Institution: University of Manchester

REF202

Unit of Assessment: 8 (Chemistry)

1. Unit context and structure, research and impact strategy

Overview

The core mission of the Department of Chemistry is to advance chemical knowledge, and to use that knowledge to overcome challenges facing society. Underpinning this mission is the strategic aim to sustain world-class ability in fundamental chemical research, including: nurturing brilliant early career researchers (ECRs); encouraging a culture of openness and diversity; provision of cutting-edge infrastructure; reaching out to other disciplines, industry, public services, policy makers and the general public.

The Unit is within the Faculty of Science and Engineering (FSE). Research is based in four buildings: the Chemistry Building, Manchester Institute of Biotechnology (*MIB*), Dalton Cumbrian Facility (*DCF*) and the Photon Science Institute (*PSI*). The Department is one of the largest in the world with >70 permanent academic staff, >360 PhD students, >160 postdoctoral researchers, >50 M.Sc. researchers and >120 M.Chem project students every year. We host >80 international visitors every year at senior and ECR level.

Highlights since REF2014 include:

- Open research awards from UKRI as PI >£76 million(M) on 31/07/2020.
- A Royal Society Research Professorship to Leigh (2016-).
- Seven ERC Advanced Grant Holders (Flitsch, Larrosa, Leigh, Leys, Schröder, N.Turner and Winpenny); this is the largest accumulation of ERC AdGs in Europe.
- Election of Morris, Scrutton and N.Turner as Fellows of the Royal Society (FRS), joining Leigh.
- Queens Anniversary Prize award (2019) to **MIB** for pioneering expertise in industrial biotechnology (IB).
- Award of thirty-two RSC prizes, including nine in 2020.
- Thirty-two appointments have been made, ten at professorial level. Eleven of these new colleagues hold externally funded fellowships.
- A £55M investment in refurbishing the Chemistry building, including a new Centre for Radiochemistry Research (*CRR*) that will host a National Nuclear User Facility (NNUF2) enabling synthetic transuranic chemistry in the UK.
- Leadership of multiple multi-institute initiatives in engineering biology/biotechnology including BBSRC/EPSRC **SYNBIOCHEM** Centre (£10.2M) and the EPSRC Future Biomanufacturing Research Hub (**FBRH**, £10M from UKRI and £5.7M from industry).
- Multiple UKRI equipment awards giving world-leading capability in X-ray diffraction, NMR and EPR spectroscopy, mass spectrometry (MS), magnetic characterisation, and radiochemistry. Industry has invested in new mass spectrometers and The University of Manchester (UoM) has invested in a characterisation suite for porous materials.
- Access to new multidisciplinary facilities within the National Graphene Institute (*NGI*, opened 2015), the Graphene Engineering Innovation Centre (*GEIC*, opened 2018) and the Henry Royce Institute (*Royce*, operational since 2020).
- >2200 outputs including >80 papers in *Science* or *Nature* group.

All statements in this document refer to the assessment period (01/08/2013 – 31/07/2020) unless otherwise stated.

Research structure

The Head of Department (HoD) delegates research strategy to a Director of Research and line management to six heads of research groupings: Analytical methods and physical chemistry (**AMP**), Chemical biology and biological chemistry (**CBBC**), Computational and theoretical chemistry (**CAT**), Inorganic chemistry (**INO**), Materials chemistry (**MAT**), and Organic chemistry (**ORG**). Staff are encouraged to work across groupings. Colleagues who work closely together, have on occasion, been placed in different groupings to increase cross-fertilisation of ideas.

Research strategy

After REF2014 we reviewed and simplified our strategy under a new Head of Department. We:

- adopted a new structure to integrate staff joining us from the Faculty of Life Science;
- adopted a structure that maintains strengths in core chemistry (*e.g.* INO and ORG) while growing activity at the interfaces (*e.g.* with CBBC and MAT) and that attracts new staff and that enables all staff to develop their own disruptive ideas;
- promoted a diverse portfolio of research grants ranging from fellowships to large collaborative grants;
- internally peer-reviewed submission of manuscripts to increase the quality of outputs;
- embedded EDI (Equality, Diversity and Inclusion), *e.g.* strong participation in the FSE Dame Kathleen Ollerenshaw Fellowships;
- identified opportunities for impact and supported these through sabbaticals and targeted funding;
- used UKRI strategic equipment funds, industry and *Royce* to improve infrastructure.

We believe research leadership must let researchers flourish by letting them pursue their own goals and develop their own collaborations. Where close collaborations build a powerful team we encourage such teams to grow, for example in biotechnology, molecular magnetism, catalysis. Implementation details are given in Section 3. We have moved out of some areas or transferred elsewhere (*e.g.* environmental radiochemistry is now within the Department of Earth and Environmental Sciences).

Our research strategy is not driven by statistics, which never capture the whole picture, however the indicators in Table 1 reflect the success of our staff over the REF2021 period. On 31/07/2020 researchers in the Department of Chemistry held >£76M in open peer reviewed UKRI grants as PIs (Table 1). These numbers place us first among UK Chemistry departments for EPSRC, BBSRC and overall UKRI grants. At REF2014 we reported £43M in open grants, which included European and industrial funding.

Table 1. Open UKRI research awards,^a ERC awards and Nature index on 31/07/2020 for the Unit

Institution	Value EPSRC/£	Value BBSRC/£	Total UKRI [♭] /£	ERC awards	Nature Index ^c
Manchester	52,838,994	22,219,003	76,577,522	12	3

a. Data from <u>https://gtr.ukri.org</u> on 24/02/21; the numbers exclude eleven EPSRC, five BBSRC and one NERC awards totalling £5,839,100, £2,473,485 and £5,966 respectively with start-dates post 31/07/20.

b. Also includes NERC and STFC.

Manchester was third in the UK in the 2020 Nature index for Chemistry, based on outputs in leading journals (<u>https://www.natureindex.com</u>). For Unit papers assigned to the Chemistry subject category by SciVal (1594 papers), 20.5% are in the top 10% most cited.

Progress since REF2014 and how our plans have been implemented

Shortly after REF2014 a university restructure added twelve colleagues in biological chemistry; we restructured internally to bring together strengths in biological chemistry and revised our strategy under a new Head of School. Refurbishment of the Chemistry Building was an objective in REF2014. This is underway (completion 2024) and will provide expanded synthetic laboratory space and a brand new CRR, able to handle trans-uranic elements; this will form a NNUF2.

We targeted increasing our involvement with industry and our success is noted below.

■ AMP: We have grown three strategic areas, where we are either unique or world-leading. We have discontinued gas phase physical chemistry as we were no longer competitive.

In NMR, methodological developments include "pure shift", which increases chemical resolution by almost an order of magnitude, and further increases the power of DOSY for mixture analysis. An open-source software package for data analysis has been downloaded >1000 times to date.

New methods have been developed for identifying low-level impurities in pharmaceuticals, and for quantitation and for mixture analysis. NMR research in life processes has advanced understanding in protein conformation changes, enzyme catalysis of phosphate and methyl group transfer, and aggregation and amyloid formation. Biotherapeutics that remove amyloids have been studied. A 700 MHz NMR spectrometer with unique reaction monitoring capabilities was obtained as EPSRC strategic equipment.

Within MS, new methods have been developed for biology and medicine, including early-stage diagnosis of Parkinson's disease (PD). We have established facilities for massive data storage and manipulation for synthetic biology. Use of TOF-MS for surface imaging is being developed within the *Royce*, funded by the EPSRC Strategic Equipment Fund. Waters[™] (<u>www.waters.com</u>) fund our Chair of MS.

The **DCF** is a unique £28M facility for radiation chemistry research geographically near the nuclear industry; this delivers impact within the UK's nuclear programme. Researchers from >30 universities and >30 companies collaborate with **DCF**, with >100 international visitors in 2019. **DCF**-based researchers have measured and modelled pressurisation of storage cans by hydrogen. Other studies have examined radiolytic formation of hydrogen in storage ponds containing sludges derived from Magnox cladding. Additional funding of £2.2M (largely from **Royce**) has been obtained to upgrade the analytical facilities in DCF.

Published highlights: development of ultra-high-resolution pure shift NMR and its extension into DOSY and TOCSY (*Angew. Chem. Int. Ed.* **2014**, *53*, 6990; *J. Am. Chem. Soc.* **2014**, *136*, 11867); discovery of volatile biomarkers of PD (*ACS Cent. Sci.* **2019**, *5*, 599); enhanced ion yields from TOF-MS (*Anal. Chem.* **2015**, *87*, 2367).

■ CAT: After retirements (Hillier, Connor) we are building around three areas: electronic structure, especially of heavy elements; biological processes; advanced materials. We recruited: Kaltsoyannis as a leader in electronic structure of heavy elements, linked to the nuclear industry for example through the multi-disciplinary *DISTINCTIVE* and *TRANSCEND* consortia, both involve universities and industry working on decommissioning and waste management; Skelton (UKRI FLF) studies lattice dynamics in advanced materials, linking to *Royce*; Chilton (RS URF and ERC StG) provides theoretical insight into molecular magnetism. These new appointments add to existing strengths modelling biological processes and method development (Popelier).

CAT maximises impact by making software available: detection of key atoms governing chemical processes (Popelier); <PHI> downloaded by ~9,000 users in 88 countries to model magnetic data (Chilton); tools and workflows for studying heat transport (Skelton).

Published highlights: enzyme catalysis (*Nature* **2019**, *574*, 722; *J. Am. Chem. Soc.* **2020**, *142*, 10240), understanding of U-M bonding (*J. Am. Chem. Soc.* **2016**, *138*, 3333), phonon mapping in $Bi_2Sn_2O_7$ (*Chem. Sci.* **2020**, *11*, 7904), high blocking temperatures in molecular magnets (*Nature* **2017**, *548*, 439).

