Pharmacology and the creation of a new radiochemistry laboratory. The nanomedicine activity has led to new materials, such as polydendrons (e.g., WO 2009122220) and new approaches to solid drug nanoparticle synthesis (*Rannard, Nature Nano. #1*). The medicinal chemistry group has contributed to the lead-optimisation of 4-aminoquinoline, quinolone and peroxide-based antimalarials (*O'Neill, ACIE #1, PNAS #2, JMC #3*) with the 4-aminoquinoline Isoquine receiving candidate selection status and entering clinical trials in humans in under five years. (Phase 1 with GSK/ Medicines for Malaria Venture (MMV) in 2008).

Energy and Catalysis: Since 2011, Liverpool has appointed seven new staff in these areas, initiating new research programmes in photocatalytic reduction of CO_2 (**Cowan, Teobaldi**), biomass conversion (**Lopez-Sanchez**), selective scission of C-H and C-C bonds for fuels and value-added chemicals (**Sergeev**), thermo-materials (**Shchukin**), electrochemical energy storage (**Hardwick**) and ionic conduction (**Blanc**). The new ECR staff have already won £3.5M external grant support as PIs since Q3 2011. Achievements include the development of new catalytic methods for C-C coupling (*Berry, JACS #2; Iggo, JACS #3*) and asymmetric hydrogenation (*Xiao, JACS #1, #2*), and the discovery of the Iridicycle catalysts through collaboration with Pfizer and AstraZeneca (*Xiao, ACIE #4*), which have been commercialized by YPT and Strem.

Functional Interfaces: Strong links have been developed with new projects involving SIRE staff, particularly with **Hardwick** (battery interfaces) and **Cowan** (photocatalysis), as well as with the Theory cluster. Key contributions have been made in the areas of 2D surface chiral crystallisation and enantiomer self-organisation (*Raval, Nature Chem. #1*), in covalent coupling directly at a surface via C-C and C-metal-C bond formation (*Raval, JACS #3*), in understanding hydroxyl co-adsorption and wetting of metal surfaces (*Hodgson, Nature Mat. #1, PRL #2*), by demonstrating cellular uptake and intracellular targeting of bio-functionalised gold nanoparticles (*Brust, ACS Nano #1, #2*) and coherent tunneling through single molecular wires (*Nichols, Nature Nano. #1*).

Theoretical and Computational Chemistry: Staff contribute to core research in all the other themes. Links to the Energy theme are driven by the appointment of **Hofer** as Director of SIRE and **Teobaldi** (photochemistry). We have obtained new insights from theory about molecules on

surfaces, including the crucial role of electron traps for the reactivity of the photo-catalytically active rutile surface (*Teobaldi, PNAS #1*), new processes such as dipole-directed growth (*Hofer, Nature Nano. #4*), cooperative reaction dynamics (*Hofer, Nature Chem. #2*), reaction-induced migration (*Hofer, Nature Chem. #1*), switching (*Persson, PRL #1*), and orbital imaging (*Persson, PRL #2*).

Strategic research aims for the next five years:
The Department plans to expand its research activity in line with the strategic themes identified above. It is proactive in seeking new funding opportunities, tackling RCUK Challenge and BIS "Eight Great Technologies" areas, and in influencing EU policy. Immediate plans include:

- Building on investment in the MIF by appointing nine new academic staff positions committed by the University (2013-16), including a leadership position in Formulation to support the unique capability in high throughput formulation created by the MIF, plus another Chair in Measurement, with other positions allied to MIF research themes and to SIRE.
- Strengthening Medicinal Chemistry with an appointment (2013/14) in Medicinal Chemistry, joint with Pharmacology (Institute of Translational Medicine), to support the development of new candidate anti-infective and anti-cancer drugs and coordinate transition of existing late lead molecules into preclinical evaluation in preparation for Phase 1 clinical trials.
- Establishing a new Open Innovation Centre in Anti-microbial Surfaces, linking Functional Interfaces and Medicinal and Bio-nano Chemistry themes to create a cross-disciplinary scientific grouping to tackle microbial activity on materials and interfaces relevant to industry.
- Growing biotechnology as a new strategic research activity, through MBR and MIF, to provide facilities for cloning, fermentation, protein isolation, and characterisation of a wide variety of macromolecules. This will significantly enhance our existing activities in currently expanding areas such as medicinal chemistry, biomass conversion, and antimicrobial surfaces.

