Institution: University of Birmingham

Unit of Assessment: UoA 8 - Chemistry

a. Overview

The School of Chemistry (SoC) at the UoB has a distinguished academic record and a bold vision for maximising the academic and commercial/end-user impact of the research that it undertakes. It has a layered research structure as shown in the table below, consisting of four research units that underpin three outward facing themes for the application of its core activity, under the banner of *Chemistry for Health and Sustainability*.

School of Chemistry: *Chemistry for Health and Sustainability*					
School Organisation	***Purpose***	***Research Building Blocks***			
Outward Facing Research Theme	Knowledge Application	Chemical Biology and Drug Discovery	Materials Chemistry and Energy	Imaging in Chemistry and Biomedicine	
Research Units	New Knowledge	Biomolecular, Supramolecular and Nanoscale	Molecular Synthesis and Catalysis	Physical and Theoretical Chemistry	Solid State Chemistry

The research units covered by the submission are as follows:

Biomolecular, Supramolecular and Nanoscale Chemistry (BSNC) Strengths: Molecular and biomolecular recognition, including molecular assemblies such as nanoparticles, helicates, adapted biomolecules (peptides, DNA) and their physical properties; solution and surface-confined molecular/polymeric materials and entities.

Molecular Synthesis and Catalysis (MSC) Strengths: Development and applications of organic synthesis and homogenous catalysis, including enhancing the efficiency of synthesis, establishing and exploring new reactivity concepts and developing strategies to rapidly access complex molecular scaffolds.

Physical and Theoretical Chemistry (PTC) Strengths: Experimental physical chemistry, including spectroscopy, imaging, electrochemistry and electrocatalysis; computational and theoretical methods probing structures (e.g. clusters and related assemblies) and processes (photochemical reactions).

Solid State Chemistry (SSC) Strengths: design, synthesis and characterization of new materials including fuel cell and battery materials; ion-exchange materials for nuclear waste remediation; magnetic materials; materials for hydrogen storage and delivery; superconductors; thermoelectric materials; diffraction studies using synchrotron X-rays and neutrons.

b. Research strategy

Overall Vision and Summary: The strategic aim of the SoC in this REF period has been to focus investment and growth in research that can be linked to areas of *interdisciplinary and exploitable activity.* To reflect this vision, an overarching banner of *Chemistry for Health and Sustainability* was set up in 2009, with three outward-facing research themes created to connect with, boost and increase the applicability of the SoC's existing core research. This strategy, which aligns with the UoB's strategic priorities and is overseen by the SoC *Research and Knowledge Transfer Committee*, has improved the SoC's research position compared to RAE2008, as follows:

- Increased investment in core research base (staff, students, equipment and grant income)
- Increased cross-discipline interaction and connectivity with academia and industry

Examples of this increased vitality in the REF window compared to RAE2008 include: number of staff returned up 27%; research income/year up 55%; PhD graduations/year up 70%; average PhD numbers/year up 43%; double the number of patents filed or published; strong links to 3 doctoral training centres, including one run by the SoC (leading to a further CDT award in Nov 2013).

Development of the Research Units: The four units have evolved from the 3 core research areas described in RAE2008 (*Molecular Processes and Theory*, *Materials Chemistry* and *Molecular* Synthesis *and Chemical Biology*), and reflect the overall increase in core research strength in the REF window, with 9 new members of staff in this return. Five of these appointments have been made under the flagship *Birmingham Fellowship* scheme (see Section c for more details).

Outward Facing Research Themes: The bold vision for these themes is to offer a route through which core chemistry research activity undertaken by the SoC, which has always been strong, may be applied and exploited more effectively. In particular they ensure that the core chemistry research undertaken is linked to local (e.g. the Birmingham Fellowships), national and international research initiatives and priorities (e.g. within the EPSRC research themes of *Physical Sciences, Energy*, *Healthcare Technologies* and *Manufacturing the Future* as well as EPSRC Grand Challenges such as *Dial-a-Molecule* and *Directed Assembly*). Furthermore they facilitate the SoC's vision to apply research across disciplines to generate impact, an approach that is in line with the findings of the 2009 EPSRC/RSC *International Review of Chemistry*, which highlighted the importance of interdisciplinary research. The themes are broadly in line with those proposed for development in the RAE2008 submission, which were noted favourably by that panel. Each theme is linked to a Centre for Doctoral Training. Further details are outlined below:

<u>*Chemical Biology and Drug Discovery*</u> (Champion **Simpkins**): This theme taps into the well-documented changes in strategy and working practices in the global pharmaceutical sector, which means increased use of outsourcing, and partnering of academic multidisciplinary teams in outreach projects, and pre-competitive research. It also facilitates links with the School of Biosciences (in particular on current UK synthetic biology initiatives), the recent investment in Pharmacy at the UoB and to chemical activity in the £4.5M Midlands Integrative Biosciences Training Partnership (MIBTP), a doctoral training partnership funded by the BBSRC, involving the UoB, the University of Leicester and the University of Warwick (2012-2018).