■ **CBBC:** This group integrates world-leading activity in biocatalysis, protein engineering, synthetic biology and biomanufacturing, and fundamental interdisciplinary biosciences. The main focus is on IB. We have uniquely established:

- a fully integrated and operational foundry for microbial production of fine and speciality chemicals through the **SYNBIOCHEM** Centre (£10.2M, Scrutton, Takano, N.Turner 2014-21);
- the EPSRC Future Biomanufacturing Research Hub (*FBRH*, £10M UKRI and £5.7M industry, Scrutton, 2019-27) coordinating UK academic, High Value Manufacturing catapult, and industrial capabilities to enable the complete biomanufacturing innovation pipeline in pharmaceuticals, value-added chemicals, engineering materials, and advanced biofuels;
- four networks in the UK biotechnology and bioenergy sector through *BioCatNet* (N.Turner), *IBCarb* (Flitsch and Field), *NPRONET* (Micklefield) and the EU-funded network *CarboMet* (Flitsch) (BBSRC funded, 2014-19).

We have been awarded the Queen's Anniversary Prize for Higher and Further Education (to MIB, 2020) and three ERC Advanced Grants. Scrutton and N.Turner were elected FRS in 2020. Notable



recent grants include the Wellcome Director's award (£10M total, £3.3M to Manchester, Cai) and a **Royce** award for rapid protein evolution (£2.1M, Green and Scrutton). We network with 115 industrial partners (international pharmaceutical, chemical and energy companies), such as GSK, AstraZeneca, BASF, DSM, Codexis, Dr Reddys, Merck, Syngenta, Shell, and Prozomix. From these we have secured significant industrial investment, *e.g.* **FBRH** (£5.7M), CoEBio3 (£3.2M), Shell partnership (£2.5M), and Prosperity Partnership (£3M). Since REF2014, our research has also led to spin-out companies, including BioShape (Flitsch/Barran), C3 Biotech (Scrutton) and Iceni Diagnostics (Field).

Published highlights: Enzyme catalysis (*Nature* **2015**, *522*, 497; *Nature* **2016**, *539*, 593; *Nature* **2019**, *574*, 219; *Nature Catalyst* **2018**, *1*, 977); structural biology (*Nature Chemical Biology* **2017**, *13*, 975); protein engineering (*Nature* **2019**, *570*, 219); and synthetic biology (*Science* **2017** *355*, 1040; *Science* **2016** *353*, 126; *Proc. Natl. Acad. Sci.* **2017** *114*, 1470).

■ INO: Liddle was recruited to lead, and to strengthen f-block chemistry and molecular magnetism. 2020 appointments (Mehta and Willcox) will build activity in homogenous catalysis, linking to ORG. Yang was appointed, alongside Schröder (in MAT), to refresh activity in porous materials.

Research on radiochemistry led to an NNUF2 award (£4.2M) to establish a capability to make and to study complexes of the trans-uranics. Research on porous materials has been highlighted in the "<u>UK Research and Development Roadmap</u>" (1/7/2020, p47) as an example of UK ground-breaking technology impact. The EPSRC National EPR Facility and Service was renewed in 2014 and has been used to study science from polysaccharide cleavage to actinide covalency. The molecular magnetism group published reports of the highest blocking temperatures and energy barriers in single-molecule magnets (SMMs).

Published highlights: a paradigm-challenging study of π --back-bonding between uranium and a poor π -acceptor (*Nature Chem.* **2019**, *11*, 806); isolation of metallocene anions (*Nature Chem.* **2020**, doi.org/10.1038/s41557-020-00595-w); a direct measurement of covalency in actinides (*Nature Chem.* **2017**, *9*, 578); new selective biomass conversions (*Nature Mater.* **2020**, *19*, 86); new zeolites with active sites to purify ethylene (*Science* **2020**, *368*, 1002); metal-organic frameworks (MOFs) that can uniquely and reversibly adsorb highly corrosive NO₂ (*Nature Mater.* **2018**, *17*, 691).

■ MAT: We have refreshed the area in porous materials, appointing Schröder, and built on strengths in 2D-materials (Keerthi, linked to *NGI/GEIC*). We are developing sustainable materials linking to *Royce*. Collaborations are strong with the BP International Centre for Advanced Materials (BP-ICAM). One BP-ICAM project helped reduce wear in automotive engine components with a direct impact to BP of \$1-10M (ICAM 2018 annual report). A collaborative project (ICAM15 and ICAM24) with Cambridge, Imperial and Illinois universities contributed to the development of a new fuel additive (Active Technology) for BP Ultimate Fuels.

A multi-user "energy lab" has been set-up within the *NGI* (Dryfe), capable of small-scale battery and supercapacitor cell fabrication; this supports both internal and external industrial users. Dryfe also designed a dry room and facilities for larger-scale device fabrication within the *GEIC*.

The **Organic Materials Innovation Centre** (OMIC, led by M.Turner) has built strong links in sustainable materials to Shaver (new appointment, Materials) and new staff are being recruited in organic electronics. New membrane science has been developed collaborating with Newcastle, Imperial, Edinburgh and Bath. We have extensive industrial collaborations on: graphene-based barrier materials with TWI Ltd; graphene-based coatings with Hempel; composites with Petronas. Molymen (based in *GEIC*) has been spun out from Dryfe's lab, to develop water filtration membranes based on 2D-materials. Chromition and SciTron as spin-outs have arisen since 2014 and polymers of intrinsic microporosity (PIMs) have been licensed to 3M.

The materials activity at *DCF* has studied radiation effects in spent nuclear fuel recycling within the *ATLANTIC* consortium (involving 12 UK universities), and the BEIS Advanced Fuel Cycle Programme.

Published highlights include: ballistic transport through 2D-channels (*Nature*, **2018**, *558*, 420); water-based biocompatible 2D-crystal inks for ink-jet printing (*Nature Nanotech.*, **2017**, *12*, 343); a unified kinetic three-dimensional partition model to predict crystal growth (*Nature*, **2017**, *544*,



456); separation of hydrocarbons in a functionalised MOF (*Nature Chem.* **2015**, 7, 121); sieving hydrogen isotopes through 2D-crystals (*Science*, **2016**, *351*, 68).

■ ORG: has built on strengths in three areas: homogeneous catalysis (recruiting Larrosa, Leonori); mechanistic study of reactions (Bures); supramolecular chemistry by developing mechanochemistry (De Bo). Our excellence led in 2018 to an EPSRC Centre for Doctoral Training (CDT) in Integrated Catalysis (<u>https://www.icat.manchester.ac.uk</u>, *ca.* £5.94M from EPSRC with further support from Arcinova, AstraZeneca, Bayer, Bristol-Myers Squibb, Concept Life Sciences, GSK, and others), and links to bio-catalysis within CBBC and chemical engineers from Manchester.

Supramolecular chemistry and molecular robotics are led by Leigh (Royal Society Research Professorship and EPSRC programme grant). Major progress has been made in designing programmable machines, and using knots to interlock complex structures.

Published highlights include: a programmable molecular machine that can build molecules stereoselectively (*Nature* **2017**, *549*, 374); the 2D weaving of polymer chains (*Nature*, **2020**, *588*, 429); the use of visible light to drive sustainable catalytic processes (*Science* **2020**, *367*, 1021); catalytic methods for late-stage modification of pharmaceuticals (*Nature Chem.* **2018**, *10*, 724); the taming of highly reactive free-radicals for complex molecule synthesis (*Nature Chem.* **2017**, *9*, 1198); development of a new mathematical treatment for the analysis of reaction kinetics (*Angew. Chem. Int. Ed.* **2016**, *55*, 2028).

Future strategy 2021 - 2026

Building on 2014 - 2020 our departmental strategic aims are:

- 1. Complete the Chemistry building renovation (cost £55M, delivery date 2024). This will provide new synthetic space for our >200 synthetic researchers in addition to the CRR.
- 2. Achieve ever greater translation of our world-leading biotechnology into biomanufacturing; the new EPSRC *FBRH* is core to this ambition.
- 3. Bring together research in catalysis, integrating bio- and small molecule catalysis within the Department, and heterogenous catalysis (*e.g.* Hardacre, Chemical Engineering and Analytical Science (CEAS); Haigh, Materials).
- 4. Establish the *CRR* and *DCF* as linked NNUFs contributing to our fundamental understanding of trans-uranic chemistry and impacting the nuclear industry.
- 5. Demonstrate the potential of molecular robotics and molecular weaving to provide revolutionary nanotechnologies and materials.

Plans for each of our research groupings are:

■ AMP: We will target ultraclean high-resolution NMR spectra at high dynamic range, with applications in pharmaceuticals. This includes real-time reaction monitoring, including heterogeneous reactions; improved tools for 19F NMR; new approaches to quantitation in mixtures.

Novel MS instrumentation will be developed for monitoring reactions, mapping soft and hard materials and determining the structure and dynamics of large molecules. We will increase the throughput and sensitivity of multi-omics MS, incorporating microfluidics and machine learning. We will establish a centre for MS diagnostics and prognostics focussing on neurodegenerative and infectious disease, and work with the industry led *Community of Analytical and Measurement Science* (*CAMS*) to train new mass spectrometrists.

Automation will increase at *DCF*, leading to greater sample throughput, and strengthening links to nuclear industry partners, including reactor chemistry, spent fuel recycling and synthesis/modification of materials by radiation. New capability in modelling radiation chemistry will be developed for application in the nuclear and healthcare industries.

■ CAT: Further recruitment will target three areas: development of quantum methods; molecular dynamics at larger scales (with CBBC and MAT); calculations of catalytic processes (with ORG, CBBC and INO). CAT will expand The University of Manchester's (UoM) flagship computer CSF3



and invest in cloud computing and in a new massively-accelerated GPU system (with the N8 HPC Consortium). Scientific ambitions include multiscale structure-stability methods for solvated macromolecular assemblies; a flexible, multipolar polarisable, fully quantum-based protein force field; control of vibronic coupling in SMMs, qubits and phosphors; detailed understanding of transuranic chemistry; study of enzymatic reaction mechanisms; predictions concerning thermoelectric materials, polymorphism in molecular crystals, thermal control in battery electrodes (with Faraday Institute).

