Unit of Assessment: B8 Chemistry

1. Unit context and structure, research and impact strategy

1.1 Background/context

Warwick's Department of Chemistry has become a UK leader over the last 25 years, ranked =6 in REF2014 with 34.8 FTE. Success in the REF2021 period has stemmed from our 2014 objectives, driven by (i) a culture of excellence in fundamental research, both within chemistry and at interfaces with other disciplines; (ii) investment in world-class infrastructure and facilities; (iii) an entrepreneurial spirit, including extensive interactions with industry, facilitated by effective routes to translation and generation of real-world impact with an international reach; (iv) a focus on recruiting and strongly supporting outstandingly talented early-career researchers.

The strong REF2014 performance provided a platform to strengthen the department further. An internal 'Strategy Renewal' (2017/18) – required by the University every 10y for all departments as a re-evaluation and re-invigoration process – identified (i) established strengths to build on, (ii) new research areas to expand into, and (iii) a need to recruit early-career staff, given a predominance of mid-career academics: a consequence of many staff appointed in the 1990s and 2000s building high profile careers at Warwick, coupled with recruitment of established academics at professorial level. This Strategy Renewal has been transformative, facilitating delivery of world-leading research and impact now and in the long term.

This REF cycle has been defined principally by investment in people (section 2), with appointments in targeted areas. This expansion has resulted in 48 (46.8FTE) staff being returned for REF2021: 18 professors, 13 associate professors, 10 assistant professors (4 with proleptic appointments when fellowships end) and 7 independent research fellows. Shared appointments with other Warwick departments, and indeed other institutions, reflect our interdisciplinary and collaborative ethos, with Warwick Medical School (WMS) hosting <u>Perrier</u> and <u>Gibson</u> (30% FTE); <u>Stansfeld</u> and <u>Corre</u> split 50:50 between Chemistry and the School of Life Sciences (SLS); <u>Challis</u> and <u>Perrier</u> split 80:20 with Monash *via* the Warwick Monash Alliance (section 4.1). Continuing excellence across the board throughout this REF cycle is demonstrated by sustained high grant income [averaging > £8M per year, consistently top 5 in the Russell Group (RG) for T&R staff, section 3]; a researcher population averaging *ca*. 170 PhD students and 62 postdocs; an increase of *ca*. 30% in annual publication numbers (to \approx 280 from WoS) compared to REF2014; and sustained external recognition through prestigious fellowships and awards (sections 3, 4).

Interdisciplinarity (a founding principle at Warwick) remains integral to our research. Our culture – and the Faculty of Science, Engineering and Medicine of which we are part – nurtures collaboration both within and between departments without barriers (REF5a, 2.9): this, and the central position of chemistry amongst the sciences, means that Chemistry's research is pivotal to university-wide ventures such as the Warwick Integrative Synthetic Biology Centre (WISB), several collaborative Centres for Doctoral Training (CDTs; REF5a, 3.8 and 3.9.1), and the 'Global Research Priorities' (GRPs; REF5a, 2.9.1):

• CDTs across the range of chemistry from mathematical modelling to biomedical technologies (section 1.4) provide platforms for collaborative projects with Physics, Engineering, SLS,



WMS, WMG, Mathematics and Computer Science as well as supporting significant interactions with academic and industry collaborators.

- The strongly collaborative university research environment, including shared management of major facilities through Research Technology Platforms (RTPs section 3), is organised to support multi- and interdisciplinary endeavours.
- Cross-department research centres (REF5a, 2.9.4) and institution-wide GRPs unite academics to address some of humanity's most urgent questions: chemistry is pivotal to the *Energy; Innovative Manufacturing & Future Materials* (acting as co-lead with WMG); and *Health* GRPs.

Internally, four Research Clusters reflect the department's core strengths, providing a focus for recruitment of new staff and organisation of research activity; many staff belong to >1 cluster.