<u>Imaging in Chemistry and Biomedicine</u> (Champion **Hannon**): This theme promotes novel approaches to imaging for biomedical and engineering applications and connects with a range of industrial sectors, including those that develop imaging technologies and instrumentation as well as biotech companies for whom imaging is key to their developments. It also underpins chemical activity in the £7.2M EPSRC-funded Centre for Doctoral Training (CDT) in *Physical Sciences of Imaging in the Biomedical Sciences* (PSIBS), run by the SoC at the UoB (2008-2018). PSIBS coordinates projects between the SoC and many disciplines at the UoB (Physics, Biosciences, Computer Science, College of Medicine and Dentistry, Chemical Engineering, see Section d for further details). The success of PSIBS and its interdisciplinary ethos has led to the recently announced £7M *Physical Science for Health* CDT, again hosted by the SoC, to apply a range of physical sciences to address key health challenges.

<u>Materials Chemistry and Energy</u> (Champion **Anderson**): This theme underpins the strong collaborations with other Schools at the UoB and reflects energy research being 1 of 6 cross-council strategic priority areas for RCUK. At the UoB it connects chemical activity in: (i) the £5.5M UoB CDT in *Hydrogen, Fuel Cells and their Applications*, funded by the EPSRC (2009-2018) on behalf of the Midlands Energy Consortium; (ii) *The Birmingham Centre for Nuclear Education and Research*, launched in 2010 to provide the nuclear expertise and capacity to support the UK's investment in the nuclear power sector and (iii) the *Industrial Doctorate Centre in Formulation Engineering* (EngD) run by the School of Chemical Engineering. *Advanced Materials* and *Energy* are two of the *Eight Great Technologies* for investment, as identified by Government (June 2013).

Industrial Engagement Strategy: The RAE2008 feedback noted links with industry as an area for development, and the SoC has addressed this through the creation of outreaching themes as outlined above. This strategy has resulted in a significant boost to industrial collaborations, through activities such as CASE/industrial studentships, CDTs, ITNs, an industrial fellowship and supported postdoctoral projects (see Sections d and e for details). Since 2008 the School has published over 30 publications with industrial partners, ranging from large multinational companies (e.g. P&G, AstraZeneca) to SMEs. The focus on applicability has led to a surge in the number of Records of Invention arising from the SoC (1 in 2009, 1 in 2010, 7 in 2011, 17 2012 onwards) made via the UoB technology transfer company *Alta Innovations.* Similarly, the number of patents filed or published by staff in this unit's return during the REF window (either through UoB or elsewhere)

has risen rapidly, with 21 in total and 14 since 2011 (up from <10 in RAE2008).

***Infrastructure Strategy**:* As part of a programme to underpin core research activity and facilitate interdisciplinary activity, the UoB has refurbished two laboratories to house a suite of state-of-the-art equipment, funded through the *Science City Research Alliance.* This was recently bolstered by recent EPSRC *Core Capability* funding (see Section d for more details on both of these schemes). The UoB has also supported the PSIBS CDT with refurbishment of student and staff office space and installation of a computer suite. Looking to the future, recent fruitful discussions with the UoB over developing the infrastructure strategy further have led to detailed plans being drawn up for a complete £37M refurbishment of the SoC, starting in the next REF window.

c. People, including:

i. Staffing strategy and staff development

Staffing Strategy Overview: The SoC is considerably boosted by it being part of a large institution with an extensive engineering and medical community. This has provided it with a real opportunity during this REF window to strengthen its staffing position by focusing on areas of core research that are relevant to institutional research strategies. A cornerstone of this strategy has been the creation of the *Birmingham Fellowship* scheme (permanent positions with 5 years protected time for research) to enhance existing academic strengths and contribute to the growing culture of collaboration and interdisciplinarity. The SoC has so far attracted five UoB fellows to positions since 2011 (out of a total of 60 across the UoB), which reflects the positive international profile of the SoC and the commitment of the UoB to strengthening the research base of the SoC. The new appointments amount to nine in total and are distributed over the four research units: UoB Fellows - **Baranoff** and **Fernandez-Trillo** in BSNC**, Chakrabarti** and **Rodriguez** in PTC, **Schnepp** in SSC; Lecturers - **Peacock** in BSNC, **Fossey** in MSC and two more senior appointments, **Slater** and **Read** in SSC. The result of this investment is a higher return of SoC staff than previously (28 versus 22 FTE staff in RAE2008, the smallest number in the Russell Group at that time), with ca. 1/3 comprising these 9 new appointments. As examples of the applicable chemistry research being brought in, **Baranoff** brings his immense experience on photovoltaic cells in the Grätzel group and patent expertise to the UK academic community, which is relevant to the *Materials Chemistry and Energy* theme; **Fernandez-Trillo**, a joint appointment with Pharmacy, brings expertise on novel polymeric materials for drug delivery and synthetic biology, which relates to the *Chemical Biology and Drug Discovery* theme; **Read**, recruited from the Atomic Weapons Establishment, studies solid-state materials for nuclear energy applications, which also directly taps into the *Materials Chemistry and Energy* theme. The connectivity through these themes works both ways with the expertise in NMR polarisation techniques for metabolite analysis of **Günther** (Professor of Biophysical Chemistry and director of HWB-NMR, the UK's largest NMR facility) and the nanomedicine expertise of **Ali-Boucetta**, both located in the UoB medical school and linked to the SoC via the *Chemical Biology and Drug Discovery* theme (in fact as part of the UoB Pharmacy initiative, two other Medicinal Chemistry appointments, including Butterworth from AZ are now housed within the SoC research labs). Likewise **Mayhew** (School of Physics) brings expertise in analytical chemistry and instrumentation and **Winn** (School of Biosciences) expertise in computational analysis and modelling of biological molecules and processes. Of staff submitted at RAE2008, retention levels are good with only Rayment leaving to become Director of Physical Sciences at Diamond Light Source in 2008. Support for X-Ray diffraction research has also been boosted by the arrival of **Dr Louise Male** (from the EPSRC National X-Ray service) for single crystal diffraction and **Dr Jackie Deans** for powder diffraction (through *Science City Research Alliance* funding, Section d). The SoC has hosted 49 different PDRA researchers as research staff in the REF window, working in 20 different research groups.