■ **CBBC:** We aim to become the national centre for Biocatalytic Pharmaceutical Manufacturing with further industrial collaborations. This strategy aligns with the government's agenda to develop and reshore pharmaceutical manufacturing, and to 'build a Northern Powerhouse'. Our current partnership with the Bill & Melinda Gates Foundation and our strong existing links with the national Centre for Process Innovation and The Medicines Manufacturing Innovation Centre places us to lead these initiatives.

In Synthetic Biology, we will diversify and scale-up biosynthetic methods and metabolic engineering by connecting fundamental research in microbial genetics, directed evolution and enzyme engineering through synthetic biology, engineering biology, robot-enabled genetic manipulation, flow catalysis and industrial scale-up. This will link with the *FBRH*. Our overarching ambition is to build partnerships across the energy, materials, personal and health care, pharmaceuticals, and bulk chemicals sectors, to maximise the impact of biotechnology, biocatalysis and synthetic biology.

■ INO: We will develop major transuranic capabilities in the new CRR using an integrated suite of gloveboxes and characterisation equipment. We will target neptunium and plutonium analogues of established thorium and uranium complexes, with two principal strands: (i) covalency of actinide bonding using metal-ligand multiple bonds as exemplars; (ii) with the National Nuclear Laboratory (NNL) study speciation of coordination complexes relevant to the nuclear fuel cycle and environmental behaviour.

We aim to renew the EPSRC National Research Facility (NRF) for EPR Spectroscopy (*ca.* £5M due 2021). EPR will be used to study actinide covalency. The molecular magnetism group will use EPR to study potential qubits with European collaborations targeting performance of 2- and 3- qubit gates and develop strategies using nuclear spin to perform error correction. We will also study relaxation within SMMs and behaviour on surfaces using advanced X-ray spectroscopies (with Baker, AMP). A major aim is to build SMM-based devices using established European collaborations.

We will grow activity in catalysis, including: use of heterobimetallic complexes; main group cages; low coordinate f-block complexes. This will involve strong collaboration with ORG.

■ MAT: We will recruit new staff to replace key staff (O'Brien, Yeates). The first, Romanov (RS URF) with expertise in OLEDs arrived after 31/07/2020. Strong interactions will be built with *Royce*; *e.g.* investment (£3.6M) in sustainable materials involves M.Turner, and further posts will be recruited in 2021. Sustainable materials will also link to *FBRH*. Dryfe will occupy new tailored "dry rooms" to develop energy storage technology in *Royce*.

New inks based on 2D-materials will be made (Casiraghi). New photoactive materials will be developed (M.Turner, Romanov) and integrated with devices. New resist materials for nanofabrication will be exploited (Winpenny). We will study the new chemistry that can emerge from reactions in confined spaces (Keerthi).

The OLED and resist work will be translated through spin-outs, Chromition and Sci-Tron, both supported by Innovate UK. The digital histopathology screen platform developed by the former, offers the potential to detect cancer in a single biopsy and is being developed with the Greater Manchester Academic Health Science Network. Resists licensed to Sci-Tron are being studied by US industrial partners.

■ ORG: "*Molecular robotics will be one of the next major scientific areas*" was predicted in The Scientific Report issued around the Nobel Prize in Chemistry in 2016. Through the Leigh group we aim to remain at the forefront of this field, developing scientific tools and strategies to provide revolutionary molecular nanotechnologies. Over the next decade we aim to: use molecular robots



to move and build things; programme the robots for specific tasks, including tasks impossible with conventional technology. We plan to build on recent breakthroughs in molecular knotting and weaving to lead a new area of woven molecular materials.

Within catalysis, we will become a centre of excellence for radical and photo-catalysis (Greaney, Leonori, Procter) and aim to become world leaders in understanding of catalytic reaction mechanism (Larrosa, Bures). We will use mechanical control to initiate catalytic processes (De Bo). This activity underpins the CDT in Integrated Catalysis and involves strong collaboration with CBBC and INO.

Enabling impact

Working towards impact is integral to our research, aligned with the University strategy given in the Institutional Statement (IS) section 2.iv:

- Research group leads are challenged to produce plans and show impact for their groupings, and this challenge is passed down to individual academics.
- PhD studentships with significant industrial co-funding are supported.
- Knowledge transfer is one of four promotion criteria, with equal esteem to research (section 2.iv, IS).
- Sabbaticals are awarded that allow spin-outs to develop.
- Our Workload Allocation Model (WAM) recognises industrial engagement.
- We encourage staff to bring industrial partners into grant applications.
- Departmental services are available to local industries, especially SMEs, building links.
- The Unit works with the University's Knowledge Exchange team obtaining EPSRC Impact Accelerator Awards, Impact Fellowships and Knowledge Transfer Partnerships; 10, 1 and 6 were awarded respectively between 2014 and 2020.
- Visiting professorships from significant industrial partners are supported, *e.g.* Kai Baidenus (BASF), Joe Adams (GSK).
- Invention disclosures are discussed with the University of Manchester Innovation Factory (UMIF), which provides proof-of-concept funding and supports patent applications.

In **AMP** all three major sub-groupings, NMR, MS and **DCF** interact with >60 industrial partners. This ranges from supporting a Chair (Barran) and buying equipment (Allergan, MS) to fully funding projects (typically in **DCF**) and PhD studentships (all). Analysis software is made available through an industrial partner (NMR).

In **CAT** we have strong impact through freeware. Direct involvement with the nuclear industry (NNL, NDA, Sellafield Ltd, Cavenish Nuclear, AWE, TÜV SÜD) is achieved by Kaltsoyannis' involvement in major consortia.

In **CBBC** industrial involvement includes multiple large grants with substantial industrial contributions, and networks with industrial partners. PhD studentships are funded by industry through UKRI Case studentships, CDT programmes, CoEBio3 industry club. A Director of Commercialisation drives industry engagement.

In **INO** there are major interactions with the nuclear industry (NNL, NDA). The EPR NRF supports a range of industrial partners, ranging from brewers to bulk chemicals.

In **MAT** there are multiple spin-outs and licensing agreements. OMIC was founded specifically to develop and translate novel organic materials in partnership with local industries.

In **ORG** our CDT in Integrated Catalysis is supported by multiple industrial partners. PhD studentships are partly or wholly industry supported. Training courses are delivered to industry.

Our selected six impact case studies demonstrate the value of our approach:

■ C4X Discovery: generating market-leading drug candidates from cutting-edge technology – Almond was granted a secondment (80% to C4XDiscovery, 2010-2015) and a reduced teaching load to facilitate impact.

■ Enabling radioactive effluent treatment and high hazard reduction at Sellafield and the management of plutonium (2 cases): the Unit hosts facilities for working with radioactive materials that during the assessment period were unique in UK academia. These enabled experimental



work in support of the effluents impact case, and preparatory work for experiments with gram quantities of plutonium that were carried out in NNL's Central Laboratory, and contribution to the plutonium impact case. Both impact cases were supported by the provision of PhD studentships.

■ New paradigms for 3D materials analysis using polyatomic projectiles: changing capacity and industrial practice. Lockyer was granted sabbaticals (2 x 6 months, 2014 and 2015) to visit groups in Japan to drive impact. Two PhD studentships were awarded in support.

■ DOSY and Pure Shift NMR: changing practice and performance in the chemical industry. Use of an EPSRC Impact Accelerator Award to support a fellowship (*ca.* £74k) was vital. Reduced teaching loads enabled external training courses to facilitate impact: 2017 Pureshift workshop; 2018 DOSY NMR workshop (Campinas, Brazil); 2018 Advanced Practical NMR Methods course (Stockholm University).

■ Sustainable chemical manufacturing through enzyme discovery, biocatalyst engineering and education in IB: N.Turner was granted a sabbatical (2017-18) and a reduced teaching load (2013-2020) to develop industrial partnerships. UMIF led negotiations on licensing, including a license with Prozomix to make all CoEBio3 biocatalysts commercially available.

There are other strong examples of impact: *e.g.* the use of PIMS in respiratory masks, technology that is now licensed to 3M; diagnosis of PD by MS; exploitation of quantum dots *via* Nanoco.

Interdisciplinary research

Much of our research spans boundaries, reflecting the research interests of our (see above). For example, interdisciplinary collaborations with materials scientists (*Nature* 2020, **588**, 429) or biologists (*Science* 2017, **355**, 1049) or physicists (*Science* 2016, **351**, 68) have produced exceptional publications. SciVal classifies our outputs as: chemistry, 1594(70%); chemical engineering 757(33.5%); biochemistry, 700(30%); materials science, 520(23%). Many outputs are included in >1 category.

Departmental staff lead one of the University's interdisciplinary research institutes, the **MIB**, and are strongly involved in the **Dalton Nuclear Institute**, **NGI**, the **PSI** and **Royce**. The unit's research in **MIB** inspired UoM to chose IB as one of only five research beacons. Staff in the **MIB** have won the RSC interdisciplinary prize in two of the last six years.

Explicit calls for PhD studentships exist between the Department of Chemistry and CEAS to build links. We consider multidisciplinary candidates for all posts (*e.g.* Cai, Casiraghi, Takano). We support appointments of chemists to other departments, including: Hardacre, Lee and Sarkisov (all CEAS), Shaver and Lewis (both Materials). We have offered advice, allowed access to facilities and supported grant applications from these chemists. Our appointment strategy builds strong interdisciplinary links.

Specific interdisciplinary research was discussed above, and more details are given in Section 4.

Open research environment

We have closely followed the University's policy (section 2.v, IS). For Open Access (OA) we also support submission to the ChemRxiv for pre-prints. The department encourages sharing of downloadable freeware.

The Library seeks to improve the discoverability of chemistry research, tweeting about open access papers via its @UoMOpenAccess account. The University's OA Innovation Fund covers article processing charges (*e.g.* £19k in 2018/2019 alone). The Library provides research data management support to researchers, completing outline checks and full reviews of data management plans (section 2.v, IS).

