Institution: Cardiff University

Unit of Assessment 8: Chemistry

1. Unit context and structure, research and impact strategy

1.1 Context and structure

The School of Chemistry is a leading research centre committed to an ethos of rigorous interdisciplinary research in the chemical sciences, underpinned by outstanding research facilities and infrastructure. Our mission is to create fundamental scientific understanding and societal impact, through our ambitious strategy of delivering innovative research in collaboration with a wide range of international partners. Following our highly ranked REF2014 submission, and having achieved a strong performance in delivering education and impact through research, Chemistry was identified by Cardiff University (CU) as a key priority area for investment. Consequently, the School has grown considerably since REF2014, delivering a 20% growth in research active staff, resulting in 44 Category A staff (39.35 FTEs) (Section 2.2).

The School has successfully grown research income over recent RAE/REF cycles (**£49.7M in REF2021** compared to £27.7M in REF2014 and £13.8M in RAE2008) leading to our highest ever cohort of PDRAs and PGR students. This has been supported by a multi-million pound investment by CU into refurbished laboratory space, as well as expansion into a **£131M Translational Research Hub** in Spring 2022 (Section 3). Over this REF period the School produced **2100 publications**, delivered a range of impact (see Impact Cases and Section 4), was awarded the first ever **Regius Professorship** in Wales, played leading roles in national research initiatives (e.g. **UK Catalysis Hub, National XPS Centre**), established the UK's first **Max Planck Centre** in the Physical Sciences, engaged with national and international scientific communities through organised conferences and outreach, and embraced the principles and practices of DORA whilst embedding all these activities within a **culture of inclusiveness**.

Following REF2014, the School was transformed from a traditional Inorganic, Organic, Physical (IOP) structure into five new research sections (see below) to take advantage of our strengths and renewed opportunities. At the July 2020 census, the current and former (*underlined*) academic PI staff members, along with current PDRAs and PGR students, in these sections are:

- **Biological Chemistry** PIs: *Allemann, Jin, Luk, Loveridge, Pickett,* ***N.Richards (Head)****, Tredwell, Tsai*. PDRAs: 17; PhDs: 24; Publications (in REF period): 234; Patent applications: 1; Grants: £6.85M.
- **Catalysis & Interfacial Science** PIs: *Bartley, Bowker, Catlow, Davies, Dimitratos, Hammond, Edwards, Golunski, He, Hutchings, Kiely, Logsdail, Meenakshisundaram, Roldan-Martinez,* ***Taylor (Head)****, Wass, Willock*. PDRAs: 23; PhDs: 76; Publications: 621; Patent applications: 11; Grants: £25.06M.
- **Materials & Energy** PIs: *Easun,* ***Harris (Head)****, de Leeuw, Dzade, Leoni, Paul, Hatcher, Nanavati, Wu*. PDRAs: 6; PhDs: 13; Publications: 617; Grants: £8.62M.
- **Molecular Synthesis** PIs: *Amoroso, Bonifazi, Browne, Buurma, Casini, Fallis, Melen, Morrill, Newman, Pope, Ward,* ***Wirth (Head)***. PDRAs: 10; PhDs: 52; Publications: 423; Patent applications: 2; Grants: £4.52M.
- **Spectroscopy & Dynamics** PIs: *Beames, Carpenter, E.Richards, Knowles,* ***Murphy (Head)****, Platts, Polyak*. PDRAs: 3; PhDs: 17; Publications: 204; Patent applications: 1; Grants: £4.6M.

Additionally, cutting across and drawing membership from all these research sections, catalysis research is delivered through the flagship **Cardiff Catalysis Institute** (CCI) (Director: *Hutchings* 2008-19, *Wass* 2019-), designated a **University Research Institute** (URI) in recognition of its international achievements and reputation. Since 2014, catalysis research through the CCI has collectively raised over £28M and generated over 850 publications from across all research sections in the School, serving not only as a driver for catalytic science, but also enabling staff to collectively form unique partnerships that address diverse multidisciplinary research challenges. In the current REF cycle, computational chemistry (led by *Catlow*) has considerably strengthened the core CCI disciplines. The CCI is now one of the lead institutions for major international catalysis

initiatives, including the **EPSRC UK Catalysis Hub**, **Max Planck Society Maxnet** on Energy (2015-20), **Max Planck Centre** in Catalysis (2020-25) (Section 4) and hosted the **EPSRC CDT in Catalysis** (2014-2022).

1.2 Research strategy

Our strategic vision is to advance interdisciplinary research through the fundamental and basic understanding of chemistry. Our School is committed to solving significant societal challenges, whilst contributing to national economic growth through new discoveries. Several research areas were already well established in REF2014, particularly Catalysis and Chemical Biology, and we have since grown considerable strengths in other areas including Materials, Synthesis, Spectroscopy and Computational Chemistry. Since REF2014, all research sections have flourished, driven by **strategic and diverse academic appointments** (Section 2.2). Substantial improvements in **core instrumentation and space** (Section 3) have provided new world class facilities, underpinning our success and leading to the dramatic increase in postgraduate research student numbers. Building on these existing core strengths, **six new cross disciplinary priority Research Themes** (**RT**), will drive our continued growth over the next REF period. These multiple themes, to which all staff contribute, represent agile groupings with a critical mass of researchers, ready to respond to cutting edge and future challenges in the chemical sciences:

- **RT1 Catalysis:** This theme spans biological, homogeneous and heterogeneous catalysis, underpinned and supported by theory and characterisation, with broad expertise across the discipline that expands beyond traditional catalysis silos to deliver research of fundamental and technological importance. Areas of specific and targeted growth include catalysis for environmental remediation, water treatment, methodologies for fine chemical synthesis, new materials, and decarbonisation of petrochemicals and fuels (including CO_2 conversion, sustainable synthetic fuels and intermediates, clean oxidations and hydrogenations, replacement of toxic, precious, or geopolitically-unfavourable metals). Working with partners in industry (producing 27 industry-funded projects since 2014), we exploit this research to deliver innovation and impact through the development of new catalytic processes. **Selected publication highlights include**: Small molecule activation by intermolecular frustrated Lewis pairs; Identification of single-site gold catalysis in acetylene hydrochlorination; Stable amorphous georgeite as a precursor to a high-activity catalyst; Efficient green methanol synthesis from glycerol; Aqueous Au-Pd colloids catalyse selective CH_4 oxidation to CH_3OH with O_2 under mild conditions.
- **RT2 Biological chemistry:** This theme focuses on a range of problems at the interface of chemistry, biology, medicine, and ecology. School specific strengths exist in biocatalysis, mechanistic enzymology, bioorganic and bioinorganic chemistry, synthetic biology and biomolecular interactions, biomolecular NMR and MS, biophotonics and optogenetics, medicinal chemistry, organic synthesis, pheromones and other semiochemicals of plants. **Selected publication highlights include:** Chemical ligation and isotope labelling of dynamic catalysis effects by DHFR; Chemoenzymatic assembly of isotopically labelled folates; Investigation of structural rearrangements of the Ca^{2+} and voltage-activated (BK) channel; Optically switchable regulation of protein function in live mammalian cells; Plasmodium-associated changes in human odour attract mosquitoes; Formation of hexacoordite Mn(III) in Bacillus subtilis oxalate decarboxylase.
- **RT3 Hierarchical functional materials & energy:** Research here focuses on the tailored synthesis of organic-and inorganic-based materials and their study as functional architectures, for engineering light-harvesting systems, storage and conversion of energy, optoelectronic devices, sensing and molecular imaging. Areas of unique strength include organic synthesis of pi-conjugated molecular graphenes, polymer mediated drug-delivery systems, flame-retardant polymers, functional nano-fluidic devices, chemistry and physics of solid inclusion compounds, dynamic properties of crystal growth mechanisms, and metal-organic frameworks (MOFs). **Selected publication highlights include:** Borazino-doped polyphenylenes; Synthesis of the first BN-doped nanographene; Population and hierarchy of active species in Au-Fe oxide catalysts; Complexation of polyoxometalates with cyclodextrins; G-quadruplex organic frameworks for light-harvesting; Determining molecular orientations in disordered materials.