Synthesis and Catalysis encompasses fundamental and applied aspects of the innovative molecular design and advanced synthetic methodology which underpins all of chemistry from new medicines to materials. Notable work includes development of new anti-cancer metallodrugs (Sadler, Nat. Chem. 2018 and 2019; Scott, Chem. Sci. 2019); asymmetric transfer hydrogenation catalysis (Wills, Angew. Chem. 2020); new syntheses of macrocyclic peptides as drug leads (Shipman, Chem. Sci. 2019); photo-redox activity of metal clusters (Pike, Chem. Sci. 2019); using mechanical entanglement to alter homogeneous catalyst regioselectivity (Chaplin, Angew. Chem. 2018); understanding exceptionally efficient supramolecular catalysis inside a synthetic host (Ward, Nature Chem. 2016). Industry links are exemplified by commercialisation of hydrogenation catalysts [Wills, Johnson Matthey (JM)] and drug discovery with SMEs (Fox, Epsilon3Bio and RxCelerate; Marsh, Valiseek).

• Chemical, Structural and Synthetic Biology (CSSB) employs a highly interdisciplinary approach to elucidating and exploiting the molecular basis of biological phenomena with applications in areas including drug resistance, food security and industrial biotechnology. Members have contributed significantly to CDTs (Corre, co-director of CDT 'Synbio') and research centres (Challis, theme leader in WISB) in Synthetic Biology. Research highlights include ground-breaking observations of hierarchical protein dynamics using solid-state NMR spectroscopy (Lewandowski, Science 2015); unravelling the mechanisms of polyketide antibiotic biosynthesis (Challis, Nat. Commun. 2016; Tosin, Chem. Sci. 2016; Jenner and Challis, Nat. Chem. Biol. 2018; Challis Nat. Chem. 2019; Lewandowski and Challis Nat. Chem. 2019; Dias, Nat. Catal. 2019) and discovery of a novel Rieske oxygenase involved in carnitine metabolism (Bugg, PNAS, 2014). Strong links with industry are showcased by £500k Syngenta co-funding of a £3.5M BBSRC strategic 'Lola' award (2013-2018; PI Challis), a fully-funded collaboration with Achaogen on development of novel β -lactamase inhibitors (2017-2018, Challis), and formation of the spinout company Erebagen (Challis, 2020).

• **Materials and Polymers** embraces materials from solid-state inorganics to soft matter, particularly polymers. Applications encompass materials for photovoltaics, electronics, ferroelectrics, catalysis, petroadditives, agrochemicals, personal care and medicine. This cluster's work is often strongly linked to industry *via* research collaborations and knowledge transfer, and the cluster boasts three of our five recent Royal Society Industry Fellowships (RSIFs) (Scott, Gibson, Walton) and two spinout companies (Haddleton, Scott). Research highlights include: precious metal oxides developed as electrocatalysts with JM (Walton, Angew. *Chem.* 2014); copper nanoparticles for electronic devices (Hatton, Nat. Commun. 2017); induction of ferroelectricity in perovskites (Senn, Nat. Commun. 2018); controlling, with



precision, placement of monomer units in a polymer chain (<u>Perrier</u>, *Nat. Commun.* 2016); a new approach for sequence control in multi-block copolymers (<u>Haddleton</u>, *Nat. Chem.* 2017); and new 'antifreeze' materials for cryopreservation of cells (<u>Gibson</u>, *JACS* 2017).

• Measurement and Modelling incorporates both innovative experimental measurements, and theory/simulations. Experimental work is notable for development of unique instruments and devices (in electrochemistry, mass spectrometry, spectroscopy and surface analysis). Many members have contributed significantly to EPSRC CDTs in Molecular Analytical Science (<u>Unwin</u>, Director) and Diamond Science and Technology (<u>Macpherson</u>, co-Director). Experimental highlights include new sensor systems based on conducting diamond (<u>Macpherson</u>, *JACS* 2019); invention and use of the Warwick Electrochemical Scanning Probe Microscopy platform (<u>Unwin</u>, *JACS* 2019); use of STM imaging to analyse polymer structure at the atomic level (<u>Costantini</u>, *Sci. Adv.* 2018); developing nature-inspired sunscreen formulations (<u>Stavros</u>, *Nat. Commun.* 2019); photoelectrochemical production of solar fuels in microgravity for space travel (<u>Brinkert</u>, *Nat. Commun.* 2018); applications of FTICR mass spectrometry to problems in bioanalysis (<u>O'Connor</u>, *Anal. Chem.* 2018) and petroleomics, with a recent world record for the most compositional assignments of species in a single mass spectrometric dataset (<u>Barrow</u>, *Chem. Sci.* 2019). Our other two RSIFs (<u>Macpherson</u>, <u>Stavros</u>) come from this group.