Research integrity

We have closely followed the University's policy (section 2.v, IS). All staff and PDRAs in the Department undertake mandatory ethics training and online courses organised by the University. As part of our PhD training programme, all postgraduate students must complete a bespoke, chemistry-specific 5-hour online course on Research Integrity as provided by Epigeum. This ensures our ECRs understand their professional responsibilities and promotes principles of Good Research Conduct.

2. People

STAFFING STRATEGY AND STAFF DEVELOPMENT:

A commitment to equality, diversity and inclusion (EDI) underpins our strategy; we have held an *Athena Swan Silver Award* since 2013. The EDI profile of the Unit is given in Table 2. Twentyone staff have left since REF2014, including three to other units. We have increased the gender and ethnic diversity of the staff.

Table 2. Comparative EDI statistics between REF2014 and REF2021			
Category (Number)	Female/%	BAME/%	International/%
The Unit REF2021 (75.3)	18	10	36
The Unit REF2014 (54)	13	4	13
% change in period	+5	+7	+23
Senior appointments in period (10)	10	20	40
ECR appointments in period (22)	32	18	50

Recruitment: Recruitment has EDI at its core. The language of all adverts is checked to ensure it is not subconsciously biasing applications. All shortlists are required to have male and female candidates represented unless impossible. All interview panels have male and female members.

All new posts are considered carefully, taking into account recent departures of staff, and the need to grow or maintain strategically important areas. Since REF2014, we have decided against appointments in specific areas (see **AMP** above) and moved staff resource to shape research.

The success of our policy can be seen in staff recruited. **Senior appointments**: Breitling, Cai, Currell, Field, Pitt, Kaltsoyannis, Larrosa, Liddle, Schröder, Takano. **ECRs**: Adams, Baidak, Baker, Birmingham, Bowen, Bures, Castanar, Chilton, De Bo, Green, Keerthi, Leonori, Lovelock, Mehta, Palmer, Riddell, Skelton, Tripedi, van Munster, Walton, Willcox, Yang.

Our recruitment strategy delivers excellence, e.g. new recruits hold 17 fellowships between them.

Currell, Field and Liddle were recruited to lead *DCF*, *MIB* and INO, respectively. Kaltsoyannis replaced Hillier in CAT. Larrosa replaced Clayden within ORG. We are recruiting in MAT to replace staff that have departed since REF2014.

The demographics of the department remain good. In strategic areas, proleptic appointments are made, *e.g.* NMR (Castanar), EPR (Bowen), porous materials/MOFs (Yang).

Staff development: Newly appointed staff are set challenging probationary objectives by line managers for the three year probation period; fairness of objectives across the Department is ensured by a Senior Mentor and the HoD. Progress is monitored by an annual Probation Committee chaired by the HoD. New staff have a mentor (not the line manager) who provides informal advice and assistance. All attend a New Academics Programme (NAP) at Faculty level that provides training and leads to membership of the Higher Education Academy (section 3.3, IS).

Researchers on five-year fellowships are also set probationary objectives and are transferred to long-term positions at the end of their fellowships, subject to meeting these objectives.

On the rare occasion (~8% of cases) a probationary staff member makes insufficient progress against objectives, this is discussed with the individual, line manager and mentor and further training and mentoring immediately put in place.

Training: Training is discussed at an annual Personal and Development Review (P&DR). Funds are provided for external management training events including Entrepreneurship training. We use BBSRC funded Future Talent Mobility accounts to develop international collaborations. Equal percentages of female and male staff take such training.

Once through probation, staff are trained for leadership roles by acting as "deputies" to research group leaders or other senior management roles. We find "training through doing" works better than just training courses; this approach is supported by academic research (*e.g.* Evans, "Implicit and informal professional development", <u>https://doi.org/10.1080/19415257.2018.1441172</u>).

Support for ECRs

We build from the university policy (section 3.3, IS). The University has received the HR Excellence in Research Award from the European Commission.

The Unit provides ECRs with mentors, PhD studentships (typically two each since 2014), start-up for small equipment, and travel funds for conferences and to establish collaborations (70% of travel fund awards made have gone to female ECRs). ECRs have free access to departmental analytical services such as NMR, X-ray, MS.

ECRs have a reduced teaching load (typically 50%) during probation. The University's New Academics Programme (NAP) provides training on writing research proposals. The Department provides access to a database of successful proposals. All proposals are internally peer-reviewed and mock interviews are mandatory for all fellowship applicants: a policy that is particularly pertinent to ECRs.

There is an excellent programme of courses available from the Faculty (see PGR section below), and all PDRAs have annual P&DRs at which training needs are identified. The award-winning website, "An Academic Career", was developed by the University of Manchester Careers Service and provides outstanding support to ECRs. The Department established a Postdoc Committee in 2012, run by postdocs, with a budget and guidance from the Director of Research. The Postdoc Committee is largely autonomous and organises activities, *e.g.* regular coffee mornings, events to support PDRAs with fellowship applications.

The quality of support offered is evidenced by >100 PDRAs from the Unit moving to academic positions world-wide since 2014.

Sabbatical leave and fellowships

We value opportunities for staff to spend a period of time concentrating on research and strongly encourage applications for external fellowships.

Sabbatical leave is considered annually for all eligible staff; a detailed plan is required, which can be developing new research or teaching ideas, or developing impact. A family-friendly approach is adopted, and sabbaticals may be taken locally. The Department's sabbatical policy has contributed to impact case studies. During the REF period, we have had at all times an average 4 FTE permanent staff on external research fellowships and 1.8 FTE on sabbatical.

External roles

The Department encourages staff to take external roles in academia, industry, and the public sector. Flexible working, reduced workloads, sabbatical leave, and the provision of administrative support are used to support such roles. 29 staff have held visiting professorships and influential external roles including: the REF2014 and REF2021 panels (Flitsch; sabbatical leave) and ERC starting grant review panel (Takano/Barran).

The Department welcomes visitors from academia and industry. For example, the strategic appointment of Joe Adams (GlaxoSmithKline; Visiting Professor) played a key role in the Department's CDT bid in Integrated Catalysis. Vernon Gibson FRS is a Visiting Professor building links to BP-ICAM. Since REF2014, the Department has hosted >100 senior academics from all over the world.

Recognition and reward for research and impact

Promotion: Line managers proactively encourage applications and consider all staff for promotion. The Personnel Committee helps develop paperwork before forwarding to Faculty. If applications fail, feedback is given, and actions planned. During the REF period, there were 7 promotions to Professor, 13 to Reader, and 13 to Senior Lecturer level. Since REF2014, two staff (both female) were promoted directly from Research Fellow/Lecturer to Reader.

Promotion considers career-breaks and part-time working. The Personnel Committee monitors sabbatical applications and cases for additional increments. Women are as likely to hold senior roles as men in the Department: in our 2017 Athena Swan return, 55% of female academics, *cf.* 52% of male, were Professors. All female staff employed prior to 2016 hold promoted positions.



The University's promotion criteria explicitly include 'Academic Enterprise and Knowledge Transfer' with parity to research. Major impact is rewarded by accelerated promotion and the provision of resource, including PhD studentships.

Workload: Research income and supervision are recognised in our WAM. For our leading researchers this means a light teaching load. We balance this through teaching-focused staff on open-ended contracts who are tasked with developing our teaching, not just delivering it. Our teaching is highly rated (>90% satisfaction at NSS for >10 years to 2019).

Prizes: Senior members of each research grouping are tasked with nominating colleagues for external prizes and this is discussed at P&DRs. This is particularly important for female and BAME staff to redress under representation in prize-winning.

RESEARCH STUDENTS:

Our procedures follow the University policy (section 3.3, IS).

PGR recruitment and funding

Recruitment follows University admissions policy. Programmes and positions are advertised making clear that we welcome applicants regardless of gender, ethnicity, disability, sexual orientation and transgender status. PGRs mostly approach supervisors directly based on the reputation of the researcher. All appointments are made on merit. All applicants are interviewed by at least two academic members of staff before appointment.

President's and Dean's Scholarships provide • University (23%) • BBSRC DTP 7%) • BBSRC iCASE (11%) outstanding international and national UGs the chance to pursue a PhD in Manchester. The Unit has hosted 19 of these Scholarships since REF2014. • Students



The Unit was home to 344 PGRs on 31/07/2020.

Chemistry's PGR students are funded from a variety of sources, including 41% supported by UKRI funding (see Figure 1) including multiple CDTs (see Section 4). "Other" includes A*STAR, alumni, Royal Society, and MRC funded. PGR students hail from 46 countries, with 50% UK, 18% EU/Europe, 10% China, 7% Saudi Arabia, 11% other Asia, and 4% from the Americas, Australia and Africa.

Our Director of Internationalisation works with the Faculty and University to design and implement an internationalisation strategy. A Faculty Summer School (4 weeks, started in 2019) promotes Manchester and the postgraduate opportunities to overseas students. The University has targeted recruitment in China, India, Hong Kong, Saudi Arabia, Nigeria, Malaysia and Mexico. This has led to funded links, for example 2+2 programmes such as the Singapore A*STAR (12 Chemistry PhDs to date) and Tsinghua 2+2 launched in 2020.

Monitoring and support mechanisms

PGRs are assigned a supervisory team consisting of a main and second supervisor, and a mentor to offer pastoral support. Annual progression reviews ensure students are making adequate progress; personalised training packages are devised for all PGRs. Our rigorous progression threshold after year 1, assessed by an academic outside the supervisory team, ensures that PGRs unlikely to complete a PhD, withdraw at an early stage.

PGRs present their research at the Department's Annual PGR Conference twice: posters in second year and talks in third year. Every year students also present posters on their research and take part in a '3-minute thesis talk' competition during the University Postgraduate Summer Research Showcase.