- **RT4 Computation & modelling:** Within this theme, emphasis lies in the development of computational methods for electron correlation, electron density analysis, QSAR, advanced methods of molecular dynamics and importance sampling, thermal and electronic transport calculations, correlated and many-body methods applied to the solid state. There is a strong interest in software development, and in the effective exploitation of high-performance parallel computers, supporting our research in adsorption / reactivity of oxide and metallic surfaces, microporous materials, mechanistic studies of organic reactions, structure and function of bio-molecules, proton exchange and transport in solutions, simulation of drug-receptor binding, and simulation of phase transformations in solids. **Selected publication highlights include:** Bio-inspired CO_2 conversion by FeS catalysts; Understanding the role of molecular diffusion in liquid-phase Beckmann rearrangement; Revealing the unique mechanism of Au-NHC compounds binding to DNA G-quadruplexes; Polaritonic coupled-cluster theory.
- **RT5 Enabling technologies for sustainable synthesis:** This theme impacts not only on chemistry, but also fosters new interdisciplinary collaborations with engineering, mathematics, and computer science. It achieves a deeper understanding of modern chemical organic synthesis tools (e.g. flow chemistry, mechanochemistry, electroorganic synthesis) by integrating with robotics, AI and machine learning to demonstrate expedient and automated discovery of new materials. Collaboration with computer scientists enable the interfacing of discovery platforms with remote touchscreen intelligent control and programming robotic devices to execute bespoke optimising algorithms, for rapid learning and discovery. **Selected publication highlights include:** Providing a quantitative approach to predict rate constants for aqueous racemisation; Use of mechanochemistry to alter reaction kinetics; Machine-assisted syntheses of substituted Ir(III)-pyrazolate luminescence complexes; Electrochemical generation of hypervalent iodine; An easy-to-machine electrochemical flow microreactor.
- **RT6 Development of advanced spectroscopies:** Here we focus on the development and applications of advanced spectroscopic and characterisation techniques, to unravel fundamental properties of materials and biostructures, including a new X-ray birefringence imaging technique, new powder X-ray diffraction methods as well as *in situ* SS NMR studies for structure determination from non-crystalline materials, time resolved and perturbation methods in EPR, and cavity enhanced laser spectroscopies. We apply these developments to mechanistic understanding of chemical and biological pathways in catalysis, understanding structure and dynamics of reactive intermediates, selective detection of trace atmospheric gases and radicals. **Selected publication highlights include:** development of a new EPR microwave resonance cavity; Infrared-driven unimolecular reactions of CH_3CHOO Criegee intermediates; *In situ* K-edge X-ray absorption of single-site Au/C catalysts; X-ray birefringence imaging; The role of peroxy radicals in benzaldehyde oxidation; An *in situ* NMR strategy for mapping time-evolution of crystallisation processes.

School research leadership is provided by the Research Committee (RC), chaired by the Director of Research (DoR), with the Head of School (HoS), Director of PGR Studies (DPGRS), Director of Impact (DoI), Heads of Sections, Research Support Manager and School Manager, as well as ECR and Safety representatives. Since REF2014, the RC has expanded to include safety and Equality, Diversity and Inclusion (EDI) as standing agenda items, fully embedding them within our research culture. Research is a central agenda item at regular senior management meetings.

1.3 Progress against REF2014 research strategy and future five-year plan

Progress in successfully implementing our REF2014 strategic aims are summarised as follows:

1. *To recruit further high-quality academic staff to expand critical mass in Biological and Synthetic Chemistry (both organic and inorganic):* From 2014-2020, we recruited high-quality full-time staff (Section 2.2) and **gained critical mass in all research sections**, particularly Biological Chemistry, Molecular Synthesis and Materials. Appointments include Chairs in Medicinal Chemistry (*Casini*), Biological Chemistry (*N.Richards*), Organic Supramolecular Chemistry (*Bonifazi*) and Catalysis (*Wass*). Other recruitments include academic staff in Biological Chemistry (*Jin, Luk, Tsai, Tredwell*), Molecular Synthesis (*Browne, Melen, Morrill*), Catalysis (*He, Logsdail, Roldan*); Spectroscopy and Dynamics (*Beames, E.Richards,*) and Materials (*Easun, Wu*). Additional part-time appointments (*Catlow FRS, Pickett FRS, Kiely*) and fixed

term ECRs (*Dzade, Hatcher, Nanavati, Polyak*) were also made, creating a **sustainable research culture** that is supportive of staff at every career stage.

2. *To attract and support high-calibre researchers by externally funded fellowships:* Many of our **ECRs were awarded prestigious Fellowships** including those funded by the Royal Society (*Hammond, Easun, Hatcher*), UKRI (*Melen, Dzade, Logsdail*) and Wellcome Trust (*Jin*).
3. *To increase recruitment of high-calibre and international students to postgraduate research (PGR) and postgraduate taught (PGT) degree programmes*. **PGR student numbers and applications have doubled since REF2014**. **PGT numbers have grown to approximately 40 p.a.**, following the introduction of new programmes in Medicinal Chemistry and Advanced Chemistry, complementing our existing programmes in Catalysis and Biological Chemistry. This was achieved through increased grant funding (e.g. Catalysis CDT), and by establishing dedicated PGR support (Section 2.8).
4. *To extend our equipment base and facilities*. Central to the expansion of the School, **CU invested over £7.8M** in Chemistry to support new research infrastructure and facilities since REF2014, including new SAX instrumentation, high-field liquid and solid-state NMR, and expanding MS services. Responding to the growth in research activity and academic recruitment, extensive **new research space (>1065 m^2)** was created, and **existing space** was repurposed **through a further £3.15M refurbishment investment** (Section 3.2).
5. *To relocate the School in a new purpose-designed building:* A new ***Translational Research Hub - TRH*** (opening Spring 2022) will act as a hub for fundamental science, with translation into application realised and delivered by co-location with industrial partners. **This £131M project**, part of CU's >£300M Innovation Campus investment (see REF5a), will deliver internationally leading, bespoke facilities for the School's catalysis research (150 researchers) and *state-of-the-art* equipment; e.g. in situ AC-STEM funded by Welsh European Funding Office (WEFO) and Wolfson Foundation (Section 3.2).

Following the successful outcomes of our RAE2008 and REF2014 research plans, over the next five years we will rise to the challenge and deliver the next stage of our strategic objectives. We will continue to grow the School and strengthen our wider influence, impact and standing based on the successful implementation and achievements of the following five key pillars:

1. To invigorate and strengthen, through strategic staff appointments, the success of **our six priority research themes**;
2. To sustain and foster **our culture of innovation**, driven by high impact research, and by deploying the full potential of the TRH facility as a platform for collaboration with industry, delivering new spin-outs, patents, licencing and consultancy activities;
3. To develop and innovate **our PGR/PGT programmes** to meet the changing and dynamic needs of the modern chemistry sector, offering new academic and research opportunities, such as Chemical Ecology, and an MBA in Chemistry;
4. To intensify and enhance **our civic mission** towards the Welsh economy, society and health, through engagement with the Welsh Government (WG) and partner organisations;
5. To drive and shape **our future research agenda** in interdisciplinary science in Wales and the UK, by becoming lead partners on large scale research grants & major international strategic partnerships, and through committee participation and elected Fellowships of Learned Societies.