Staff development and career support. The UoB was awarded the HR Excellence in Research accreditation in September 2011 and has implemented its Concordat action plan (September 2013). Organisational level process, policies and activities include annual performance and development review (PDR) schemes, leadership development programmes provided by the *People and Organisational Development Unit* (POD) and recurrent central funding to maintain development provision for researchers. Courses include IP training, grant-writing workshops and science communications training, which is important for outreach. The SoC has an active mentoring scheme in place for probationary staff and early career researchers (ECRs) and a

sabbatical scheme for established staff. Feedback and advice on research proposals and papers are coordinated though its core research units. In line with the SoC strategy to promote exploitation pathways from core research, members of staff have attended the UoB *Medici Enterprise Training Programme* in the REF window, which aims to identify and develop business skills to protect and successfully commercialise academic research. The SoC supports female staff who have had childcare-related career breaks to re-establish their research, for example with funds to buy additional research support and meet childcare costs to attend conferences.

Personal Research Fellowships: Three prestigious awards were awarded to SoC staff in the REF window that align with the drive by the SoC to develop and apply areas of core research: **Fossey** - *Royal Society Industry Fellowship* (2012-2016) provides 50% salary and a budget to work on a project with Syngenta transferring UOB scientific discoveries to the anti-malarial and agrochemical arena. *SoC support* – reduction in JSF's teaching and admin load by 50%, with a part time replacement teaching fellow appointed; **Pikramenou** - *Leverhulme Trust Research Fellowship* on "*Multimodal nanoparticle agents to target delivery in cells*" (2012-2014). This award has strengthened Pikramenou's links with the medical diagnostics community at the UoB. *SoC support* – extended teaching cover to increase the running time to 2 years instead of the normal 12 months; **Tucker** - *EPSRC Leadership Fellowship* on "*Functional DNA-based Assemblies*" (2009-2014, £1.74M). This award has allowed Tucker to apply various concepts from the supramolecular chemistry domain to nucleic acid chemistry research, resulting in collaborations related to medical diagnostics and therapy. *SoC support* - 3 PhD awards and cover for teaching and administration.

International Staff Appointments: Three of the 5 UoB fellows have been attracted to work in the SoC from overseas – **Baranoff** (Switzerland), **Rodriguez** (Switzerland), **Schnepp** (Japan) and the other two are foreign nationals (**Chakrabarti** from India and **Fernandez-Trillo** from Spain) who have remained in the UK, having first worked at other institutions. **Peacock** was appointed having been a postdoc in the Pecoraro group (USA). The SoC has had particular success in attracting high-quality international research fellows on the EU Marie Curie funding programme with 9 postdoctoral fellowships being awarded in the REF window (see Section d for recipients). The SoC has received various visiting academic fellows in the REF window, including Dr Fuyi Chen (Northwestern Polytechnic University, China); Dr Haydar Arslan (Zonguldak University, Turkey); Prof. Dr. Sergio Antonio Marques Lima (UNESP, Brazil). Outgoing fellowships include a *Natural Science Foundation of China* fellowship to **Fossey** to collaborate with Wei-Ping Deng (Shanghai) and a *RSC-SAFEA Visiting Researcher Programme* award to **Johnston** (Beijing).