Our Director for Postgraduate Studies is assisted by 1.5 administrators and chairs our Postgraduate Committee with PGR representation. A web-based system records progression milestones for each PGR. Disabled students receive additional support through the Disability



Advisory Support Service (DASS). Our Student Support Services give counselling, careers and academic support. PGRs have access to the on-line PGRLife, that brings together all the information a PGR needs.

Since REF2014, 271 PhD students have graduated (a 19% increase on REF2014) of which *ca.* 92% have entered employment or further study within 6 months of graduating. Completion rates (within 5 years) have risen from 84% (2010 cohort) to 88% (2014 cohort).

Skills development and preparation for future careers for PGRs

The Unit engages with the Faculty's Researcher Development programme. In 2019 128 PGRs attended, mainly first year, averaging 2.6 courses each. A Graduate Teaching Assistant training course is compulsory and most attend the course on Research Essentials and engage in one or more other courses, including in Impact and Engagement, Career Management, and Wellbeing and Personal Effectiveness. Courses on research integrity and export control are given on-line and are compulsory.

The Unit is involved in multiple CDTs (see section 4) which provide training in interdisciplinary working and additional training in transferable skills.

The University Careers service provides specialist postgraduate support for Chemists and Biological Scientists. This support continues after graduation.

Recognition

Outstanding Achievement Awards (OAAs) are presented during biannual staff symposia to PGRs and PDRAs who have made a major contribution: winners give presentations to the whole Department. For EDI we ensure at least 33% representation among OAA winners from each gender per symposium; BAME researchers win more OAAs than might be expected given the ethnic profile of the unit.

Chemistry PGRs have also received Manchester Doctoral College Excellence Awards: Recent winners include 'Best PGR Output 2019' (Zhang) and 'PGR of the Year 2018' (Kassem). Fifteen PGRs have been awarded EPSRC Doctoral Prizes to transition into independent research.

The Unit proactively supports its PGRs in applying for external awards. For example, since REF2014, Reaxys International Prize 2019 Finalist (Zhang), Salter's Award 2017 (Thomas), Dalton Emerging Researcher 2015 (Chilton) and 2018 (Goodwin).

Equality, diversity and inclusion

A commitment to EDI is embedded in our culture with supporting structures and policies; all staff and students are treated with respect and dignity to enable them to realise their potential. Training courses "*Unconscious Bias*" and "*Diversity in The Workplace*" are compulsory for all staff and attendance is monitored. The Unit holds an Athena SWAN silver award. The University has been awarded the Race Equality Charter (section 3.2, IS).

The Department EDI Committee coordinates and monitors our progress on EDI. The Chair is a member of the Departmental leadership team (where EDI is a standing agenda item). The Committee includes academic and support staff, PDRAs, PG and UG students and is diverse in terms of gender and ethnicity. We also use a biennial survey of staff to monitor attitudes and awareness of EDI. An action plan for EDI initiatives arose from our Athena Swan renewal, which is reviewed by both the EDI Committee and the Leadership Team regularly. We run regular events to highlight the contributions of women and gender-diverse people to STEM.

The DASS assists staff and students in applications for Disabled Student Allowance and Access to Work to fund specific equipment and/or reasonable adjustments required to conduct research. DASS provides a personal plan for each individual, which the Department implements.

There are staff networks across the University, including the LGBT, BAME and Disabled Staff Networks, which directly support staff with protected characteristics.

The main processes for sabbatical leave and secondment were described above. These are monitored in terms of gender and, aggregated over several years, there is an indication that women are less likely to apply. We are discussing with staff the barriers to applying for leave and

are actively seeking applications from women for sabbaticals from 2020 onwards.

The Unit has a strong commitment to flexible working and opportunities for this, along with other University policies, are advertised to staff annually. Many academics use informal flexible working agreements, but formal commitments are increasing to ensure fairness and account for caring responsibilities. Flexible working is advertised in new roles unless impossible. Engagement with UoM peer support groups for new parents is encouraged. We have quiet rooms, where mothers can express milk. We go beyond University policy and offer 12 months PDRA funding to staff on parental leave to help them run their research groups.

Staff and research students returning from leave, including parental leave, review workload with their line manager, to ensure they are supported in the transition back to work. We also support "Keeping In Touch" days so staff do not feel isolated from work whilst they are on leave. We consider and support any flexible arrangements that are necessary for returning staff, responding if their situation changes. Where staff are managing ill health, an on-going review to make necessary accommodations is undertaken with the line manager informed by expert advice from the University's occupational health service.

We monitor gender in promotion and progression; in the period 2014-2019, 12% of promotions were women; this is disappointing but may be due to demographics: we had four female professors at REF2014, as now, and in period we have appointed ECRs who will be promoted from 2021 onwards (see Table 2). This will be monitored closely. Promotion is available to full-time and part-time staff. Circumstances such as maternity leave or illness can be shared by the applicant and are taken into account by the promotion panels. The additional training course "*Recruiting Staff at Manchester*" is mandatory for appointment/promotion panels. The HoD and Deputy (a gendermixed team over the past few years) review staff lists to identify candidates for promotion and pay review to encourage those who might not put themselves forward.

In preparation of our REF submission we followed university procedures for selecting outputs (section 3.4, IS). The submitted outputs have been reviewed through a Equality Impact Assessment and no statistically significant discrepancies could be identified between the submission and the gender and ethnicity profile of our staff.

Support for staff with protected characteristics: Support is embedded in our policies: we employ a Disability Confident scheme in job advertising; have gender-neutral toilets; provide overseas travel guidance; run promotion workshops targeted at underrepresented groups; run Staff Network Groups (ethnicity, religion, ability, parental/caring, gender); have same-sex partner leave for new parents; analyse student questionnaire returns for bias; involve Occupational Health on work conditions; have zero-tolerance "Report & Support" procedures on harassment.

3. Income, infrastructure and facilities

Research funding and strategies for generating research income:

Our strategy is to give creative researchers as much time and support as possible. We have not favoured research that is core chemistry or interdisciplinary: our only consideration is quality. We targeted a culture that is supportive and ambitious. We have minimized unproductive activity as far as possible. Actions during the period include:

- We hired outstanding ECRs and supported them with PhD studentships (two each), start-up funds (typically £20k, but where needed up to £50k) and free access to departmental services. In parallel we set ambitious probationary targets and mentored them to meet these targets. Almost all ECRs (>70%) that started since 2014 have received significant external funding and have published in world-leading journals. Six have won external prizes.
- We made ten Chair appointments to lead in key areas.
- We introduced a detailed WAM to free time for world-leading researchers; typically, they will only offer one lecture course and take final year masters students for research projects. To maintain excellent teaching, we hired outstanding teaching focused staff and we offer them career progression, including promotion to chair.



- We share timely intelligence on external funding opportunities and pro-actively encourage applications to prestigious schemes (*e.g.* ERC or UKRI Fellowships).
- We support significant external proposals (>3 years PDRA funding) with matching funds or posts (*e.g.* PhD studentships).
- We have a rigorous internal peer review process.
- We have upgraded all departmental facilities through EPSRC and BBSRC awards providing state-of-the-art equipment for X-ray diffraction, MS, NMR and EPR spectroscopy, magnetic characterisation and synthetic biology. Services are supported by dedicated research staff to deliver the best possible experiments and training.
- We share successful grant proposals across the Department.
- We run in-house training for grant writing for ECRs.
- We provide excellent administrative support for costing grant proposals and senior administrators to support major funding bids.
- Department studentships and equipment funding are used to generate preliminary results for grant applications. We prioritise the support of ECRs.
- We encourage staff to share manuscripts prior to submission, especially with colleagues with a track record of publishing in high impact journals; high profile papers are a major factor in obtaining external funding.
- Annual P&DRs set ambitious objectives and monitor progress for all staff.
- If a colleague is regularly unsuccessful with funding applications, we assign a mentor, and encourage collaborative proposals to build confidence and expertise.

On 31/07/2020 the Department had the largest EPSRC grant portfolio (£52.8M) and the largest portfolio of active BBSRC grants (£22.2M) of any UK Chemistry department. The Department has also enjoyed a near 3-fold increase in European funding (£44.4M) since REF2014 (£16.5M). This is associated with ERC fellowships. The Brexit agreement should allow high levels of European funding to continue.

Major and prestigious grant awards and links to outputs

During the REF2021 period, the Unit has been awarded multiple prestigious fellowships and grants. Given the high number, Table 3 illustrates one major award per PI in (many hold more than one), and one output per award.

There is a strong link with research outputs. For example, SYNBIOCHEM has produced >460 outputs and Leigh's programme grant "Molecular Robotics" has produced >40 research articles.

Table 3. Illustrative outputs for major and prestigious grants in REF2021 period			
PI	Award	Example high quality research output	
Flitsch	ERC Advanced	Real-time screening of biocatalysts in live bacterial colonies <i>J. Am. Chem. Soc.</i> 2017 , <i>139</i> , 1408.	
Larrosa	ERC Advanced	Cyclometalated Ruthenium Catalyst Enables <i>Ortho</i> -Selective C-H Alkylation with Secondary Alkyl Bromides <i>Chem</i> 2020 , 6, 1459	
Leigh	ERC Advanced	Rotary and linear molecular motors driven by pulses of a chemical fuel. <i>Science</i> 2017 , <i>358</i> , 340.	
Leys	ERC Advanced	Structures of carboxylic acid reductase reveal domain dynamics underlying catalysis. <i>Nature Chem. Biol.</i> 2017 , <i>13</i> , 975.	
Schröder	ERC Advanced	Reversible coordinative binding and separation of sulphur dioxide in a robust metal-organic framework with open copper sites. <i>Nature Materials</i> 2019 , <i>18</i> , 1358.	
N.Turner	ERC Advanced	A reductive aminase from <i>Aspergillus oryzae</i> . <i>Nature Chem.</i> 2017 , <i>9</i> , 961.	
Winpenny	ERC Advanced	Conformational flexibility of hybrid [3]- and [4]-rotaxanes, <i>J. Am. Chem. Soc.</i> 2020 , <i>142</i> , 15941.	