1.4 Research impact

Impact is a high priority strategic area for the School, overseen by the DoI who Chairs the Impact Committee, providing an effective support mechanism to introduce best practice. Impact is central within the Personal Development Review (PDR) of individual staff, with emphasis on identifying opportunities and development resources (including rewarding impact-active staff in workload allocation (Section 2.6). A healthy and dynamic pipeline of impact cases is monitored by the DoI, ensuring nascent cases are supported appropriately (examples in Section 4.3). For research within the URI remit, impact is facilitated by bringing together diverse researchers with

key stakeholders. The CCI has outstanding industrial links with a strategic focus on translation of fundamental research into application.

1.5 Interdisciplinary research

A culture of interdisciplinary research is successfully delivered in the School, directly evidenced by our research themes, and facilitated through the RC (Section 1.2). The DoR participates in College and University Research Forums that remove barriers and strengthen collaborations between the CU disciplines. Demonstrating the vitality of interdisciplinary research, Chemistry staff lead two CU **Interdisciplinary Doctoral Training Hubs** themed on *Sustainable Plastics* and *Biosensors and Diagnostics*, reaching across several Schools to create two new student cohorts. Chemistry collaborates with the schools of Architecture, Biosciences, Computer Science & Informatics, Dentistry, Engineering, Mathematics, Medicine, Pharmacy & Pharmaceutical Sciences, and Physics & Astronomy. We are lead partners in the CU **Materials Network** and the **Cardiff Institute for Tissue Engineering Research** (CITER).

In addition, URI networks (including the CCI) act as a focal point for interdisciplinary research in key areas of strength. For example, a URI on water research brings together biology, ecology, engineering, social science and external stakeholders (Welsh Water), with chemistry-led projects on water treatment (e.g. *Easun, Hutchings*). We have also made a joint academic appointment (*Tredwell*) with the Wales Research and Diagnostic **Positron Emission Tomography Imaging Centre** (PETIC), strengthening biological chemistry research.

1.6 Open Access (OA)

The School is compliant with all funder requirements and Concordat on Open Research Data, ensuring full online access to scientific information (free of charge to end-users). Open data is managed through CU *Converis* system, with mandated datasets assigned a unique DOI. The Open Access Coordinator) manages OA for the School, overseeing training, recording and ensuring compliance with funders' requirements. All post-print files and bibliographic details for outputs are held in CU's digital publications repository. 100% of Category A staff are registered on ORCID.

1.7 Research ethics and integrity

Research Integrity training is mandatory for all academic staff and PGR students. We comply with all ethics protocols, while our Ethics Officer is responsible for managing ethical issues through the School's Research Ethics Committee. The Ethics Officer monitors procedures, reviews issues, ensures researchers receive correct documentation, and conducts three-yearly reviews, reporting outcomes to the Cardiff University Open Research Integrity and Ethics Committee (ORIEC). The School's Research Ethics Committee also considers research proposals involving human participants, human material or human data. Researchers regularly update the Committee for monitoring, providing written reports to comply with standard accountability procedures, with a retrospective review on project completion.

2. People

2.1 Staff development strategy

The School developed a **strategy to enable all staff** (regardless of grade or career pathway) to attain their full potential, by providing access to a range of professional and personal training courses, including wellbeing and mandatory courses in EDI and Unconscious Bias. At institutional level, CU became a *Global Stonewall Diversity Champion* in 2019 and the top UK University in the ranking for the fourth year running, climbing to 10th place in the *Top 100 Employers List*. CU has held an Athena SWAN Institutional Bronze award since 2009, and recently created Deans for Research Environment & Culture, and EDI (2019). CU also has a network for LGBT+ staff and postgraduates, entitled *Enfys* (see REF5a). Our School holds an **Athena SWAN Bronze award** (2019), with a clear action plan implemented through our EDI committee. In 2018, CU introduced a mandatory *Leadership & Management* training course for senior staff (including Professors and Senior Line Managers), which all Chemistry senior staff have completed. ECRs take an additional *Academic Practice* training programme, leading to Fellowship of the Higher Education Academy (FHEA). Upon successful completion of probation, all staff participate in an annual PDR, receiving

regular guidance and support for career progression; overall the School has >98% annual completion rates (in the past five years). The School has provided funding for two female academic staff to attend the *Aurora National Leadership Programme*, designed for HE institutions to take positive action to address the under-representation of women in leadership positions in the sector.

2.2 Staffing and recruitment strategy

The School has expanded considerably since REF2014, strategically recruiting new staff across all career stages, growing capacity in our research themes, whilst also **ensuring robust succession and progression planning**. Currently the School hosts 44 research active T&R academic staff, increasing from 35 in REF2014, supported by a further five FTE academic staff on the T&S career pathway.

Following REF2014, the School identified staff retiring and leaving as a prodigious opportunity to progressively revitalise research activity, strategically recruiting many new staff to underpin the five research sections and establish the new innovative research themes (Section 1.2). Recruitment expansion was also facilitated in-part through a **CU staff and capital investment plan** (£7.8M). Strategic new appointments were made in Biological Chemistry (two Professors, *N.Richards, Casini* and four ECRs, *Jin, Luk, Tredwell, Tsai*), Organic/Inorganic/Materials Chemistry (one Professor, *Bonifazi* and five ECRs, *Browne, Easun, Melen, Morrill*, *Wu*), Catalysis (one Professor, *Wass* and three ECRs, *He, Logsdail, Roldan*) and Spectroscopy (two ECRs, *Beames, E.Richards*), all supporting our research themes. Simultaneously, a number of new part-time appointments of renowned scientists were also made, including *Catlow FRS* (Catalysis), *Kiely* (Electron Microscopy) and *Pickett FRS* (Chemical Biology), whilst *Bowker, Carpenter* and *Hutchings FRS* were retained in their senior positions. We also recruited two independent software engineers (*Nanavati, Polyak*) and two externally funded Research Fellows (*Dzade, Hatcher*).

As a consequence of the strongly supportive research environment in the School, the accomplishments of some staff appointed since 2015 has facilitated their move to prestigious new academic positions in the current REF cycle, including *de Leeuw* (PVC-Leeds), *Bonifazi* (Vienna) and *Casini* (Munich). We are also proud that we facilitated ECRs to achieve their career choice to take up positions in other Schools outside Chemistry including *Browne* (Pharmacy, UCL), *He* (Material Science, NU Singapore) and *Hammond* (Chemical Engineering, Imperial). We have a clear strategy for replacement appointments, with recent examples including a Chair in Catalysis (*Pera-Titus,* September 2020) and a Medicinal Chemistry Lecturer (*Serpi,* October 2020), with more appointments to follow.

In 2015, we introduced changes into the text of our job adverts, to include positive statements about gender equality, inclusivity, and flexible working policies to facilitate staff to achieve a good work-life balance. Academic recruitment panels now include at least one female staff member. Importantly, the HoS writes to all academic position candidates following their interview, giving detailed feedback on their performance at interview.

The average age of our academic staff has decreased significantly since REF2014 (84% of staff are below 60 years, with 52% under 50 years.), demonstrating the **long-term vitality of our environment**. In addition to our nurtured home talent, we have a large number of international staff (c*a*. 30%) coming from 13 different countries. Commensurate with this growth in staff, the School has seen a progressive increase in the total number of PDRAs; up from 52 at census date in REF2014 to a maximum of 74 during this REF cycle. After recruiting 13 ECRs onto fixed-term University Fellowships in 2014-15, all were converted to open ended permanent positions, and four were additionally promoted to SL or Reader. All of our ECRs successfully secured funding in this REF cycle including multiple UKRI responsive mode grants. The School thus continues to build its reputation as a place for **nurturing new talent**.