c. People, including:

i. Staffing strategy and staff development

The Department recruits internationally excellent researchers into targeted research areas that match our longer-term research strategy. Our approach is to recruit a balance of established senior academics, to provide leadership in new research areas, as well as lecturers and ECR fellows to provide critical mass across the research areas identified. Recruitment is based on excellence in research in an international context, with the majority of the new academic appointments being non-UK nationals (four UK, five EU and one US). New appointments in Energy and Catalysis, as part of SIRE, comprise a Chair (**Shuchkin,** from Max Planck Institute, Golm) and six academics, including both experiment, **Blanc, Cowan, Hardwick, Lopez-Sanchez** and **Sergeev** (from Berkeley, USA), and theory, **Teobaldi**. **Lopez-Sanchez** and **Sergeev** also contribute to the Catalysis theme, while **Blanc** also contributes to Materials and drives the Department's solid state NMR capability. Other new appointments are, **Adams** and **Boulatov** (from Illinois, USA) in Materials, and **McDonald** (Q3 2013) who will contribute to the Medicinal and Bionano theme. New staff receive an institutional induction and training, including academic teaching and grant writing courses. They are supported by an academic mentor from Chemistry to guide them in research grant strategy and other aspects of research planning. New staff have a 30% teaching load, which increases over four years, and are supported with a studentship and other start-up costs. Chemistry has a policy of expansion, with 10 new academic positions planned (see b above) in the period 2013-16. The University is a signatory to the Concordat to Support the Career Development of Researchers and has Bronze Athena Swan status. SPS supports equality and diversity in recruitment and is currently applying for Bronze Athena Swan status in its own right. Female staff comprise 22% of our research staff and 40% of academic staff are from outside the UK.

All staff have a Professional Development and Review (PDR) annually. PDRs are based on a Portfolio of Activity that provides a record of staff activity and outputs, informing the discussion about workload and career development, and providing evidence for reward or promotion cases. PDR includes a discussion of strategy, direction, publishing and grant plans, to enable a managed approach to research development, aligned with departmental priorities. PDRs identify training and development needs in skills, knowledge or experience that might prevent individuals from seeking leadership roles, whether academic or outside the University Sector. A Leadership Programme available via the University of Liverpool Leadership Framework (validated by the Institute of Leadership and Management) provides participants with evidence of relevant development. All staff are eligible to apply for research leave. For example, **Carnell** spent six months in the

Manchester Interdisciplinary Biocentre (2012), while **Nichols** won a Visiting Professorship and Fellowship from the Otto Mønsted Foundation (2010) and spent four months at DTU, Denmark, publishing four co-authored papers, including two JACS, and winning an EU grant "Electronanomat", all with Ulstrup. **Cooper** led the proposal for MIF while on a three month sabbatical at UC Santa Barbara in 2012. Promotions in the period include **Cosstick** and **Higgins** to Professor, **Claridge** to Reader, **Volk** and **Berry** to Senior Lecturer.

The Department takes great care to develop early career staff and support them in winning personal research fellowships, particularly by mentoring and internal reviewing of grant applications. New Chemistry staff take the University's Centre for Lifelong Learning ECR programme, which supports the development of leadership and team management skills, as well as developing skills to improve individual research performance. Three Chemistry staff took part in the 2012 Leadership in Science workshop run by Imperial College Business School for early to mid-career researchers in engineering and science. ECR staff are encouraged to take leadership roles, for example **Lopez-Sanchez** has been appointed Director of the new MBR and **Hardwick** is the EU network coordinator for SIRBATT, a £4.4M programme in grid scale energy storage.