Casiraghi	ERC	Water-based and Biocompatible 2D Crystal Inks for All-Inkjet
	Consolidator	Printed Heterostructures.
		Nature Nanotech. 2017, 12, 343.
Liddle	ERC	Back-bonding between an electron-poor, high-oxidation-state
	Consolidator	metal and poor π-acceptor ligand in a uranium(V)–dinitrogen complex. <i>Nature Chem.</i> 2019 , <i>11</i> , 806.
Mills	ERC	Isolation and electronic structures of derivatized
	Consolidator	manganocene, ferrocene and cobaltocene anions.
		Nature Chem. 2020, https://doi.org/10.1038/s41557-020-
		00595-w
Green	ERC Starter	Design and evolution of an enzyme with a non-canonical
		organocatalytic mechanism.
		Nature 2019 , <i>570</i> , 219.
Leonori	ERC Starter	A Photochemical Dehydrogenative Strategy for Aniline
		Synthesis
		Nature 2020 , 584, 75.
Procter	EPSRC ECF	Metal-Free CHCH-Type Cross-Coupling of Arenes and
		Alkynes Directed by a Multifunctional Sulfoxide Group.
		J. Åm. Chem. Soc. 2016, 138, 790.
Scrutton	SYNBIOCHEM	Conversion of alcohols to enantiopure amines through dual-
		enzyme hydrogen-borrowing cascades.
		Science 2015, 349, 1525.

Organisational infrastructure supporting research and impact

A major refurbishment of the Chemistry building is underway (£55M, 2019-2024). Six floors will have new laboratory layouts. An initial phase has provided a new nitrogen generation facility, loading bay, solvent store and new electrical transformers for the building. The building will remain fully operational throughout.

Support infrastructure

The **NMR service** runs >200,000 experiments *p.a.* on 15 high field spectrometers, supporting >50 research groups from across the University. NMR access is provided for external users including local universities and SMEs (*e.g.* Nanoco, Synthite, BWA, Chromition, C4X, Sci-Tron).

The **MS Facility** provides an analytical service for >100 research groups and runs >30,000 samples per year. The facility has over 20 instruments to cover most requirements, including one of the best accurate mass instruments available, and regularly analyses samples from other N8 Universities and industry (*e.g.* BP, Rolls-Royce, AstraZeneca, Allergan Biologics, Thermo Scientific, and Waters).

The **X-ray Facility** is equipped with the highest performance single crystal diffractometer in the world outside central facilities, in addition to 3 other high-quality single crystal diffractometers, 2 powder XRD instruments and 1 SAXS instrument. >1500 single crystal structures and >7000 powder samples are analysed *p.a.* XRD analysis is also provided to other universities and to industry (*e.g.* C4X, Econic Technologies, Hexcel, Nanoco, AstraZeneca).

The facilities and expertise in the **Organic Materials Innovation Centre** are available to all SMEs, helped by links to the Knowledge Centre for Materials Chemistry. OMIC is currently supported by 18 grants from industry and boasts 162 interactions. Building on a foundation in polymer science, OMIC now also embraces 2D materials.

The Department also maintains an **Analytical and Separations Suite** (Polarimetry, UV-VIS-NIR, FTIR, HPLC, GC), **Microanalysis Service** (CHNS, ICP-OES, Halide, DSC, TGA), and **Glassblowing** (two scientific glassblowers), **Electronic** and **Mechanical Workshops**. Nineteen technical staff are associated with Analytical and Research activities, and eight work in the Mechanical and Electronic Workshops. Staff in the *MIB* enjoy further support from a pool of 44 technical staff. The Unit is actively involved in a technician apprentice programme training *ca*. eight apprentices *p.a*.



UoM has extensive High Performance Computing (HPC), which is extensively used by the CAT research grouping. This includes the flagship, c. 14,000-core Computational Shared Facility, and the c. 4,000-core HPC Pool. This hardware is well-supported by excellent Research IT staff, who also provide chemistry-specific software support, Research Data Storage and Management, Research Software Engineering, and Research IT training. Standard services such as email, cybersecurity and IT purchasing are provided to all University staff and students

Chemistry researchers enjoy strong support from the UoM Library through sector-leading research services, including research data management and research metrics (section 4.2, IS). The Library's 'OA gateway' has been instrumental in maximising compliance with the REF OA policy. Metrics-driven reports enable benchmarking of chemistry research.

Equality and diversity

We follow university guidance on EDI in all training activities (section 4.1, IS). For example, we offer targeted training and mentoring in fellowship and funding applications to under-represented groups. We have a strong collaborative ethos, with collaborative grants accounting for 75% of open grants by value. 32% of our grants have a female PI or Co-I.

All laboratories have disabled access.

Specialist research infrastructure

The **EPSRC UK National Research Facility** for **EPR Spectroscopy** (£4M, renewed in April 2016; led by Collison and McInnes) offers state-of-the-art experimental techniques to >200 users *p.a.* for multi-frequency continuous-wave and pulsed EPR spectroscopy, and associated data modelling. We have a world-leading capability in handling sensitive and radioactive materials, leading to many international collaborations (*e.g.* UC Irvine; EPFL; MIT).

The **DCF** (led by Currell) has capabilities in ion beam and gamma irradiation, material modification and characterisation; these facilities are used by >60 academic and industrial users *p.a.* Dedicated on-site expert experimentalists help users design, develop and deliver experiments and to interpret data and outcomes. Funding (**Royce**, ~£2.2M), has provided new irradiation sources, dissolved gas probes, a TOF-SIMS, a differential centrifuge, and an electron energy loss spectrometer, and a new biolab to facilitate work at the biology interface.

The **Michael Barber Centre for Collaborative MS** (MBCCMS; led by Barran and Lockyer) develops and uses MS, particularly ion mobility MS. The MBCCMS has two SEOs, an EO and four technicians and supports >60 industrial and academic groups. We host 21 mass spectrometers funded by BBSRC, EPSRC, the university and industry. Waters support the MBCCMS Chair (£0.8M) six CASE students and makes in-kind contributions to instrument development (>£1M). Allergan have donated two mass spectrometers to the MBCCMS (£0.7M) as well as two other mass spectrometers to the MS Facility. Industrial users include AstraZeneca, Covance, Allergan, Bristol Myers Squibb, UCB Pharma, Fujifilm: all have funded CASE studentships.

The **CRR** recruited Kaltsoyannis and Liddle to lead, repositioning itself to focus on understanding actinide chemistry rather than environmental radiochemistry. It is now being rebuilt (cost of £8.5M) and will host a NNUF2. Since REF2014 the CRR has continued to train radiochemists and nuclear scientists, repairing a key skills pipeline in a skills-shortage area.

Further specialist infrastructure funded with £3.5M from **SYNBIOCHEM** and £2.2M **Royce** includes: liquid handling robots for high throughput directed evolution and synthetic biology protocols; next generation sequencing; automated colony picking; and analytical instrumentation (5 mass spectrometers and HPLC/SFC).

Collaborative use of research infrastructure including major facilities

For diffraction: macromolecular crystallography was allocated over 900 hours of beamtime at Diamond Light Source (DLS). For small molecule crystallography, 42 days was allocated since 2014, including 6 days for high pressure studies.

For X-ray spectroscopies at DLS: 116 days have been awarded to study MOFs, and a further 74 days to investigate actinide bonding and molecular magnetism. The MOF group also has



beamtime at European Synchrotron Radiation Facility (*ca.* 8 days/year) Oakridge National Laboratory (*ca.* 10 days/years) and Advanced Light Source (*ca.* 8 days/year).

Neutron spectroscopy from the MOF team: 30 days/years split roughly 50:30:20 at ISIS Neutron and Muon source (on TOSCA, IRIS and WISH). For molecular magnetism around 20 days have been awarded on ISIS and at the Institute Laue-Langevin.

Radiochemistry work has been supported at the U EXAFS beamline (at DLS), by one month at the Helmzholz-Zentrum Dresden-Rossendorf for Np and Cm chemistry, and eight weeks at the Central Laser Facility.

The CAT section makes extensive use of ARCHER, the UK's National Supercomputer with >380M allocation units (nominal value \sim £200,000),

Benefits-in-kind

The Unit has had around 40 industrial funded studentships either in full, or in part as CASE or as part of CDTs. In addition, industrial partners are involved in multiple research projects as listed elsewhere. Allergan have formed a fruitful partnership with the MBCCMS, and have donated two mass spectrometers including a Bruker Rapiflex and Waters Xevo QToF (worth *ca*. £0.7M) to the unit.

Industry make extensive use of our research facilities (>20 companies in 2019-20), and these contacts help build impact.

4. Collaboration and contribution to the research base, economy and society

Research collaborations, networks and partnerships and how they deliver impact

The Unit has filed >50 patents and launched 7 spinouts since REF2014.

Within *MIB* there are over 80 funded cross-campus collaborations and ongoing national and international collaborations with over 500 different research institutions worldwide. The *MIB* led 4 of the 13 National BBSRC networks in IB and bioenergy (*NPRONET*, *IBCARB*, *BIOCATNET* and *BIOPRONET*). *MIB* leads the Biocatalysis & Biotransformation Theme for the UK Catalysis Hub (£3.1M; N.Turner).

There is a major collaboration with Shell Global Solutions (Leys lead, £2.4M from Shell, 2016-2021) to develop new biocatalysts to derive novel green production routes to commodity chemicals. Two patents have been filed by Shell (Leys co-inventor) with key papers in *Nature*, *Nature Chem.* and *Nature Chem. Biol.* Several awards co-funded by DSTL and ONRG (over £1.5M) are driving the emerging field of synthetic biological materials.

The research centre **CoEBio3** uses an 'industry club' model to engage with research users and beneficiaries. This model is in its 4th round of funding and typically raises £0.75-1M from 8-10 companies per phase (*e.g.* GSK, AZ, Merck, Pfizer, BAS, Novartis, Syngenta, Dr Reddy's, from a total of 20 over the four phases). This model allows beneficiaries to shape the Centre's research agenda and has led to the impact underpinning the CoEBio3 impact case, 'Sustainable Chemical Manufacturing Through Enzyme Discovery, Biocatalyst Engineering and Education in IB'.