Equality and Diversity*:* The UoB has a strong commitment to equality and diversity, as evidenced through its Equality Scheme and membership of the Athena SWAN Charter (Bronze Award) and Stonewall. The UoB has staff groups for disabled, LGBT and minority ethnic staff, which are promoted to staff at induction and via the intranet. The SoC has a relatively young age profile (all but 4 staff under 50 years old) and has had a steady increase in the number of female academic staff over the past ten years (3 in 2004, rising to 8 in 2013 or 25% of the total number of academic staff), with 50% of the p/g cohort female. The SoC has demonstrated its commitment to Athena SWAN values by the establishment of a working group in 2012 (soon after the UoB gained its Bronze Athena award), which led to the SoC being given a Bronze Award in October 2013. Through Athena SWAN seminars (e.g. inviting York Chemistry), conference attendance (RSC, Joliot-Curie), network meetings (RSC Women in Science evenings), establishment of focus groups for p/g and postdoc researchers and its support of UoB activities such as the *Academic Network for Women*, the SoC has raised awareness of gender and equality issues with all staff. These have informed changes in practices and a plan of action, which includes implementing a transparent workload model for teaching and adopting a policy for scheduled meetings that accommodate caring responsibilities. There is also a commitment for data monitoring and reporting for gender balance across all school activities, changes in outreach activities to encourage a more diverse student population and proactive support for promotions and arrangements of return from maternity leave. The drive to increase awareness of equality and diversity issues is also met through the UoB's *Diversity in the Workplace* online training course, which is compulsory for all staff.

ii. Research students

Postgraduate Admission Data: The total number of FTE postgraduate students enrolled on doctoral (PhD) programmes in the SoC in each year (from 1 August 2008 to 31 July 2013), as well

as the headcount number of new PhD students enrolling each year, are shown in the table below:

	New Intake				
Year	Chem PhD	CDT PhD	Total Entry	FTE Chem Total	FTE CDT Total
2008/2009	21	5	26	80.1	2.8
2009/2010	31	10	41	83.7	11.9
2010/2011	22	13	35	75.3	22.0
2011/2012	24	15	39	76.7	34.8
2012/2013	22	15	37	64.2	47.1

The FTE Chem Total column indicates the increase in PhD student numbers in the REF window (FTE PhD average/yr 76.0) compared to RAE2008 (FTE p/g average/yr 53.1). The PSIBS CDT, introduced in 2008 (see Section d), has boosted PhD numbers further. These students are registered in the SoC throughout their 4-yr programme, with their main project starting in Year 2, which involves supervisors from various schools, with strong representation from SoC staff.

Postgraduate Completion Data: As detailed in REF4a, there have been 118.15 FTE graduations in the REF window (excluding PSIBS graduation data which is not yet available), with an average of 23.6 awards/year, up by 70% on the RAE2008 return (average 13.9 awards/year), which again indicates the increasing vitality and strengthening research position of the SoC.

Approach to Recruitment and Policy*:* To ensure optimal quality in the chemistry p/g cohort, all prospective students, including internal candidates, are interviewed by two members of staff to probe their ability and motivation for research. Furthermore to qualify for a School-funded scholarship, the minimum entry requirement is a 4-year undergraduate masters (MSci or MChem) with marks of 65% or above. Projects are advertised through an online p/g prospectus. In line with the aspiration to apply and exploit core research in areas allied to outreaching research themes, in 2013 the SoC introduced a one-year Masters by Research (MRes) programme in *Chemistry for Biomedical Imaging* as well as two one-year taught postgraduate masters programmes (MSc) in *Chemical Biology and Biomedical Imaging* and *Drug Discovery and Medicinal Chemistry*. These programmes strengthen collaborative interactions with other schools, for example with researchers associated with the UoB Pharmacy initiative.

Supervision Arrangements, Training and Support: Each student is provided with a supervisory team consisting of a *Lead Supervisor*, a *Second Supervisor* and a *Mentor*. The *Second Supervisor* acts as an academic advisor on research skills, training and UoB requirements but can also act as a *Co-supervisor*. The *Mentor* is responsible for the pastoral support of the Student and is chosen from one of the School's Welfare Tutors. Each starting p/g student undertakes a *Personal Training Programme*, which includes courses on safety training, laboratory demonstrating, ethics and IP as well as English language courses for international students. Students attend research seminars organised by their research unit and whole School seminars. Written work consists of a literature review and end of year report (Year 1) and a research paper (Year 2). Students are also required to present a poster (Year 2) and give a formal research lecture (Year 3) at the Annual Postgraduate Symposium. Students regularly attend the annual UoB-run postgraduate careers conference, with SoC staff contributing by speaking at the *Careers in Academia* session. Evidence for the quality of the training environment comes from available data on first destinations for leaving PhD graduates from the SoC in the REF window, with 49% having obtained a postdoctoral position in the UK or abroad and 27% obtaining industrial positions (the remainder largely work in the public sector, teaching or in non-industrial employment).