The School offers skills training workshops to PDRA staff (teamwork, project management, scientific writing, collaboration, grant writing, and peer review). PDRA staff run their own quarterly Forum, which provides input to the Department's planning, and are supported in writing Fellowship applications. Five Chemistry staff won Royal Society URFs in the period. Jelfs, Weaver, Trewin and Ingleson won URFs as PDRAs before moving to Imperial (x2), Lancaster, and Manchester. Current RS URFs include **Gastaldo** (previously a Marie Curie Fellow) and **Fogg**. New lecturers **Cowan** and **Boulatov** won EPSRC Early Career Fellowships and **Teobaldi** an EPSRC Career Acceleration Fellowship, while Nayak and Liu won Marie Curie Fellowships. Other ECR staff who have moved to new positions include Bradshaw (Reader, Southampton), who was mentored to obtain an ERC starter grant, and Khimyak (now Professor at UEA). Many staff from the Department have gone on to research positions in different academic institutions, both in the UK (e.g., Palgrave, UCL) and abroad (e.g., Evans to Alfred R Bader Chair at Queen's, Ontario; Demont, Rennes; Leary, IMDEA Madrid; Petty, Holy Cross, MA, USA; Humblot, CNRS, Paris).

The Department encourages continued research activity by Senior Emeritus staff, who have contributed >90 papers, research income and valuable expertise. For example, Schiffrin published 23 papers and raised more than £1M research income in the period. We are regularly hosts to international visitors, e.g. in Materials, Kaskel (Dresden), Felser (Mainz), C.N.R. Rao (IIT), B. Raveau, S. Kitagawa (Kyoto), J. Fréchet (KAUST/Berkeley) have all visited recently. Many of these visits result in collaborative papers, with *ca.* 35% of our papers having an international co-author.

To support research activity, the Department has reduced the teaching load on research staff by recruiting three new full time University Teaching Fellows, two (Gaynor, Sedghi) directly into the Department and the third (Reilly) to support Chemistry teaching in the new Central Teaching Laboratory (CTL). Additional support for the Department's research activity has been made in the form of a dedicated Safety Officer position (Crowe-2012, Jones-) to coordinate safety policy and implementation and assist in the training and induction of new research staff. New support staff (a technician and administrator, joint with Physics) were recruited to support research activity in SIRE, while 14 new technical and support positions are planned (2014-6) in support of MIF.

ii. Research students

Academic Year	2008/9	2009/10	2010/11	2011/12	2012/13
PhD Students registered	106	106	109	119	123
FTEs	80.8	84.5	84.5	89.5	93.5

In 2012/13 the Department had 123 active PhD students (94 FTEs), a 15% increase over the REF period (see table) and a 50% increase over the end of RAE2008. The wide variety of countries of origin, ethnicity and religions amongst our research students testifies to the Department's commitment to diversity and equality of opportunity in student recruitment, with 40% of current PhD students being female. Our PGR Student Admissions Policy maintains academic standards by ensuring we employ objective assessment methods to recruit the highest calibre of UK and international PGR students. Entry to MPhil or PhD study requires a research Masters, or a 1st or 2.1 Honours degree (or equivalent) in Chemistry or appropriate related discipline. Applicants are

assessed by reference to prior academic achievement, then interviewed by a selection panel including the prospective supervisors. The Department aims to make a decision within one month of receiving the application.

A system of dual supervision, and the involvement of two additional members of staff as assessors in the annual progression reviews, evaluates all aspects of the quality of the student's work and addresses their needs in developing the necessary research skills. This structure provides multiple points of contact with the Department if problems arise. Progress Monitoring occurs by a review at three months, then annually, and is managed by the PGR Coordinator (**Kozhevnikov**). Students produce a short report at three months, containing a literature survey, and agree objectives and a project outline, with annual reports thereafter. The annual review includes a *viva voce* examination by the independent assessors, providing the student with practice at defending their work and justifying the approach taken. The assessors' report informs the decision for progression and provides useful feedback to the student and supervisors. Year 2 reports follow a communication style, to teach preparation of a publication, and students present a Poster on their research as part of the University PGR Development Programme. In the final year, all PGR students present a 20 minute talk on their PhD work to their research division. Students are expected to publish in high quality journals and present their work internationally; for example Forster (a PhD. student with **Hodgson** & **Raval**) published his PhD research in Nature Mat., JACS, ACIE, PRL and Chem. Sci.