2.3 Supporting ECR staff

Training courses specifically targeted at PDRAs and ECRs are available, with participation strongly encouraged. PDRAs are given the opportunity to develop their academic skills, by assisting in undergraduate (UG) workshops, through delivery of laboratory-based classes and through the School's *Post-Doctorate Lecture* programme. Occasionally, senior PDRAs with a demonstrable aptitude for teaching are given responsibility for delivering UG lecture components;

some have successfully moved to new academic posts (e.g. *Freakley*, Bath; *Kondrat*, Loughborough; *Miedziak*, South Wales; *O'Malley*, Bath; *Terranova*, Buckingham*; Wilcox*, Manchester).

Fellowship applications are thoroughly supported by the School, including the provision of practice interviews. During the REF period, **seven ECRs were awarded externally funded Fellowships** from the Royal Society (*Hammond, Easun, Hatcher*), UKRI (*Melen, Dzade, Logsdail*) and Wellcome Trust-Henry Dale (*Jin*), along with three Marie Curie Co-Fund Fellowships and several Marie Curie individual fellowships that are recruited annually. The School takes a proactive role in **supporting the long-term career aspirations of talented PGR researchers**; two former PGR students (female) progressed to permanent academic positions in this REF cycle. ECRs receive a **generous start-up package** whilst their teaching and administrative loads are managed accordingly in the first three years of appointment (increasing from 25%, 50% to 75%). This workload management greatly facilitated their success allowing them to focus on research.

The University provides training courses for all staff when applying for research funding; e.g. the EPSRC New Investigator Forum, the Royal Society URF support programme and EU Fellowship support programmes. Opportunities are available for ECRs to sit on mock panels. All staff have access to a library of research applications, reviewers' comments and PI responses. The School operates **a mandatory grant application peer-review scheme**, with feedback from two or more colleagues. No applications >£50K are submitted without undergoing formal internal peer review. After four years in post, our **ECRs participate in committees within the School**, in a deputy capacity, principally to learn about the role and gain experience of academic management duties without the administrative burden.

2.4 Research leave & flexible working schemes

CU runs an ongoing University Research Leave scheme (6-12 months) which is available to all academic staff, and the **Cardiff Disglair Lectureship** scheme facilitates longer periods of research leave, alongside funding postdoctoral researchers transitioning into their first teaching and research position (see REF5a). Applications for flexible working arrangements are also encouraged and supported in the School. Six staff members (three-female; three-male) have availed of this flexible working opportunity, with periods ranging from three months to four years, and we have a comprehensive *Returners Support Scheme* in place to assist staff returning after extended leave.

2.5 Stimulating exchange

A significant proportion of our PGR students obtain industrial experience, through direct collaboration and/or placements. Since 2014, the School has attracted 11 fully funded PhD studentships (*ca*. £160K each with partners including DSTL*, FIRS Laboratories, RSR Ltd, ExxonMobil*), 14 students through a matched-funding CU initiative, eight UKRI iCASE studentships (*Johnson Matthey, Jaguar Land Rover, BP*), and nine students through the Knowledge Economy Skills Scholarship (*KESS* – WEFO and industry funding), all of whom spend time in industry. Several students have projects linked to the Diamond Light Source. Involvement of industrial partners is also manifested through our external advisory boards (e.g. the CCI board). One ECR held a two-month secondment at BBC Wales, gaining experience in science communication and broadcasting. EPSRC IAA funding has also led to two PDRAs undertaking secondments with *Greenergy* and *Johnson Matthey*.

Our annual seminar series provides a regular vibrant forum for all staff and students, and we are currently moving to a blended delivery programme with on-site and virtual guest speakers. They are planned by the ECR seminar committee (enabling them to build collaborative networks) by soliciting suggestions from across the School. Final selection is decided in consultation with the RC. Crucially, guest speakers have lunch with PGR students during their on-site visits, enabling students to discuss their research with leading experts.

2.6 Recognising, rewarding and supporting impact

The School operates a **Workload Allocation system** published annually with tariffs covering teaching (modular, non-modular, scholarship), PGR supervision research, engagement, management and citizenship, including a generous 600 hours allocated to Research. Staff with

funded research grants (and student supervision) are therefore transparently accounted for through reduced teaching and administrative contributions. For non-professorial staff, successful performance is recognised through promotion (overall 14 successful promotions to SL, Reader or Professor in current REF cycle) or through the annual *Outstanding Contributions Awards* scheme. For Professorial staff, a bi-annual *Senior Salary Review* is conducted, and excellent research performance is rewarded. For staff developing research impact, a generous workload tariff is provided, with delivery facilitated through internal funding; e.g. 37 Impact Acceleration Awards of £920K value in the review period (Section 4.3).

2.7 PGR recruitment

In the 2014-20 period, PGR applications increased by 180%, up to a high of 279 in 2019. All posts are advertised via the university website and *FindaPhD.com*. Up to 60 PGR students start annually(*via* October/January/April/July entry points), with the total number enrolled each year increasing from 2014-15 to 2018-19, **representing a near doubling of PGR numbers compared to REF2014**. The small drop in 2019-20 was largely due to uncontrollable external factors (e.g. Covid-19) and resultant deferrals to enrolment. The quality of international PGR applicants is maintained via a mandatory interview process; the proportion of non-EU international PGR students has increased to 26% in 2019-20. We also host *ca.* 50 (capped for best experience) visiting PGR students annually, mostly from overseas, supporting a vibrant research culture based on *ca.* 250 PGR students. PGR recruitment is overseen by the School's monthly Academic Recruitment Group.

	2014-15	**2015-16**	**2016-17**	**2017-18**	**2018-19**	**2019-20**
Applications	*153*	*225*	*247*	*237*	*279*	*159*
Starters	*46*	*60*	*57*	*58*	*57*	*38*
Enrolled total	*120*	*148*	*167*	*187*	*200*	*182*
Thesis submission	*74%*	*82%*	*86%*	*100%*	*87%*	*96%*

Recruitment from diverse backgrounds is funded via EPSRC DTA, CU studentships, including Vice-Chancellor Scholarships, KESS and China scholarships (CSC). Industry, iCASE and UKRI are all commonly used, with further funding from the EPSRC Catalysis CDT.

Since 2014, the School has attracted 11 fully funded PhD studentships (*ca*. £160K each) and eight iCASE awards. The Catalysis CDT attracted a total of 61 MRes starters (11 2014-15, 13 2015-16, 12 2016-17, 13 2017-18, 12 2018-19), in addition to 58 fully funded School/College/University PhD studentships (11 2014-15, 7 2015-16, 14 2016-17, 13 2017-18, 4 2018-19, 9 2019-20). We support international applicants looking for funding *via* CSC (total 6), Commonwealth Scholarship (1), VC Scholarship (2), and CONACyT (3). We also have four Marie Skłodowska-Curie ITN PGR students, across two different EU projects. Involvement in other CDTs include one PGR student who is part of the Bath Doctoral Training Initiative for Biosensors.

2.8 PGR monitoring and support

Students have one or more supervisor(s), and a review panel of two independent academics. Progress monitoring events occur at three, nine, 15, 21, 27, 33, 39, 45 months, with progression recommendation by the review panel at nine, 21 and 33 months. For each event, students submit a research plan, skills audit/self-assessment record, and a record of supervisor(s) meetings, while supervisors submit a report. At nine, 21 and 33 months, the students also submit a longer-form report (plus thesis plan at 33 months); an interview with the review panel determines the progression recommendation. The DPGRS reviews all PGR monitoring events, implementing corrective action if necessary; additional support is available through our dedicated PGR Office. This rigorous process has facilitated the **increased thesis submission rates** (see Table above).

All PGR students and academic staff are enrolled on a dedicated online PGR module which supports all aspects of PGR activity (including counselling, health and wellbeing services; training, including ethics and integrity, unconscious bias, and equality and diversity; safety forms; career development; thesis submission checklist; demonstrating guidance; feedback mechanisms and PGR Forum/SSC/Board dates/minutes). All PGRs further benefit from numerous training courses

from the Doctoral Academy and the GW4 Alliance (universities of Bath, Bristol, Cardiff, and Exeter).