Progress Monitoring: A formal mid-year *Review of Progress Meeting* involving the student and Supervisor(s) takes place at 6, 18 and 30 months after registration. A formal end of year *Review of Progress Meeting* takes place during the 12th, 24th and 36th months of registration (i.e. near the end of each year of study), involving the student, supervisor and second supervisor, which is used to inform the School Progress Panel at the end of each year. The four year PSIBS PhD programme has a separate operating structure but has a similar recruitment, monitoring and support structure: applicants interviewed by 3 members of staff; students have 3 supervisors and an independent mentor; monthly and quarterly supervision reporting monitored by the Steering committee; annual reports, presentations and vivas for progression.

d. Income, infrastructure and facilities

Research Grant Income: There has been a significant increase in grant income in this REF window, with a 55% increase in the yearly average to £2.95M, totalling £14.77M (NB - REF4b data excludes the PSIBS CDT funding), compared to RAE2008 (£1.90M/year, totalling £12.50M). This increase can also be represented by grant value capture/year (average of £2.34M for 2007/8 onwards, compared to an average of £1.47M/year for 2000/01 - 2006/7 inclusive), with the last four years seeing consecutive increases. EPSRC grant income has been particularly healthy in the REF window (25 grant awards to SoC staff as PI, amounting to £14.2M, compared to £5.6M in the RAE2008 window). A snapshot of current EPSRC grant income per capita (Sep 2013 data on active grants, with staff numbers based on latest HESA data) puts the SoC 12th overall among UK chemistry departments for current PI funding levels. Highlights include **Johnston** being PI on the £1.6M EPSRC Critical Mass Grant "TOUCAN" (EP/J010804/1) and CI on the £3.2M EPSRC Programme Grant "Simulation of Self-Assembly" (EP/I001352/1). Staff joining the SoC on their first academic appointment in the REF window have also been particularly successful, with **Peacock** and **Fossey** winning *EPSRC First Grants* and **Schnepp** and **Baranoff** receiving *EU Marie Curie Career Integration Grants*. Each award has been supported by the SoC with a matched PhD studentship. **Rodriguez** brings with his appointment a *Netherlands Organization for Scientific Research* (NWO) VENI grant (€250k). The significant amount of funding from the EU includes €1.9M for 9 postdoctoral fellowships (IEF and IIF) to the following research groups: **Davies** (3), **Baranoff** (2), **Hannon**, **Fossey**, **Worth** and **Johnston**. Examples of awards involving industrial support include **Preece** being part of a €3M interdisciplinary project '*Hybrid Molecule/Nanocrystal Assemblies for Photonic and Electronic Sensing Applications*' (HYSENS, 2011-2014), involving 5 academic institutes across Europe and 3 industrial partners. Also **Horswell** has participated in *Surface Electrochemical Reactivity in Electrocatalysis: A Combined Theoretical and Experimental Approach* (ELCAT 2009-12), a €3.1M Initial Training Network (ITN) for PhD students and young researchers involving *Johnson Matthey*. Other examples of industrial support and partnerships include **Fossey's** *RS Industrial Fellowship* and several PhD studentships (collaborations summarised in Section e). Recent awards illustrating the success of outreaching theme priorities include: (i) EPSRC consortium DISTINCTIVE (with *NDA*, *Sellafied Ltd*) a multi-institutional grant involving **Read** and **Hriljac**, bringing together decommissioning and nuclear waste management research as well as training for the next generation of researchers; (ii) COOPERA-TB, an EU ITN (€1.2M) involving **Cox**, UoB Biosciences and *GSK*, focused on tuberculosis drug discovery.

Research Facility Awards: SoC staff have also made extensive use of national and international synchrotron X-ray, neutron and computing research (eg HECToR involving the Materials Chemistry HPC consortium) facilities, with facility time awarded in open competition. The total in-kind income for facilities is £6.92M, which comprises eligible research council facilities (£3.87M, REF4c data) and overseas facilities (£3.05M, mainly the Swiss Light Source at the Paul Scherrer Institute and the Advanced Photon Source at the Argonne National Lab).

PSIBS Doctoral Training Centre: The EPSRC £7.2M DTC for *Physical Sciences of Imaging in the Biomedical Sciences* (PSIBS) began in 2008 to facilitate the training of high-quality engineering and physical sciences graduate students in a multi-disciplinary environment at the life sciences interface. It is a cross-campus activity involving and integrating all STEM schools on campus, enabling both chemical biology and biomedical imaging research and is led from the SoC by **Hannon** (PI and Director). All its projects involve co-supervision by physical scientists, computer scientists and biomedics and this has given great impetus to and support for the SoC's links to the Medical and Dental and Life Science Schools that was a key part of the SoC's outreaching strategy after RAE2008. The particular focus of PSIBS research is on the development of imaging techniques and the computational analysis of image data to enable and support future breakthroughs in biology and biomedicine. It has formed a partnership with 18 companies, including *GE Healthcare*, *Perkin Elmer* and *Smith and Nephew*. The new £7M Physical Science for Health CDT (announced Nov 2013) demonstrates the successful evolution of PSIBS and will apply a range of physical science (and notably chemistry, polymer science and nanoscience) to address key problems in the new biomedical foci of ageing, trauma and cardiovascular disease.