The Department seeks to maintain the highest standards of research governance and many of the underlying themes (professional conduct, health and safety, confidentiality, project planning) are integrated into our PGR development programme, which is aligned to the national Researcher Developer Framework. The University PGR Development Team offers intensive three-day themed skills workshops to first year PGRs, including topics specific to SPS. The Graduate School Skills Programme is compulsory for all research students and provides six weeks of developmental activity during the PhD. The programme has an interdisciplinary approach to professional development to encourage teamwork and foster the formation of a PGR community.

Feedback from our annual PGR survey led the Department to revise its Induction Programme, which now includes a full introduction to PGR procedures, Departmental research facilities and safety training. All information is also available on VITAL, the Postgraduate area of the University website. PGR students are supported by additional study and skills training relevant to their programme of research. Students take either a taught M level module or one of several bespoke PGR modules, chosen in consultation with their supervisor. Organic chemistry students are also required to complete a series of six literature assignments, with awards for the best performance (Kenner Award) and best talk (Sir Robert Robinson Award). All PGR students are required to attend research Colloquia in their area and Department Research Seminars (ca. 20 p.a., attendance monitored).

Research training is internationally recognised in many areas, e.g., in Materials through our participation in the SOPRANO Marie-Curie ITN, the Summer Schools run with UCSB International Centre for Materials Research and one day meetings at Liverpool. Other international programmes include CHEXTAN, SMALL, PRAIRES and ARTIST EU-RTNs, the NOVELOX EST activity, and via the AntiMal International PhD Programme, organised in collaboration with the European Molecular Biology Laboratory, Heidelberg, in medicinal chemistry. A joint training scheme with DICP in Energy and Catalysis is supported by BP. The Department aims to promote exchange between academia and commercial sector through CASE studentships, as well as recruitment and secondment of students to industry. For example, **Rosseinsky** has a student who spends extended periods working at Johnson Matthey's research laboratory.

d. Income, infrastructure and facilities

The Department's Research Income totals £33M during the REF period, a 70% increase in funding rate from RAE2008. £20M of income came from the Research Councils, Royal Society and BIS/TSB, £7M from the EU and the remainder from charities and industry. £43M new research grants have been started in the period (a rate 100% greater than RAE2008), with Bradshaw (now Southampton), **Brust**, **Cooper** and **Rosseinsky** all winning European Research Council (ERC) grants. The total award value in a selection of high value programmes, which exist alongside a broad range of smaller programmes tackling specific problems, is highlighted below.

The exceptionally strong funding generated by the Materials cluster emphasizes the nationally and internationally leading nature of this activity. Materials synthesis is backed by an EPRSC Programme Grant of £8M to Liverpool with a further £0.5M for allied work at UCL, an ERC Advanced Grant of £3.3M and a £1.4M programme in functional materials backed by the RS. An ERC award also supports work in tectonic materials (£2.5M), with other major programmes including nanomedicines for HIV/AIDS (£1.6M, £1.1M, £1.8M), stem cell tracking (£1.8M), an integrated approach to adaptable porous materials (£0.9M, £0.6M) being funded by the EPSRC, as is a new £1M fellowship in Chemomechanics. In line with strategic priorities, we have further strengthened interactions with industry, as exemplified by the Centre for Materials Discovery. The CMD, established in the previous period, represents Europe's largest suite of instrumentation for parallel materials discovery. The strength of outputs has led to a renewed investment in CMD from Unilever (£2.8M), along with the new MBR (£2.6M) being developed with Unilever under the Regional Growth Fund and a £0.6M investment to integrate new Radio-chemistry labs into Nanomedicine. Specific strength in polymer and supercritical fluid science has also produced a key funding interaction between **Cooper** and BP to fund a new (£1M) high pressure research lab.