Mentoring and supporting PGR scientists is facilitated in several ways. The HoS meets all PGR students twice per year. Through a quarterly PGR Forum, nominated PGR Representatives and the DPGRS liaise with the whole PGR cohort, key discussion points form the agenda and actions for subsequent PGR Staff-Student Committees and PGR Boards. PGR students also hold membership on School committees (e.g. Athena Swan; Safety). Submission of confidential feedback is encouraged, allowing the School to triage issues, formally record extenuating circumstances and process rapid actions. PGR students complete an exit survey allowing us to reflect upon their experiences and improve School policy. PGR is a standing agenda item at RC, SET and School Board, providing managerial oversight of all PGR related matters.

3. Income, infrastructure and facilities

3.1 Research funding

The School has witnessed a dramatic uplift in Research income performance in the current REF cycle, primarily stimulated through our enabling strategy of strengthening the core equipment and research facilities. Some of the highlights evidencing this performance are outlined below. Our total research grant income over the assessment period has **grown to £49.7M, up from £27.7M for the REF2014 period** (79.4% increase). We received competitive funding from EPSRC, BBSRC, MRC, NERC, STFC, EU, RSC, HEFCW, Welsh Government, WEFO, Innovate UK, DSTL, MoD, US Secretary of State of Defence, Leverhulme Trust, Wellcome Trust, Wolfson Foundation, Royal Society, Diamond Light Source, Academy of Medical Sciences, Analytical Chemistry Trust Fund, Bill and Melinda Gates Foundation, Biochemical Society, British Council, Combatting Terrorism Technical Support Office, Daphne Jackson Foundation, Stapledon Memorial Trust and National Nuclear Laboratory. **Research awards from industry have also grown (52 awards, £6.01M)**. Our research spend increased considerably (REF4a income data); from 2013-14 to 2018-19, annual income increased from **£2.14M to £3.91M** (+83%) for UKRI, from **£42K to £433K** (+1031%) for UK Charity competitive processes, and from **£3.92M to £6.18M** (+58%) for all income. Our income also increased in absolute terms per FTE.

Research grant applications are aligned with the School's research strategy and are managed through our five research sections (Section 1.1). All staff are supported in grant writing, as a core component of the annual PDR process, with specific emphasis on supporting ECRs through interaction with Line Managers and support programmes (Section 2). Our strong collaborative environment encourages ECRs to work with more senior colleagues on funding applications. The School operates a **Rolling Grant Pipeline**, staff discuss their grant application plans with Line Managers, along with an annual meeting with the DoR and Research and Innovation Support Manager (RISM) to construct a live pipeline document that evolves through the year. The pipeline facilitates our strategic planning of applications, avoids bottle necks in submissions, and provides on-going administrative support up to the point of submission and beyond.

The School partnered or leads on a range of large-scale grants, with total funding of £21M from EPSRC. We are a central institution to the **Catalysis Hub**, with **£9.1M directly awarded to Cardiff** (Section 4.1). Another example is an EPSRC **Centre-to-Centre Grant** (£1.53M), to investigate fundamental aspects for conversion of CO_2 to sustainable fuels. This approach builds on our success in the EPSRC **Low Carbon Fuels Call** (£1.88M).

3.2 Operational infrastructure, including specialist equipment

To support the strategic growth of all research staff and students, we **significantly increased our estate footprint since REF2014**. Housed in the historic Main Building of CU, we have expanded post-REF2014 to occupy new research space in the South Wing (increasing by 22% to 7717 m^2). The new facilities have predominantly been allocated for research laboratories, **providing an additional 1065 m^2 of new space**, allowing expansion of existing facilities and creating new ones. Simultaneously the School has also refurbished and repurposed existing research space within its original footprint through **CU investment of £3.15M**.

These new facilities were created to support our strategic research themes, underpinning all research groups, including: laboratories for organic and inorganic synthesis, materials preparation,

biological chemistry, heterogeneous/homogeneous catalysis, and dedicated computational research space. The *Catalysis CDT Research Training Laboratory* was also established and fully equipped. A number of facilities focusing on specific equipment were created, including laboratories for high-field EPR, Mass Spectrometry, SEM and data processing suite, solid-state NMR and high-throughput multifunctional catalyst testing reactor suite.

Having occupied **Main Building** since 1927, our estate infrastructure will undergo a significant transformation in early 2022 when the **CCI relocates into the nearby TRH building** on the new CU *Innovation Campus*. The TRH will bring together all catalysis researchers, co-housed in purpose designed laboratories to engender interdisciplinary research, including the computational modelling groups. Vacated space in Main Building will be refurbished primarily for new UG/PGT teaching provision. The TRH building is part of a **£131M investment by CU** to deliver world-leading facilities for the CCI, alongside the *Institute for Compound Semiconductors*, and part of an overall **>£300M investment in the new Innovation Campus**. New facilities include an analytical suite for catalyst characterisation (330 m^2), and laboratories for catalyst preparation/testing (830 m^2). The TRH also contains externally accessible industrial collaboration laboratories (210 m^2), featuring configurable space for commercially focused projects, creating an important driver for innovation, enterprise and impact. The TRH will house a new EM facility with a suite of TEM and SEM instruments, including a unique next generation analytical **in situ AC-STEM funded by Wolfson Foundation £0.75M, WEFO £3.66M and CU**.

The School has also **established substantial new equipment** to support research, mainly through external funding and matched CU support, including a new X-ray Photoelectron Spectroscopy facility for surface analysis (Sêr Cymru £543K, and Cardiff *Research Infrastructure Fund*) along with a School funded experimental officer post (*Morgan*). This facility underpins our catalysis and materials research and is complemented by the Cardiff led EPSRC National Facility in Photoelectron Spectroscopy (Section 4.1).

Since 2014 the School has invested heavily in its core MS and NMR facilities, with financial support from EPSRC (£0.98M) and CU. **New MS equipment totalling £1.60M** (Perkin Elmer TGA-FTIR-GCMS, Waters Synapt LCMS, Waters Xevo LCMS, Agilent 7900 ICPMS, Bruker Autoflex MALDI-MS, and Thermo Finnigan Orbitrap Exact GCMS) has been installed in a suite of custom refurbished laboratories, strengthening our existing MS facilities. The Xevo (for small biological molecules) and Synapt LCMS (for analysis of biomolecules) instruments underpin much of the research in RT2. The *TGA-FTIR-GCMS* identifies volatiles evolved during controlled heating of solids, supporting projects in bioenergy, biomass processing and high-performance materials, underpinning research in RT3. Analysis and characterisation of proteins, peptides and polymeric materials uses the Autoflex Speed MALDI-MS system equipped with a Time-of-Flight mass analyser, whilst ultra-high resolution GCMS is achieved using the Orbitrap Exact system.

To complement our widely used 600 MHz and other NMR spectrometers, a **£1.26M investment established four new NMR spectrometers** (Bruker solid-state 400 MHz, Bruker 500 MHz with Prodigy Cryoprobe, two Bruker 300 MHz), in addition to upgrading the existing 400 MHz systems, underpinning the successful outputs and grant income in all Research Themes. The solid-state NMR instrument is equipped with two CPMAS H/X double resonance probes for the characterisation of heterogeneous catalysts and functional materials. The 500 MHz liquid NMR system has an auto-tuneable cryogenic Prodigy broadband multinuclear dual resonance probe for analysis of ^{1}H, ^{19}F nuclei and nuclei in the frequency range ^{15}N to ^{31}P, with a 60-port sample changer allowing fully automated data collection. Both 300 MHz liquid NMR systems have a dual resonance probe for the observation of ^{1}H and ^{13}C nuclei, with 60-port auto-changer providing fully automated data collection.