Infrastructure and Facilities: In 2012, the UoB was one of four institutions (with **Johnston** the UoB lead) sharing a £3.5 million award from the EPSRC to create a high-performance

supercomputing hub called *MidPlus*, which provides extra computing power and data storage and complements existing computational facilities on campus. This investment greatly adds to the regional infrastructure and will aid collaborations and engagement with local business and industry. The SoC has an established suite for solid-state materials characterisation as well as the *Centre for Chemical Analysis* containing state-of-the-art centralised chromatography (HPLC), NMR spectroscopy, mass spectrometry and X-ray diffraction in the Haworth building, which has attracted ca. £60k of commercial income since 2008. These facilities have benefitted from two major funding awards in the REF window:

Science City Research Alliance (SCRA). This is a regional initiative, set up between the UoB and Warwick, providing £55M in investment from Advantage West Midlands and the European Regional Development Fund for state-of-the-art facilities and equipment to encourage growth and support science and technology. The SoC has benefited from new equipment under the Advanced Materials theme (£2.2M in total, comprising AM1 led by Greaves and AM2 led by Preece) along with the refurbishment by the UoB of 2 laboratories to house the equipment (AM1 Diffraction Facility £0.8M and AM2 Nanofacility £1.4M). The equipment includes two X-ray powder diffractometers, a Raman spectrometer, an X-ray fluorescence spectrometer, UV/vis, fluorescence and NIR spectrometers and NMR console upgrades. In addition to facilitating core and interdisciplinary research and training outcomes, the investment has led to new partnerships and commercial income from over ten different companies, based largely in the West Midlands. These span the range from small start-ups, through to established regional engineering businesses and international companies.

Core Capability for Chemistry Research*:* In 2013, the SoC received a £1.4M investment funded through an EPSRC competitive grant led by **Simpkins** (EPSRC contribution: £0.9M; UoB contribution £530k) to upgrade a variety of equipment housed in the SoC as part of the drive to enhance its research facilities. The items of equipment include a travelling-wave ion mobility mass spectrometer (IM-MS) with both matrix assisted laser desorption ionisation (MALDI) and electrospray ionisation capabilities, a multinuclear diffusion probe for 300 MHz NMR microimaging system (micro-MRI), with 1H and X-nucleus capability (i.e. 19F, 31P), and two X-ray diffraction instruments to analyse both crystalline and non-crystalline samples. This equipment enables a diverse range of core research to grow within the SoC.

e. Collaboration or contribution to the discipline or research base

Contributions to the wider research community: As part of the growing national trend towards work with other disciplines, both from within the same institution and with other institutions, the SoC contributes some of its large equipment (NMR, XRD) to the *M5 Universities Group*, which was set up in 2012 to boost research collaboration, improve efficient sharing of equipment and facilitate bids for high-end equipment. As another example of inter-institutional collaboration, the SoC (led by **Anderson**) has played a central role in the UoB's participation in the Midlands Energy Consortium (MEC) and has been represented on the Management Board of the Midlands Energy Graduate School (MEGS) since its inception in 2008. This activity within the MEC led to the funding in 2009 of the £5.5M UoB EPSRC-funded CDT in *Hydrogen, Fuel Cells and their Applications*, with now over 50 PhD students actively engaged in research in fuel cell and hydrogen related projects involving 30 academic staff and research fellows across three institutions. **Anderson** and **Slater** are currently members of the Science Board of the H2FC SUPERGEN Hub. SoC staff have also been involved in shaping policy and funding priorities, for example with **Slater** being an Invited International Expert for the UK Government organized "*Low Carbon Cars: Exploring the Challenge of bringing Electric Vehicles to Market International Experts' Meeting*" in 2008. The resulting recommendations infomed the subsequent G8 summit meeting. **Anderson**, **Peacock**, **Pikramenou** and **Tucker** have been involved with the EPSRC *Directed Assembly Grand Challenge Network*, with Peacock recently becoming one of its Network Champions. **Tucker** also coordinated the UK supramolecular chemistry community's response to the 2011/12 EPSRC research portfolio review of *synthetic supramolecular chemistry*. The resulting report, channeled through the RSC, contributed to the EPSRC's decision to maintain its strong level of support for this interdisciplinary research area.

Research Collaborations*:* The drive to apply and extend the core research of the SoC in the REF window is linked to the plethora of active collaborations with both academia and industry, many of

them cross- and interdisciplinary, as shown in the following examples:

Academic collaborations: SoC staff are UK representatives on the management boards of 4 EU COST Actions (**Hannon**, **Pikramenou**, **Johnston** and **Worth** – specific details in leadership section). These coordinate the networking of more than 250 research teams across Europe and provide financial support for meetings and scientific missions for collaborative experiments via student exchange. These and other collaborations resulting in REF papers, patents and funding include: **Worth** – Quantum dynamics research with Fielding (UCL) and Robb, Bearpark (Imperial) resulting in EPSRC funding (EP/K037943/1); **Fossey** – Metal-catalysed organic synthesis involving collaborations in China (Shanghai and Henan) resulting in 2 REF outputs; collaboration with James (Bath) resulting in REF output and 2 patents; **Cox** – Application of organic synthesis to chemical biology with Besra (UoB, Biosciences) resulting in funding from MRC and Wellcome Trust (£1.4M platform grant), REF outputs, ITN and patent; **Hriljac** - Synchrotron studies at APS (Chicago) ISIS and DLS, resulting in collaborations (UK and US), REF outputs and *Infineum* funding (see below); **Anderson** – Collaboration with INA (Spain) on atomic scale characterization of metal nanoclusters in porous hosts, resulting in REF output 1; **Greaves** – Hydride reduction of layered solid-state structures in collaboration with groups in China (Changchun) and Portugal (Lisbon), resulting in REF output 4; **Slater** – Solid oxide fuel cell research in collaboration with researchers in Spain (Zaragoza) resulting in EPSRC funding (EP/I003932/1); **Hannon** – Chemistry-biology research on nucleic acid recognition and crystallography with leading researchers in the field (e.g. Zurich, Barcelona) resulting in REF outputs and patent; **Pikramenou** – gold nanoparticle work with UoB Medical School, leading to Leverhulme Fellowship, REF outputs and patent; **Britton** - collaboration with Forsyth (Australian Laureate Fellow) leading to 3 exchange visits and REF output 1.