An aim of our research has been to target the fields of medicinal chemistry, renewable feedstocks and energy as areas of future societal importance. International collaborations in medicinal chemistry have led to funding from Washington U., USA for Isoprenoid Biosynthesis to treat Malaria, (£0.6M) from Bayer and the IVCC on novel vector control agents for use against mosquito vectors with LSTM (£0.5M), from EU FP6 for Drug Development of FAQ4 and RKA182 (£1.3M), the Wellcome Trust Seeding Drug Discovery award (£1M) and the MRC DPFS for development of drugs to treat tuberculosis (£0.6M), with other major funding from the MRC (£1.2M). In the Energy theme, ECR staff won significant funding from EPSRC for electrochemical energy storage (£0.8M, £0.5M), sustainable processes (£0.8M) and catalysis for renewable feedstocks (£1.3M). EPSRC funded fellowships related to energy include programmes in experimental (£1.1M) and in-silico (£0.7M) photocatalysis. Funding from the ERC (£2.8M) has been secured in Functional Interfaces to study the development of nanoscale devices, from the EU for Chirality and Molecular Recognition at Surfaces (£1M), and EPSRC for Control of 2-D Molecular Organisation (£0.5M).

The Department's success in developing infrastructure and facilities that support our strategic aims and underpin our research activity is based on substantial University and external investment in expanding our research laboratories and equipment base including:

- £68M (£44M capital) for Materials Innovation Factory,
- £4.9M new laboratories for Stephenson Institute for Renewable Energy,
- £2.6M refurbished laboratories for the Micro Biorefinery programme (Unilever, RGF),
- £1.8M EPSRC supported programme to upgrade NMR, MS, X-ray diffraction and SPM.

The Department maintains a strategic focus on its core strengths, with the largest single investment in infrastructure in the period being the establishment of the Materials Innovation Factory, one of eight projects supported in the first round of the UK Research Partnerships Infrastructure Fund (UK RPIF) scheme in 2012. The MIF project commenced in Q3 2012 and is scheduled to be built by Q1 2016. It will be an internationally unique research institute, used by academics and industry partners, further reinforcing our commitment to industrial engagement. The scale of the industry interaction is, we believe, unprecedented in the UK in the area of Materials Chemistry, with at least 120 industry users to be co-located in the Chemistry Department in Year 1.

The Department has a strong base of shared facilities, upgraded in 2012/2013 in a £1.8M programme, with specialist instrumentation maintained by individual research clusters accessible either to trained users or through collaboration. These facilities include:

- Significant NMR provision including solution state (500 MHz, 400 MHz (x 2), 250 MHz and 200 MHz, with access to 800 and 600 MHz in Structural Biology) run by a dedicated NMR specialist and solid-state and high pressure NMR capability through research groups.
- Single crystal X-ray diffraction facilities (Bruker Smart Apex diffractometer, with a Mo source and cryogenic system) run by a dedicated Crystallographer (Robertson).
- CHNS-O analysis (Thermo Flash EA1112 CHNS-O Analyser and ICP-OES).
- MS capabilities including electrospray, EI, CI as well as GCMS. This includes a high resolution instrument for accurate mass measurement from ~ 250 Da up to ~ 8,000 Da.
- Full range of mechanical, electrical and glassblowing workshops

The Department has an exceptional equipment base, including advanced polymer and colloid characterization, a unique robotic synthesis capability in CMD, comprehensive single crystal and powder diffraction, including rotating anode single crystal diffractometers, SEM and extensive gravimetric and volumetric porous materials characterization. RHEED-monitored pulsed laser deposition allows thin film deposition with unit cell-level structural and compositional control. Instrumentation for electrochemical characterization of fuel cells and gas permeation membrane evaluation is available. The Functional Interfaces cluster possesses an extensive instrumentation base, including a suite of state-of-the-art UHV scanning probe microscopes (4-500 K STM, AFM). The low pressure facilities are complemented by research grade FTIR and SPM for high resolution imaging in ambient and electrochemical environments, nonlinear optical spectroscopy and nano- and femtosecond time-resolved vibrational spectroscopy. A new Grid-Scale Energy Storage grant (with Manchester) will add TERS, CARS, IR, high res. XPS and a battery test facility to allow characterisation and test of battery interfaces. Our equipment base and industrial contacts result in consultancies with a range of companies, from start-ups, such as Hydra Polymers, SMEs, such as ACAL Energy and Glassbond, through to large companies, including BASF, Bayer and Unilever.