The *DCF* and *CRR* together link the nuclear industry directly and *via* a CDT *Nuclear Energy* – *GREEN*. *DCF* facilities are used by: NNL Sellafield Ltd; EDF Energy; Wood; UKAEA; Rolls-Royce; Createc; Lein Applied Diagnostics; Canberra; Rovtech; Ionix Advanced Technologies; Forth Engineering; ABSL Space Products; Ostara Biomedical; Royston Lead; Applied Photonics Ltd; Croda International; MTA-Atomki; VFE; Precision Acoustics; Mirion Technologies; 30 universities.

Kaltsoyannis has contributed as Co-I and management board member to two multi-disciplinary nuclear consortia. *DISTINCTIVE* (2014-2018, total £8.3M with £4.9M from EPSRC) involved 10 universities and 3 industry partners; winner RSC Industry-Academia Collaboration Award 2020. *TRANSCEND* (2018-2022, total £9.4M with £4.6M from EPSRC) involves 11 universities and 8 industry partners.

These interactions are part of a long-term relationship with the nuclear industry.

OMIC had 162 funded interactions with industry in the period. Industrial collaborators include: BP; ARM; Unilever; Pragmatic Printing; CPI; NeuDrive; Novalia; KDX Ltd; NTU; DataLase Ltd; BEKO plc; International Paint; Solvay; Peptisyntha; 3M; Merck; Airbus; United Technologies; Petronas; Pervatech; Green Biologics; Crown Packaging; Akzo-Nobel; ITM Power; C-Tech Innovation; ACAL Energy; DSTL; Saudi-Aramco. Academic partners include 9 UK and 5 overseas institutions. OMIC strongly contributes to the development of Advanced Materials in the *Royce* through the Chemical Materials Discovery, 2D Materials and Nuclear Materials themes. Development of more sustainable materials is supported by infrastructure investment (*Royce*, £3.6M). OMIC is involved in the *Knowledge Centre in Materials Chemistry* (with Liverpool, Bristol, Southampton, Bolton, STFC and CPI). KCMC has delivered £23.4M in collaborative grant income since 2014 with £5.0M in Manchester.

SYNBIOCHEM (2014-21, £10M from BBSRC and EPSRC) involves >30 academic staff spanning Manchester's Chemistry and 5 further departments, and it involves 3 other UK Universities. Industrial partners include: Syngenta; GSK; LifeTech; Agilent; Croda; BioFocus; Peakdale Molecular; Key Organics; P&G; UCB; Dr Reddy's; Firmenich; UCB; Shell; BioSyntha; Hypha Discovery; Abolis Biotechnologies; Sphere Fluidics; Waters; Unilever; Prozomix/Twist, BDS Biofuels, Waters, C3 Biotech Ltd; Aeirtec; Allergan; AkzoNobel; Bio-Shape; Demuris; DSTL; Fujifilm Diosynth; Genentech; Industrial Biotechnology Innovation Centre (IBIOIC); Pfizer. 157 PhD students were trained in the Centre. 10 patents have been filed and 2 spin-out companies (C3 Biotech Ltd and Manchester BioFactory) have resulted. The Centre is a founding member of the Global BioFoundry Alliance uniting worldwide capabilities in synthetic biology.

The *FBRH* (established 2019, £10.3M, EPSRC and BBSRC; £5.7M, industry; £5M UoM) and involves industrial partners including core members: Allergan, Almac, Arcinova, Biocatalysts, BDS Fuels, Bio-propane producers, BP, Britest, C3Biotechnologies, Calysta, CoEBio3 consortium (8 companies), Croda, GSK, Ingenza, Johnson Matthey, Prozomix, Quorn, Shell, Singer, Sphere Fluidics, Unilever, and Victrex; and associate members: BAE Systems, BPE, Cambridge Consultants, Cogent Skills, DSTL, Dupont LGC, NML, Teijin Films, LabGenius, and Syngenta. Spokes reach out to UCL, Imperial College, Nottingham, UK Catalysis Hub, ICBIOC, and the Centre for Process Innovation.

International partnerships include a UK-Brazil (BBSRC-FAPESP) multi-centre five-year project (2017-2022), total value of £3.2M with £1.1M UoM (Dixon, N.Turner). These connections have led to 'strategic global partnerships' with LATAM research institutions through a cross-disciplinary BEIS/UUKi award, supporting ECRs.

The **EPSRC National Research Facility** for **EPR** collaborates with scientists worldwide, including EPSRC Programme Grant and Fellowship holders (Briggs, Cronin, Rosseinsky, Skabara), ERC grant holders (Arnold, Bogani, Grey, Ingleson, Levitt, Lloyd-Jones, Manners, Morton, Nitschke, Rosseinsky). This has led to *ca.* 250 collaborative publications since 2014, including papers in: *Science* (with Raven, Bristol), *Nature* (with Gray, Cambridge), *Nat. Chem. Biol.* (with Walton, York), *J. Am. Chem. Soc.* (with Parker, Durham; Timmel and Anderson, Oxford; Dincă, MIT).

The **Molecular Magnetism Group** is world-leading and collaborates with groups in the UK, Italy, Spain, the USA, China, Japan, Denmark and Australia. These collaborations are supported by EPSRC Quantera, COST and H2020 FET-FLAG funding.

The Unit is also involved in the EPSRC-funded **Centre in Advanced Fluid Engineering for Digital Manufacturing** (£3.1M) led by Unilever, and also involving Manchester's engineering departments.

The **CDT** in *Integrated Catalysis* (iCAT, £5M, 2019) is funded by EPSRC and industry. Industry partners include those in the UK (*e.g.* AstraZeneca, and GlaxoSmithKline) and abroad (Bayer, Germany). iCAT unites experts in biocatalysis and chemocatalysis, and groups with chemical and process engineering expertise.

We are strongly involved in two further CDTs (2019-27) based in Manchester. *Growing Skills for Reliable Economic Energy from Nuclear* (£6.3M), which will train the next generation of researchers for the nuclear industry, and *Advanced Biomedical Materials* (£6.7M), which has



strong links to biomedical industries. Both show our commitment to interdisciplinary training of PhD students.

We partner in a **CDT in BioDesign Engineering** (£7M, 2019) led by Imperial with UCL and industrial partners, which provides integrated training covering experimentation, automation, coding, data science and entrepreneurship applied to the design, realisation, and optimisation of novel biological systems for diverse synthetic biology/engineering biology applications.

BP-International Centre for Advanced Materials (BP-ICAM) with chemistry-led research (Quayle, Yeates, O'Brien) delivered reduction of wear in automotive engine components. The project was an IChemE Global Awards Oil and Gas Category Finalist, 2017. Another project with Cambridge, Imperial and Illinois Universities contributed to the development of a new fuel additive (Active Technology) for BP Ultimate Fuels.

EPSRC programme grants: 'Molecular Robotics' (£2.95M, led by Leigh; with Cambridge and Bristol), 'Heteroprint' (£5.42M, led by Skabara, Glasgow; involving Yeates and Winpenny, with Sheffield, Cambridge and Strathclyde), and 'SynFabFun' (£4.51M, led by Metcalfe, Newcastle; involving Budd, with Imperial, Bath, Edinburgh, and 11 industrial project partners).

The **International Synthetic Yeast 2.0** consortium (led by Cai) aims to build the world's first synthetic eukaryotic genome. The consortium involving world-leading groups from Johns Hopkins University, New York University, National University of Singapore, Tsinghua University.

The Department is involved in three EPSRC Manufacturing awards: 'Engineering van der Waals heterostructures' (Co-Is: Yeates, Casiraghi) with seven industrial partners; 'Manufacturing at the 7 nm node and beyond enabled by novel resist technology' (PI: Winpenny) with the California Institute of Technology and an industrial partner; 'Formulating and Manufacturing Low Profile Integrated Batteries for Wireless Sensing Labels', (Co-I: Yeates) involving four industrial partners.

Leigh is funded by a H2020-FETOPEN project (2017-2021) "Mechanics with Molecules"; this collaborative project involves the Universities of Dresden (Germany), Graz (Austria), Liège (Belgium) and research institutes CNRS (France) and CSIC (Spain) to develop single-molecule machines and test their operation on surfaces.

Consultancies and training

In addition to major industrial collaborations listed above, staff have consulted across many sectors, including pharmaceuticals (AstraZeneca, GlaxoSmithKline, Merck, Novartis, Boehringer Ingelheim), crop protection (ADAMA), energy (BP), general science (DSM), fine chemicals and custom synthesis (Syntor, MOF Technologies), biopharmaceuticals (Gilead Sciences, Lonza, Antabio), genomics (BGI), and instrument developers (Oxford Instruments).

Staff have also provided training courses in industry, *e.g.* Leonori (Syngenta), Procter (GlaxoSmithKline).

Contributions to economy and society and engagement with diverse communities and publics

Our largest contribution is in IB (see impact case for greater detail). **CoEBio3** researchers created training courses in IB including 'Biocatalytic Retrosynthesis', delivered as continuous professional development to chemists at AstraZeneca, GSK, Gilead, Novartis and Lonza. To accompany, they produced a book, "*Biocatalysis in Organic Synthesis: The Retrosynthesis Approach.*" (2018, >500 sold) and a computational tool (RetroBioCat: <u>www.retrobiocat.com</u>) downloaded >550 and read >1600 times on chemrxiv.org (on 23/10/20).

Researchers from **CoEBio3** are members of the IB Leadership Forum and co-authored parts of the report "<u>Growing the UK Industrial Biotechnology Base</u>" (2018), which is now the guiding document for UK Bioeconomy policy – with a goal of the 2030 bioeconomy being double the size from 2018.

An "Advanced Materials from Synthetic Biology" roadmap was commissioned from Scrutton by the Office of Naval Research (*Syst. Synth. Biotech.* **2018**, *3*, 105) and is used in the USA.