Non-academic and industrial collaborations: As part of the drive to explore new medicinal chemistry activity at the UoB, **Simpkins** secured an Industrial KTS collaboration through Institutional EPSRC *Additional Sponsorship Funds* (2012), involving a postdoc working with AZ to transfer compound library knowledge to the UoB. The results have informed the UoB strategy for various initiatives (e.g. Pharmacy) currently being promoted at the UoB. As part of the focus on forging closer links with industry, Dr. E. Kendrick (*Sharp Laboratories*) was recently appointed an honorary senior research fellow and collaborates with **Slater** on ionic conductors. The REF window has seen an increase in industry linked (eg CASE) studentships as follows: **Davies** – *AZ* (2010); **Grainger** – *GSK* (2008); **Simpkins** – *AZ* (2007 and 2011); **Pikramenou** – *Serascience* (2013); **Preece** has three interactions involving surface science and colloid research through the Engineering Doctorate (EngD) Scheme in Formulation Engineering at the UoB: *P&G*, leading to one patent; *Dupont Teijin Films*; *BASF,* leading to patent preparation; **Preece** also has a project on microencapsulation with *P&G* who co-funded 2 PhD studentships, leading to an EPSRC grant (EP/F068395/1, 2009-2012); **Hriljac** has a collaboration with the *National Nuclear Laboratory* related to the production, characterization and testing of nuclear wasteforms, leading to 2 PhD studentships from *NDA* (*Nuclear Decommissioning Authority*); **Hriljac** also has a collaboration with *Infineum UK Ltd* based on the analysis of synchrotron X-ray data related to biofuels and additives that includes funding a PDRA and PhD studentship (2013) and consultancy (2012-13); **Peacock** collaborates on analytical instrumentation with *Waters Ltd*, leading to REF output 4; **Mayhew** collaborates with *Ionicon Analytik* on applications of PTR-MS for threat agent detection, leading to REF output 1. **Baranoff** was recently awarded a *Samsung Global Research Outreach Award* for new materials development, leading to a funded PhD studentship (2013).

Leadership, Awards and Esteem: For fellowships to **Tucker**, **Pikramenou** and **Fossey**, see Section c. The SoC is well represented on EPSRC college (14 members Oct 2013). Other activity includes: **Anderson** - US Department of Energy (DOE) *Hydrogen Energy Program* funding panels; **Hannon** - Chairman of EU-ESF COST Action D39 on *Metallo-drug Design and Action* (08/09); Steering Committee member of COST Action CM1105 on *Functional Metal Complexes that Bind to Biomolecules*; elected committee member of the *International Society for Biological Inorganic Chemistry*; 1 *Science Foundation Ireland* review panel and 5 EPSRC panels since 2009, including Roving Panel member; **Britton** - Treasurer of the Committee of the *Division of Spatially Resolved Magnetic Resonance - Groupement Ampère*; REF output 1 on visualizing battery chemistry highlighted in C&EN; **Grainger** - Member of RSC Organic Division Council. 2009-2012; **Hriljac** - External Examiner of *Nuclear FiRST* DTC (Manchester-Sheffield), 2010-present; Member (2008-2009) then Chair (2009-2011) of a DLS Facilities Access Panel; Elected member (2013) of