Over the past 50-years, the School has established a strong track record in **EPR spectroscopy** research and this has continued over the REF period, recently moving into a refurbished laboratory to accommodate a new W-band (90 GHz) EPR instrument (EPSRC £712K). Further hardware developments extending instrument capabilities include the design of new resonators for multi-modal spectroscopy (Royal Society), design of new dual-mode resonators (EPSRC £720K), tuneable light sources for ultra-fast time-resolved photochemical studies (EPSRC Cardiff Equipment Fund) and engineered surfaces for photocatalysis (EPSRC £304K), supporting close collaborative research projects with Industrial partners; e.g. *Johnson Matthey, AstraZeneca*.

A unique £1.6M 32-bed **multifunctional high-throughput automated reactor** for heterogeneous catalyst testing was installed in 2018 and commissioned in 2020 (EPSRC £874K; supported by *Johnson Matthey*, *Invista* and the *Catalysis Hub*). The reactor is custom designed to operate over a wide range of conditions for many versatile applications. Two 16-bed modules operate independently with robotic and automated analysis for gas/solid and gas/solid/liquid reactions, providing key data for research on valorising waste streams, sustainable feedstocks, CO_2 utilisation and environmental catalysis.

The School of Chemistry plays a central role in **Supercomputing Wales** (SW) and **Advanced Research Computing @ Cardiff (ARCCA) facilities**, with high performance computing underpinning research in RTs one, three and four, including fundamental quantum theory (*Knowles*), new materials (*Leoni, Harris*), homogeneous catalysis and life sciences (*N.Richards, Platts*) and heterogeneous catalysis (*Catlow, de Leeuw, Logsdail, Roldan, Willock*). The SW project (**WEFO, £5.65M**) provides the infrastructure and support for two dedicated software engineers (*Nanavati, Polyak*), with responsibility for supporting researchers on HPC resources, whilst developing their own independent research.

Central analytical services underpin all operational research, and they are supported and managed by the School Manager and Deputy School Manager, reporting to the RC. A team of technical and professional services staff support our analytical facilities, increasing from 15 FTE in REF2014 to 19 FTE currently. CU supports technical staff to attain professional registration; as a signatory to the **Technician Commitment**, CU was awarded **Employer Champion Status** in 2018. Infrastructure technicians (*Blake, Cross, Griffiths, Halton*) support operation of the research laboratories. Dedicated technicians support analytical services, ensuring method development, local management and data dissemination and archiving (*Court-Wallace, Hicks, Perdjon, Waller, Williams*). Fully equipped mechanical and electronic workshops provide bespoke manufacturing and specialised maintenance (*Morris, Wescombe*). Seven Experimental Officers are dedicated to specialist facilities, including high-throughput catalyst testing (*Nia.Richards*), EM (*Davies*), XPS (*Morgan*), catalysis (*Shaw*), crystallography (*Kariuki*), solid-state NMR (*Hughes*), and biological chemistry NMR (*Mart*).

The School based RISM (*Moseley*) provides support on all aspects of research grant preparation, submission, and administration, liaising closely with investigators. Costings for research proposals are supported through the pre-awards team based in Research and Innovation Services (RIS), ensuring compliance with external funders' conditions, they also provide support and training for Fellowship applications. The central Contracts Team support investigators, in drafting, reviewing and negotiating research-related contracts. Additionally, the University Commercial Development team has 15 staff, providing support with IP protection, translational research, licensing and spinout company creation.

A specialised Science (Chemistry) Library is co-housed within the Main Building, with a dedicated chemistry librarian, and many specialist chemistry information resources including *SciFinder Scholar*, *PubChem* and *Chemspider*. The annual library budget is £6.4M and provides access to over 100,000 journal titles (see IREF5a).

The School **promotes EDI in its research culture**, and continually works to make infrastructure and facilities accessible to all. Examples are the modification of specific research laboratories to improve accessibility to wheelchair users, and those with impaired mobility. The move to wider ranging electronic based resources, complying with W3C International Standards on Accessibility, now widens access to these resources for those with a range of disabilities.

3.3 Infrastructure, facilities and expertise contributing to impact

Access to School equipment is available to industry and other collaborators, creating an open access culture for research to deliver impact. New impact focused facilities have been established; e.g. a new reactor for kg scale-up polymer preparation, characterisation and a twin-screw extruder to manufacture prototypes for mechanical testing and 3D printing filaments (CU funded, £294K), led to collaboration with *Kingspan*. The School positively encourages industrial collaboration, by providing studentship and seed-corn funding to create new partnerships. Staff are readily available to work with external stakeholders on projects that focus on impact; the collaborative nature of

many teams and the structured Research Groups means that a wide range of staff can feed in their expertise.

Chemistry actively engages with the CU *Innovation Network*, created in 1996 to establish contacts between business and CU for knowledge transfer, and now has more than 1,800 members from business, academia, and support organisations. IAA funding has allowed researchers to undertake secondment with industry on research projects that have a specific impact focus, with secondments to *Greenergy*, *Johnson Matthey Sonning* and *Johnson Matthey Shanghai,* the latter two supporting our impact case Golden Green Chemistry.

3.4 Collaborative and shared equipment

School equipment and infrastructure sharing has been identified as a means of **promoting collaboration and ensuring efficient use of resources** (particularly senior staff helping ECRs access specialist equipment). CU maintains a searchable equipment and facilities database, providing researchers with technical details of *ca*. 350 items of equipment available for research. This database also feeds into the national EPSRC-funded *equipment.data.ac.uk* database, publicly available to both potential academic and industrial users. Our equipment and facilities are also included in a regional equipment database maintained by the GW4 Alliance, which is committed to establishing shared infrastructure on a regional basis.

Research is also underpinned by **use of STFC facilities**, including Diamond Light Source, ISIS neutron scattering/diffraction and RAL laser facilities. EPSRC National Facilities are regularly used, with a particular focus on crystallography, NMR and XPS. The School was a lead partner establishing the catalysis research laboratory in the **Research Complex at Harwell**, maintaining a permanent presence with resident PGR students and staff.

3.5 Major benefits in kind

For UKRI applications in the assessment period, **393 letters of support from companies** and other non-academic partners were submitted, **pledging £24.7M contributions in kind and cash**, resulting in 92 successful awards and contributions of £5.38M. Sponsorship of prizes for several research meetings have been received (Section 4). Another example is that *Bruker Biospin* funded a one-year PDRA as project partners to support the establishment of a high field W-band EPR facility. We also received in kind access to many international large-scale facilities, for example, five competitively won days for neutron scattering at the Institute Laue-Langevin Grenoble (>£60k), as well as access to the European Synchrotron Facility at Grenoble, Electra Sincrotrone at Trieste, Shanghai Synchrotron Radiation Facility, and advanced electron microscopy at the US Oakridge National Laboratories.

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

4.1 Research collaborations, networks and partnerships

The School of Chemistry recognises its responsibility to promote collaboration across all the scientific disciplines, and this is reflected in the wide range of interactions that the School holds. Over 1000 publications are co-authored with external collaborators from national and international institutions, facilities and industry. In this REF cycle, staff have delivered **203 collaborative awards of total value £31.4M** and 68 of these awards were industrially collaborative projects (£5.9M, UK, EU and overseas), including a Total Research & Technology heterogeneous catalysis consortium (£879K) involving four academic partners from the EU. Another specific example of international partnership from our Catalysis Theme is our recently established **Max Planck Centre** (MPC) on Fundamentals of Heterogeneous Catalysis, which combines leading expertise in the CCI with the Max-Planck-Institut für Kohlenforschung, the Fritz Haber Institute of the Max Planck Gesellschaft FHI and the Max Planck Institute for Chemical Energy Conversion, enabling this MPC to share key resources, including industrial interactions. Our MPC is only one of three in the UK and the first in physical chemical sciences. Another major collaborative activity for the CCI is the EPSRC **Centre-to-Centre** grant on trimetallic nanoparticles for CO_2 conversion (£1.53M; *Hutchings, Catlow, Taylor,* and others), involving UCL, Utrecht and Fritz-Haber-Institute.