We are founding members of **CAMS** an industry-led initiative to promote world-class analytical science training, research and innovation by bringing together 12 industrial and 8 academic partners.

Barran's group detects biomarkers for PD, funded by Parkinson's UK and the Michael J. Fox Foundation. Their clinical trial is the largest metabolomics study of PD (>1800 samples). The first results (*ACS Cent. Sci.* **2019**, *5*, 599) attracted great media attention (*e.g.* a Canadian and three BBC documentaries, and future National Geographic film).

Since 2017 our MS facility has worked with the Department of Food and Environmental Protection Section of International Atomic Energy Agency and the UN on implementation of the UN programme of MS measurements of food samples from developing countries.

Since 2017 we have communicated our research directly *via* a YouTube channel: <u>https://www.youtube.com/channel/UCXf3CFkyGpa2eleT5wz Prw</u>. The videos have been viewed >148,000 times.

We have a strong culture of schools' liaison, including hosting >20 Nuffield students. We created outstanding MOOCs in Physical Chemistry (60,300 enrolled, winner RSC Higher Education Prize 2015) and Molecular Spectroscopy (30,214 enrolled) and IB (>44,000 enrolled). >800 A level students attended *MIB* Open days, whilst our multilingual science program provides interactive IB science sessions to language schools in Manchester.

Presentations were made at the Royal Society Exhibition (Complex Life of Sugars, 2016, Flitsch and Field) and New Scientist Live (2016-18) and at the European Open Science Forum (Manchester 2016). Annual events collectively reaching >8,000 participants include: Great British Bioscience Festival; National Science and Engineering week; Manchester Science Festival; Birmingham Big Bang Fair (Micklefield); and #ScienceX (Trafford shopping centre). Casiraghi worked with composer Sara Lowes to create "the Graphene Suite" and *MIB* has worked with artists in residence (Karen Barber and Lynne Chapman 2016) to create science-based art works displayed at outreach events nationally and in local exhibitions.

Contribution to sustainability of discipline

Significant roles in learned societies include leading contributions to the RSC:

RSC Council 2014-2019 (Flitsch), Faraday Division Council (McInnes, Dryfe), RSC Organic Division Awards Committee (Leigh, Procter), RSC Faraday Division Awards Committee (Casiraghi), Chair of RSC Organic Division Poster Symposium (Procter), RSC Chemical Biology Bioorganic Group (Webb and Wong), Chair of RSC ESR Group (McInnes), Chair of RSC Electrochemistry Group (Dryfe), RSC Radiochemistry Group (Natrajan), and the RSC Nucleic Acid Group (Micklefield).

Members of Academia Europaea (Leigh, Schröder), Liddle (Vice-president of the European Rare Earth and Actinide Society); Anderson (International Zeolite Structure Commission), Leigh (Honorary Membership of the Israel Chemical Society).

Since REF2014 the Unit trained *ca*. 8% of the UK's PhD chemists on average *p.a.*, and >100 of our PDRAs have moved into academic positions worldwide. This is a major contribution to the discipline.

Influence, contribution and recognition

Fellowships:

Since REF2014, Unit staff have been awarded an RS Research Professorship (Leigh) and 33 Fellowships: ERC AdGs (Flitsch, Larrosa, Leigh x 2, Leys, Schroder, N.Turner, Winpenny), ERC CoGs (Casiraghi, Ingleson, Layfield, Liddle, Mills), ERC StGs (Green, Leonori, Mutti), EPSRC Established Career (Liddle, Popelier, Procter, Winpenny), EPSRC Early Career (Leonori), RS University Research (Chilton, De Bo, Riddell), RS Dorothy Hodgkin (Bowen), BBSRC David Phillips (Dixon, Green), EPSRC Foresight Fellowship in Manufacturing (Webb), Human Frontiers Science Program Cross-Disciplinary (Baker), SCI Ramsay Memorial (Chilton, Keerthi), BBSRC Future Leader (Van Munster), UKRI Innovation (Lovelock), and Leverhulme Trust Research (Tuna).

Prizes

Since REF2014, we have received many accolades including election to FRS (Morris, 2014; Scrutton 2020; N.Turner 2020) and FREng (O'Brien, 2016), and the award of a CBE (O'Brien, 2016). Manchester Chemistry won more RSC prizes than any other institution in 2019 (6 prizes) and 2020 (8 prizes); in addition, Kaltsoyannis was part of the **DISTINCTIVE** consortium, awarded the RSC 2020 Industry-Academia Collaboration prize. Table 4 lists the 32 RSC awards won by 26 different academics since REF2014. Table 5 lists further prizes.

Table 4. Manchester Chemistry-based RSC Prize Winners			
2020		2017	
Bures	Hickinbottom	Greaney	Bader
Casiraghi	Gibson-Fawcett	Leigh	Perkin
Flitsch	Bioorganic	N.Turner	Stereochemistry
Green	Harrison-Meldola		2016
Liddle	Tilden	Chilton	Dalton Young Researcher
Procter	Charles Rees	Denecke	Becquerel
Schröder	Nyholm	O'Brien	Longstaff
Yang	Harrison-Meldola	Winpenny	Ludwig Mond
	2019	Yeates & Winpenny	Emerging Technologies
Barran	Theophilus Redwood		2015
Larrosa	Corday-Morgan	Liddle	Corday-Morgan
McInnes	Tilden	Natrajan	Bill Newton
Micklefield	Bader	O'Malley	Higher Education
Mills	Bill Newton	Procter	Bader
Scrutton Interdisciplinary		2014	
2018		Casiraghi	Marlow
Leonori	Harrison-Meldola	Flitsch	Interdisciplinary
Mills	Harrison-Meldola	Leigh	Pedler
Goodwin	Dalton Young Researcher		

Table 5. Further major prizes			
2015	Cai	Wellcome Trust, Frontier Innovator Award	
	Faulon	Scientific Excellence award from the French National University Council	
	Leys	RS Wolfson Merit Award	
	McInnes	International EPR Society Medal for Chemistry	
	Morris	James N Shoolery Prize	
	Procter	Liebig Lectureship, German Chemical Society	
2016	Casiraghi	Philip Leverhulme Prize	
	Leonori	European Young Chemist Award, Silver Medal	



	Leonori	UNESCO/IUPAC/ PhosAgro Green Chemistry Award
2017	Schröder	Honorary Doctorate from the Nikolaev Institute of Inorganic Chemistry, Russian Academy of Sciences
2018	Adams	BRSG - NMR DG Annual Prize for Excellent Contribution to Magnetic Resonance by an ECR.
	Popelier	Inaugural Richard FW Bader International Prize for Excellence in Electron Density Research
	Bures	Young Researcher Award from the Spanish RSC
2019	Chilton	Olivier Kahn International Award, The European Institute of Molecular Magnetism
	Larrosa	Blavatnik Award Finalist
	Leigh	Nanoscience Prize, International Society for Nanoscale Science, Computation and Engineering
	Leonori	Philip Leverhulme Prize
	Leonori	AstraZeneca Award for Outstanding Achievements in Organic Synthesis
	Liddle	Alexander von Humboldt Friedrich Wilhelm Bessel Research Award
	Yang	CCDC Chemical Crystallography Prize for Younger Scientists
2020	Collison	Bruker Prize for EPR Spectroscopy

17 Unit staff have held Visiting Professorships at top overseas institutions.

Chemistry staff have delivered over 1200 lectures since REF2014 at universities (>660) and conferences (>560). Staff have chaired the organising committees of >30 international conferences and symposia.

24 Unit staff are members of the EPSRC College, 5 have sat on BBSRC funding panels and 20 on EPSRC funding panels and have served as Panel Chair 4 times. Staff referee for funding organisations in >30 countries, with 27 refereeing for the ERC.

Unit staff have served as Editors for journals including; Chemical Science (Leigh); FEBS J (Scrutton); Progress in Nuclear Magnetic Resonance (Morris); Beilstein Journal of Organic Chemistry (Flitsch); Natural Products Review (Takano); ACS Omega (Takano); Springer Nature's Cancer Nanotechnology (Currell); ACS Biomaterials Science and Engineering (Takano); Metabolomics (Goodacre).

A further 24 staff have served on journal Editorial Advisory Boards or as Guest Editor of special issues.

Co-operation and collaborative arrangements for PGR training

We lead a CDT in Integrated Catalysis and are involved in three further CDTs running on 31/07/2020 (see p19). We were also involved in CDTs in **Materials for Demanding Environments**, **Next Generation Nuclear** and **Nanoscience** in Manchester since REF2014.

We have an established 2+2 programme with Singapore and have established a Flagship 5-year (2020-2029) 2+2 Programme with Tsinghua (see section 2).

Flitsch led the *GlycoBioM* consortium (finished 2015) and is Co-I on Chem21 within the Innovate Medicines Initiative (2012-2017). Scrutton led a Marie Curie ECR ITN training Centre '*MAGIC*' (2014-2018), training 12 PhD students. Membership of Marie Curie ITNs: *PoliMer* (Field); *Sweet Crosstalk* (Field); *GlycoVax* (Flitsch); *TINTIN* (Flitsch); *Immunoshape* (Flitsch); *PIPPI*



(Golovanov); **SASSYPOL** (Leigh); **EURO-SEQUENCES** (Leigh); **BIOMOLMACS** (Leigh); **PhotoReact** (Leonori); **Masstrplan** (Pitt).

Liddle chaired a COST Action (CM1006 – EUFEN, >120 groups from 22 countries) providing 4 training schools/conferences in f-element chemistry (2012-2015). Larrosa is a member of the Management Committee of an EU COST Action on C-H activation in Organic Synthesis (CHAOS) (2015 – 2020). We are members of COST actions in molecular magnetism (several groups) and mechanochemistry (De Bo).

The EPSRC EPR NRF trains 30-50 PGRs per year, including week-long residential courses. This has also been delivered in Brazil and Australia.