The University strongly supports computational research through continual investment in computer clusters, with the most recent upgrade (2013) providing a further 1,888 computational cores (£1M). The Theory cluster has secured access to Tier 1 computer resources on the European level through PRACE, national large scale parallel compute resources at HECToR (via the HPC materials chemistry consortium and CCP3), the Blue gene at Daresbury and the N8 machine at Leeds. Finally, continued Library investment (~£1.5M in REF period) provides electronic access to >600 chemistry journals (including all ACS journals and a Gold level RSC subscription), thousands of scientific texts (e.g., ScienceDirect Freedom Collection and Wiley Online Library Full Collection) and access to online databases (e.g., SciFinder Scholar, Reaxys, Scopus, Web of Science), with nearly 200,000 document downloads in the last 12 months directly enabling our research.

Our future funding strategy will build on the enhancement in our infrastructure and facilities achieved in this period, and the on-going investment in MIF, to expand the research themes identified in section **b**. In particular, we will exploit the new opportunities for industrial collaboration presented by the development of MIF, and for collaborative research created by the new staff associated with the MIF and SIRE research themes. Examples in place already include SIRBATT, a £4.4M EU network coordinated by **Hardwick** (£1M), and ERDF, TSB and EU funding (**Raval**) for the Anti-microbial Centre (£3.7M plus £0.9M to industrial users).

e. Collaboration and contribution to the discipline or research base

The Department's activity is based on interdisciplinary and collaborative research, with engagement nationally and internationally with both industry and academia on a number of levels, from leading large international research networks and projects through to individual collaborations with high profile academics. International academic links are supported by the University's Internationalisation policy, providing joint PhD programmes with various international partners (section b). The Department supports external links by funding joint students, by prioritising matched collaborations with industry for support and by providing sabbaticals. Inter-departmental collaborations are promoted by appointing joint staff at the interface between disciplines, e.g., in Nanomedicine the appointment of **McDonald** (Q3 2013) joint with Pharmacology.

Examples of international activities include the following:

- Extensive academic collaborations exist leading to >280 papers published with international collaborators. The Department has hosted more than 40 overseas academics including, for example, J. Polanyi, Nobel Laureate, Toronto (*Hofer, Nature Chem. #1, #2*) and H-J. Gao, Deputy Director Institute of Physics, Chinese Academy of Sciences.
- A leading role in a range of high profile networks including: **O'Neill** as the deputy head of FP6 initiative ANTIMAL (31 institutions from 10 European and 2 African countries with 6 industrial partners), **Hardwick** coordinates an EU network on energy storage (SIRBATT) consisting of 12 academic and industrial partners, while collaboration with CRISMAT, Caen (3 EU networks during period) has led to regular staff exchanges. The Department is also part of the Canadian Institute for Advanced Research (CIFAR) network in nanoelectronics (**Hofer**).
- Close academic collaborations (**O'Neill, Berry**) with the Swiss Tropical Institute, Washington University St Louis, Medicines for Malaria Venture, Gates Foundation and GSKs Open Lab

Foundation in Madrid, as well as with industrial partners including GSK, Bayer and Grunenthal.
- In collaboration with the UCSB International Centre for Materials Research, Materials chemists organised a summer school in Inorganic Materials for Energy 2012.
- Work on molecular superconductors (**Rosseinsky**, **Darling**) in partnership with Prassides (Durham), Arcon (Ljubljana), Iwasa (Tokyo) and Takata (SPring-8 RIKEN) has identified the unconventional nature of superconductivity in the highest transition temperature systems.