Another significant collaboration is the **UK Catalysis Hub**, involving several members of the School (PIs *Hutchings, Catlow,* with nine other members of staff involved in projects) with 45

partner institutions, creating collaborative projects with the Universities of Manchester, Bath, Oxford, Southampton, London (UCL), Sheffield, Durham, Bristol, Imperial and Glasgow, with 27 industrial partners contributing nearly £1.5M (including *Sabic, Johnson Matthey, Welsh Water, Unilever, Selden, BP, GSK, Lucite*). The School of Chemistry remains a leading player in this venture.

Other representative examples of **large collaborative grants** across our Research Themes include: **1**) **WEFO Supercomputing Wales** (£5.65M; *Catlow, Knowles* and others) involving Cardiff, Swansea, Bangor, Aberystwyth; **2**) **Utilisation of Solar Energy and Electrocatalytic Processes** for the Low Energy Conversion of CO_2 to Fuels and Chemicals (£1.3M; *Catlow, De Leeuw, Roldan*), led by Cardiff with UCL, QUB and *Johnson Matthey*. The School is also involved in a number of **EU doctoral training network programmes**: **3**) EU Industrial Doctorate *CHARISMA* led by Cardiff (€606K, *Bonifazi*), involving 3 academic partners and two companies, to study the concept of applied irreversibility to displays; **4**) EU ITN *PARACAT* led by Torino (€2.6M, *Murphy*) involving five universities, one research institute, three industrial partners, and two academic partners, to investigate the role of paramagnetic species in catalysis; **5**) EU ITN *PHOTOTRAIN* led by Bologna (€2.6M, *Bonifazi*), a network involving 13 global academic and industrial partners focussing on fundamental conversion of solar energy.

From our Research Theme in **hierarchical functional materials,** staff (*Fallis, Dervisi, Beames, Pope*) have developed new scientific collaborations with UK and US governmental agencies, international defence agencies and industry to commercialise methods for chemical warfare agent detection, supported by a competitively tendered technology development contract from the *Counter Terrorism Technology Support Office* (US State Department). The ongoing contract will supply thousands of colorimetric test devices and iteratively refine their use by generalist military and first-responder personnel (see Impact Case Novel high fidelity point-of-use tests for chemical warfare agents).

The School has always retained strength and excellence in X-ray Photoelectron Spectroscopy, and this unique collaborative position is exemplified through the **EPSRC National Facility in XPS** (£2.58M, *Davies*). This National Facility, led by Cardiff along with UCL and Manchester, is based on a cluster of versatile instruments in Cardiff (including UPS and ISS), with access to *in situ* EELS and angle resolved XPS primarily at the *Research Complex at Harwell*.

The School of Chemistry collaborates with a diverse range of other schools including *Pharmacy & Pharmaceuticals*, on therapeutic proteins for targeted cancer treatment (*Allemann*, BBSRC, £510K), *Medicine* to develop new devices for portable anaesthesia (*Paul*, MRC, £741K) and *Engineering* on developing new microwave resonators (*Murphy*, EPSRC, £720K). Opportunities to develop collaborations between the disciplines are supported by university-funded networks (e.g., University Research Network in Materials Science) and URIs, based on themes that traditionally cut across several disparate disciplines. Many of the URIs have significant Chemistry involvement (Section 1.5). CU also has strategic partnerships with KU Leuven (Belgium), Xiamen University (China), Unicamp (Brazil), University of Namibia (Namibia) and Bremen University (Germany).

4.2 Interactions with key research users, beneficiaries and audiences

The contribution of staff in the School to the discipline including our wider beneficiaries is illustrated through the number of lectures at conferences, meetings and workshops and organised conferences locally. These are pivotal mechanisms for staff interaction, engagement, and relationship development with potential collaborators. A focal point in the School calendar is the annual **Cardiff Chemistry Conference** (CCC), a two-day event involving lectures from 6 internationally eminent scientists, local ECR academic staff and PGR/PDRA researchers. A similar **annual 2-day CCI conference** includes lectures by 6-8 experts in catalysis research, including industrialist and academic speakers.

Successful commercial collaborations between industry and the School are exemplified by a series of **Knowledge Transfer Partnerships** with *Selden*, transferring fundamental catalysis discoveries into commercial products (£492K). Interactions with external partners have also been strengthened by the appointment of staff to advisory roles (Section 4.5), including funding councils.

Beyond academic and commercial arenas, more far-reaching connections have been made with key audiences in societal and political settings through participation with political institutions (e.g. *Science and the Assembly*). Members of the School have also participated in RS, EU and UKRI policy development meetings, across a broad range of scientific fields, including the circular economy and CO_2 conversion. Furthermore, members of the School have contributed to Welsh, UK and European governmental policy; e.g. *Catlow* on House of Lords EU Committee to hear evidence on the UK's future relationship with the EU on research and education (Oct 2020).

4.3 Wider contributions to economy and society

Based on our vision of scientific excellence, investigators aim to dedicate a proportion of their time to disseminate research results to the general public and other sectors of society. These events couple our fundamental research with the natural enthusiasm of our staff to disseminate their research. Our impact cases (see below) and projects of wider interest (including those in environment, sustainability, energy, and security) lend themselves naturally to public dissemination, making our fundamental research readily accessible to non-expert audiences. Among our outreach events, we frequently participate at the *Royal Society Summer Science Exhibition* (2014, 2017, 2019), *New Scientist Live*, *Manchester Science Festival*, *Harwell Open Day* and numerous events at the *National Museum of Wales*, *Soap Box Science* and *Pint of Science*. We also participate in University community projects, funded through the *RSC*, *First Campus* and the WEFO *Trio Sci Cymru*. Members of the School also regularly contribute to programmes on national and local (Wales) BBC radio and television, such as *In Our Time* by M Bragg (*N.Richards*) and *The Life Scientific* by J Al-Khalili (*Pickett*).

The School hosts the RSC Outreach Regional Coordinator for Wales (*Mason*), promoting RSC education activities with stakeholders and HE Institutes to support outreach activities. We organize many on- and off-site activities (e.g. *Chemical Potions* for younger audiences). These events also include teachers' engagement activities, with whom we arrange two meetings per semester to gather their advice on aligning our outreach activities with their curriculum. We also target a wider audience through social media (e.g. *Twitter, YouTube, LinkedIn, etc.*). ECRs have received funding from the RS (*Easun*) and the RSC (*E.Richards/Beames*) to support such outreach activities.

The School hosts the fortnightly meetings of the **Cardiff Scientific Society**, an external organization (established 1926), which aims to educate and enlighten members of the public on the latest scientific discoveries, with recent Presidents including *Allemann*, 2015-17; *Harris*, 2017-20 and *Catlow* 2020-22. The School also contributes to Welsh culture; the design of the 2018 *Eisteddfod Crown* (sponsored by CU) incorporated aspects of the University's research, involving quasiperiodic tiling patterns based on research in quasicrystal chemistry (*Harris*).