Diamond User Committee; **Ali-Boucetta** - REF output 1 on alleviation of nanotube pathogenicity highlighted in C&EN; **Preece** - Chair of RSC Group '*Chemical Nanosciences and Nanotechnology*; External Examiner of Imperial College *MRes in Nanomaterials*; Member of RSC Materials Chemistry Division Council; Member of the Editorial Advisory Board *J. of Experimental Nanoscience*; Member of Int. Advisory Board of *Chem Soc Rev;* member of External Advisory Board of the EPSRC CDT Molecular Scale Engineering (Leeds-Sheffield); **Winn** - Member of the Editorial Board of *Journal of Physical Chemistry & Biophysics*; **Peacock** - Evaluator for Marie Curie IIF, IEF and IOF schemes; REF output 1 on enzyme mimics highlighted in C&EN; **Johnston** - Vice-Chair and Work Group Leader of EU COST Action MP0903 NANOALLOY (2006-11); **Slater** - Member of STFC ISIS facility Diffraction Panel (2007-2011); Crystallography representative on ISIS user committee (2012-present); **Worth**: Member of Management Committee of EU COST Action CM1204 on *XUV/X-ray Light and Fast Ions for Ultrafast Chemistry* (XLIC, 2013-17); **Günther** - Scientific Director of £10M HWB Biomolecular NMR centre (UoB), the UK's largest NMR facility (7 spectrometers 500-900 MHz); **Tucker** – Edited special issue of *Supramolecular Chemistry* dedicated to the *6th Int. Symp. Mac. & Supramol. Chem.* (Brighton, 2011); Advisory Panel member for EPSRC National X-Ray Crystallography Service; REF output 3 on FcNA included in RSC themed issue on nucleic acids and highlighted in *Nature Chemistry*; **Rodriguez** – REF output 1 on CO enhancing gold catalysis (*Nature Chemistry* front cover) won 2012 CIDETEC award and highlighted in C&EN; **Pikramenou** - Management Committee member of EU COST Action MP1302 on *Nanospectroscopy* (2013-17); WG Leader of EU COST D31; **Fossey** – Member of team winning 2013 Daiwa Adrian Prize for "*Chemonostics: Using chemical receptors in the development of simple diagnostic devices for age related diseases*"; **Davies** - *Thieme Chemistry Journal Award* 2011; **Mayhew** - Chair of the Molecular Physics Group of the IoP (2012 onwards).

Plenary and Keynote Conference Lectures (selected recent examples)*:* **Preece** - 7th *Int. Conference on Materials for Advanced Technologies*, ICMAT (Singapore, 2013); **Davies** - *23rd Int. Symposium: Synthesis in Organic Chemistry* (Oxford, 2013); **Pikramenou** - *Clinical Nanomedicine & Targeted Medicine* (Switzerland); *Materials Research Society Spring Meeting* (USA, 2013); **Slater** – *19th Int. Conference on Solid State Ionics*, (Japan, 2013); *Prospects in Ceramic Proton Conducting Fuel Cells* (France, 2013). **Johnston** - *5th Asian Pacific Conference of Theoretical and Computational Chemistry*, APCTCC5 (New Zealand, 2011); *Discussion Meeting on Thermodynamics of Alloys*, TOFA (Croatia, 2012). **Mayhew** - *5th Int. PTR-MS Conference* (Austria, 2011); **Greaves** - *ZING Int. Conference on Solid State Chemistry* (Spain, 2012); **Peacock** - *12th Int. Symposium on Inorganic Biochemistry* (Poland, 2013); **Simpkins** - *22rd Int. Symposium: Synthesis in Organic Chemistry* (Cambridge, 2012); **Worth** - *5th Theoretical Biophysics Int. Symposium* (Portugal, 2011); **Günther** - British Council supported lecture series *"Can Medicine be Predictive?*" (Spain, 2013); 9th *European Meeting on Magnetic Resonance* EUROMAR (Greece, 2013); **Fossey** – *Int. Symposium on Catalysis Toward Green Sustainable Chemistry* (Japan, 2013); **Hannon** - 16th *Int. Conference on Bioinorganic Chemistry* 16-ICBIC (France, 2013).

Conference Organisation: **Hannon** - Chair of the 2014 Gordon Research Conference *Metals in Medicine*; **Anderson** – Organising committees for *14th Int. Symposium on Metal-Hydrogen Systems* (MH2014) and *Universitas 21* Energy Conference (UoB, 2008); **Slater** - International advisory board for the *2nd International Conference on Clean Energy Science* (China, 2014); **Tucker** – International Advisory Board for *6th International Symposium on Macrocyclic and Supramolecular Chemistry* (Brighton, 2011); **Pikramenou** - Scientific committee member for *Dalton Discussion on Inorganic Photophysics and Photochemistry* (Sheffield, 2012).

Chemistry Conferences at the UoB: The SoC has actively supported staff in the organization and hosting of major conferences in the REF window, each attracting 100+ delegates: *RSC SupraNano* 2008 (Chair **Preece** and **Tucker**); *Annual Conference of the RSC Spectroscopy and Dynamics Group*, SDG 2010 (Chair **Worth**); *Chirality and Supramolecular Chemical Synthesis* 2009 (Chair **Fossey**); *Catalysis and Sensing for our Environment* (CASE) 2011 (Chair **Fossey**); *RSC Chemical Nanoscience Meeting* 2011 & 2012 (Chair **Preece**); *RSC Carbohydrate and COST Meeting* 2012 (Chair **Fossey**); *RSC Midlands Electrochemistry Group Meeting* 2012 (Chair **Horswell**); *RSC Nucleic Acids Forum* 2012 (Chair **Tucker**); *High-dimensional Quantum Dynamics: Challenges and Opportunities* 2012 (Chair **Worth**)*; Theory of Atomic & Molecular Clusters VII (International)* 2013 (Chair **Johnston**); *2nd UK Nuclear Academics Discussion Meeting* 2013 (Chair **Read**).