On a national level, the Department has particularly strong interactions with industrial partners, as well as with UK based academics, and examples include:
- EPSRC funded programmes in medicinal chemistry involving industrial partners include Pfizer, AstraZeneca, Gilead, Abbott and Merck. Medicinal Chemistry works with Liverpool School of Tropical Medicine, Dept. of Molecular & Clinical Cancer Medicine, MRC Centre for Drug Safety Science (Liverpool), London School of Hygiene and Tropical Medicine.
- Direct engagement with industry in the CMD, with colocation of 12 full time Unilever staff, which has established an international reputation and delivered a wide range of scientific outputs (e.g., polymorph discovery in organic porous materials) and benefits to business (e.g., new patented Fischer-Tropsch catalyst with UK industry partner).
- Building on the Department's strong industrial links, new programmes include the KCMC, the RGF-funded MBR and the MIF. The KCMC was established in 2009 with regional partners Manchester, Bolton Institute for Materials Research and Innovation and Daresbury STFC Computational Science Group and in 2013 was supported by TSB as a Special Interest Group to roll out the engagement model nationally.
- Focussed industrial projects span a wide range of topics, including supercritical fluids (BP), catalytic studies (Lucite) and CVD precursors (SAFC Hitech).

Academics in the Chemistry Department actively take leadership roles within the community, contributing to the health and sustainability of the discipline, as evidenced through:
- Organising, chairing and co-chairing of high profile international conferences and meetings including: European Conference on Surface Science (**Hofer,** 2008), International NanoMedicine Workshop (**Rannard,** 2010), 1st UK-China Workshop on Metals in Organic Synthesis (**Xiao,** Beijing 2011).
- Delivering 38 Plenary and >260 invited talks at international conferences, as well as >300 invited colloquia (>175 international).
- Acting as advisors to the academic community, including **Rosseinsky** to KAUST Competitive Grant Panel; and on the Director selection panel, Institute of Basic Sciences, S. Korea; **Raval** as International Scientific Advisory Board, IMDEA Nanoscience Centre, Madrid (2007-2012); Scientific Advisory Committee, DIAMOND Light Source (2010-present). Staff act as panel members (38) and Chairs (4) for funding programmes and facilities access, including EPSRC.
- Holding editorial roles, for example Chemical Science (**Rosseinsky**, Associate editor 2010-2012), J. Mol. Catal. A: Chem. (**Xiao**) and Chemistry World (**Brust**).
- Holding visiting Professorships at several international institutions including A-Star ICES (**Iggo**), Université Pierre et Marie Curie, Paris (**Raval**), Chinese Academy of Sciences, Beijing (**Hofer**) and Chalmers, Sweden (**Persson**).
- Contributing to a range of committees and special interest groups, such as the IOP condensed matter structure group (**Claridge**), Treasurer of the British Society for Nanomedicine (**Rannard**), RSC Nucleic Acids Group (**Cosstick**), secretary of Macro Group UK (**Adams**).

The contribution of Liverpool chemists to the community has been recognised through a number of awards and medals in the REF period including: **Rosseinsky**, Royal Society Research Professor 2013-; inaugural De Gennes Prize, RSC 2009; C.N.R. Rao Lecture Award of the Chemical Research Society of India 2010; Hughes Medal, Royal Society 2011; **Persson**, 2012 RSC Surfaces and Interfaces Award; **Hofer**, Distinguished International Professor, Institute of Physics, Chinese Academy of Sciences 2011; **Evans**, 2009 RSC Peddler Award; **O'Neill**, RSC Malcolm Campbell Award 2011; **Fogg**, 2012 RSC Gibson-Fawcett award; **Xiao**, UK Prize for Process Chemistry Research 2008 sponsored by GlaxoSmithKline, AstraZeneca and Pfizer, and "Chang-Jiang Scholar" Chair Professorship, Ministry of Education, China, 2010-13. **Cooper**, 2010 RSC Macrogroup UK Medal for Contribution to UK Polymer Science, 2009 RSC Corday-Morgan Prize, 2009 Royal Society Wolfson Research Merit Award, Top 100 Cited Materials Scientists ISI 2012.