As innovation is one of our core strategic aims, the School has placed renewed emphasis on **developing and supporting research impact**. Therefore, in addition to our four submitted impact cases, other examples of research by our staff that will underpin future innovation activities and impact cases in the School include: **1**) new pest management potential from synthetic biology, focused on benign aphid control from engineered sesquiterpenoid natural products (*Allemann*); **2**) Fuel from air, based on patented research using solar-energy produced H_2 to reduce CO_2 to methanol for energy storage and already at 500,000 kg pa pilot plant stage in Germany (*Bowker*); **3**) Innovative disinfectant products, using strong oxidants based on in situ generation of H_2O_2 for transient bacterial decontamination (*Hutchings*); **4**) *Molpro* Quantum Chemistry Software, widely used in industry and academia; the software licence was spun out as a company in 2015 (*Knowles*); **5**) Multifunctional microemulsions as highly sensitive scintillants for detection of radiation at nuclear energy sites and effective bactericides against pathogens (*Fallis, Pope*); **6**) Electrochemical sensors for miRNA in urine, a potential biomarker for kidney disease (*Redman*); **7**) Fuels from process waste streams, producing methanol from crude glycerol waste streams (*Taylor, Hutchings*); **8**) Earth abundant catalysts for preparation of isocyanate pre-polymers, facilitating green production of commodity chemicals (*Ward*).

The development and support of these impact cases comes from a number of sources. Project **1** above (New Pest Management) benefitted from BBSRC Follow-on-Fund and Super-Follow-on-Funds (BB/N012526/1, £197K; BB/R019681/1, £551K), with results exploited as a new strategy

for crop protection / growth and promoting population sustainability in the EU (patent EP3247799). For fundamental EPSRC-supported research, impact development is facilitated through *Impact Acceleration Awards*, including scientific projects on selective oxidation of methane to methanol for efficient upgrading of low value resources, conversion of waste bio-derived molecules to fuels, and hydrochlorination of acetylene to produce vinyl chloride.

4.4 Contributions to sustainability of the discipline

At subject-based level, *Buurma* was Chair of the ECR Panel for the EPSRC *Directed Assembly* Network (2012-2016) and is currently Champion for the theme *Controlling molecular self-assembly in biological and biomimetic systems* whilst *Browne* led the Emerging Reactor Technologies sub-theme of the Grand Challenge Network *Dial-a-Molecule*. Promoting the sustainability and vitality of the discipline, several ECRs hold roles on various national committees, including RSC Dalton Division Council (*Melen*); RSC Interest Groups in EPR (*E. Richards*), Main Group Chemistry (*Melen*), Chemical Biology and Bioorganic Chemistry (*Tsai*); RSC Wales Regional Steering Group (*Logsdail*). Other members of the School have served on committees that help sustain the discipline, including: RSC Interest Groups in Colloids and Interfaces (*Paul*), Surface Reactivity and Catalysis (*Taylor, Willock, Hutchings, Bowker*), Applied Catalysis (*Taylor*), Physical Organic Chemistry (*Buurma*); Biological Chemistry, ACS (*N. Richards*); Council, Microscopy Society of America (*Kiely*).

4.5 Indicators of wider influence

The research achievements of our School have been recognized through numerous awards, prizes, honours, distinctions, and esteem indicators, including appointments to leadership roles in the research community (nationally and internationally), learned societies and professional bodies. These awards have been conferred on staff across the spectrum of career stage, highlights include:

Elections to international/national academies and learned societies: Foreign Associate, NSA, USA (*Pickett*, 2014); Member, Academia Europaea (*Catlow*, 2013; *Harris*, 2013; *de Leeuw*, 2017; *Kiely*, 2019); Member, German Academy of Sciences Leopoldina (*Catlow*, 2020); Fellow, Learned Society Wales (*Kiely*, 2015; *de Leeuw*, 2016; *Wirth*, 2016; *Catlow*, 2017; *Murphy*, 2018; *Bonifazi*, 2019; *Pickett*, 2020); Honorary Fellowship, Indian Society of Chemists and Biologists (*N.Richards*, 2020); Member, International Academy of Quantum Molecular Science (*Knowles*, 2018).

Prizes, awards and distinctions: **1**) **International Prizes**: ENI Award for Advanced Environmental Solutions (*Hutchings*, 2017); Clara Immerwahr Award (*Melen*, 2016); Bruker Award, Phytochemical Society (*Pickett*, 2016); ACS Inorganic Chemistry Lectureship (*Casini*, 2019); **2**) **Royal Society Awards**: Wolfson Research Merit Award (*Murphy*, 2014; *Wirth*, 2016); **3**) **RSC Prizes/Awards**: Faraday Prize (*Hutchings*, 2018; *Catlow* 2020); Harrison-Meldola Prize (*Melen*, 2019); Bader Award (*Wirth*, 2016); Industry-Academia Collaboration Award (*Hutchings*, 2017); **4**) **LSW Medals**: Menelaus (*Hutchings*, 2017); Dillwyn (*Melen*, 2019; *Edwards* 2020); **5**) **Other awards**: British Crystallographic Association Young Scientist Award in Chemical Crystallography (*Hatcher,* 2017); Institute of Chemical Engineering Innovative Product Global Award (*Hutchings*, 2015); **6**) **Honorary degrees**: DSc (Surrey), DSc (Neuchâtel), DSc (Hertfordshire) (all to *Pickett*); **7**) **Named Lectures**: Bergman Lecture, Berkeley (*Carpenter*); Dewar, QMUL, Xingda, Peking, Zhang Dayu, Dalian (all to *Hutchings*); C.N.R. Rao, Bangalore (*Hutchings* and *Catlow*); Lu Jiaxi, Xiamen (*de Leeuw*); Elizabeth Creak Distinguished Lecture, Warwick, Sterling B Hendricks Memorial Lecture, ACS, Rekunyk, Saskatoon, Keck Lecture, North Carolina State (all to *Pickett*); **8**) Collectively, members of the School have delivered **81 plenary/keynote lectures** during the REF cycle.

Visiting professorship appointments at foreign universities: Tokyo Metropolitan, Louisiana State, Cape Town (*Hutchings*); Shanghai Tech (*Harris*); Kyoto (*Wirth*); Parma (*Bonifazi*); Technical University Munich (*Casini*); Utrecht (*de Leeuw*); Northwest, China (*Jin*).

Appointments on international advisory boards and committees: selection panel for the Alexander Todd – Hans Krebs Lecture, German Chemical Society (*Wirth*, 2015-18); selection panel for Inaugural Bragg Prize, International Union of Crystallography (*Harris*, 2020); Vice Chair, European Section of the Electrochemical Society (*Bonifazi*).

Leadership roles in learned societies, professional bodies, government committees and research councils: Foreign Secretary of the Royal Society (*Catlow*, 2016-21); President, Faraday Division, RSC (*Hutchings*, 2012-15); Member of Council, RSC (*Knowles*, 2013-17); Chairman, Audit Committee, RSC (*Knowles*, 2015-17); Member of Council & Head of Chemistry Section, Academia Europaea (*Hutchings*, 2017-22); EPSRC Physical Sciences Programme Strategic Advisory Team (*Knowles*, 2008-14; *de Leeuw*, 2017-19); Expert panel, Research Council of Norway (*de Leeuw*, 2014-18).

Chairs of Conferences: Staff members have also chaired major international conferences in Chemistry and related disciplines; Organic Solid State Chemistry (*Harris*, 2013), Computational Methods in Quantum Chemistry (*Knowles*, 2017), Hypervalent Iodine (*Wirth*, 2018), Chemical Ecology (*Pickett*, 2019), Reactivity and Mechanism in Chemical Biology (*N.Richards*, 2021), Metals in Medicine (*Casini*, 2020).

Editorial Roles: Members of the School have held senior editorial positions (*Pickett*, *Phil. Trans. Royal Soc. B*, 2016-present; *Hutchings*, *J. Catalysis*, 1999-present), whilst 16 other staff held appointments on journal editorial boards and guest edited 12 special journal issues.

Royal Appointments: *Hutchings* received a CBE in 2018, whilst *Catlow* was knighted in the delayed 2020 Queen's Birthday honours. The School was also awarded a **Regius Professorship** in 2016, one of only twelve to mark Her Majesty's Diamond Jubilee in 2012, conferred to *Hutchings*.