Computational chemistry research spans areas from protein dynamics to electronic properties of new materials, and is central to the 'Heterogeneous Systems' CDT. Projects include new reaction discovery methods for nanoparticle-catalysed reactions of pollutant gases (<u>Habershon</u>, *J. Phys. Chem. A* 2019); theory and simulation of molecular reactions on surfaces and in materials (<u>Maurer</u>, *Nat. Comm.* 2020); and rationalisation of ice nucleation mechanisms (<u>Sosso</u>, *PNAS* 2019).

1.2 Strategic research aims during REF period

Our overriding aim this REF cycle was to build on the department's research quality and international standing from its excellent performance in REF2014, aligning with the University Research Strategy of *Excellence with Purpose* (REF5a, 1.2). We have expanded our portfolio of fundamental and applied research with 13 new academic appointments since 2017, 11 of whom are early-career staff. We excel at both internationally-leading fundamental research, and real-world applications through our close links with industry.

The Strategy Renewal process involved a 10y horizon-scanning exercise for research and teaching to 2028, incorporating the entire next REF cycle. A vigorous programme of new academic staff appointments during 2017-2020, informed by this Strategy Renewal and the institutional strategy, has substantially refreshed our research environment and allowed a REF return of 13 more researchers than in 2014, aiming to:

- Build strength broadly across the core disciplines of chemistry;
- Provide higher critical mass in specific areas of recognised excellence (polymers, solidstate materials, chemical biology, electrochemistry, computational chemistry);
- Increase interactions with other departments across disciplinary boundaries to develop new collaboration-based strengths;
- Support innovation by diversifying into new fields, and exploiting external opportunities, which are aligned with societal and industrial challenges.

Our 13 new academics match these priorities and have substantially diversified our activities. And we host a further 12 early-career fellows (ECFs) who flourish with strong institutional



support (REF5a, 3.1), providing a pipeline of outstanding young colleagues, often progressing to permanent posts (Section 2). Indeed four recently-appointed ECFs already have proleptic Assistant Professorships following outstanding performances (Wilson, Jenner, Senn, Pike).

The quality of our recent appointees is illustrated both by their successes at winning prestigious fellowships, and the rapid establishment of collaborations with other departments. <u>Días</u> (appointed 2019; Biomolecular structure) and <u>Stansfeld</u> (appointed 2019; computational biochemistry, 50:50 with SLS) strengthen links with SLS; <u>Bartók-Pártay</u> (AI and Machine learning, appointed 2019; EPSRC-ECF from 2020) brings us closer to Engineering, Physics and Computer Science. <u>Maurer</u> (computational chemistry, appointed 2017; UKRI-FLF from 2019) has initiated collaborations with colleagues from Physics, Engineering, Maths, and SLS; <u>Sosso</u> (computational chemistry, appointed 2017) had published with colleagues from Physics and WMS by 2019. We anticipate similar successes, both within and beyond the chemistry department, from our more recent appointees.

Research integrity. Our research is conducted within the University's established research ethics structures (REF5a, 2.11). All researchers engage with the Epigeum *Research Integrity Certification and Assessment programme*: we work closely with the Research & Innovation Services (R&IS) Research Governance Team to ensure that ethics approvals are in place where required. An R&IS Research Development Officer provides support for matters relating to research ethics, ensuring a consistent and clear approach throughout the department. A 'Research Ethics and Practice' course for PhD students guides research students through the relevant approval processes.

1.3 Future plans for research

The outcomes of the Strategy Renewal exercise – identification of areas for new appointments and a decision to focus on early-career researchers to meet our strategic goals – have directly informed our vision for the department's future. Expansion of the academic staff contingent constitutes both a major institution-level investment in the department's future, and a statement of intent about our forward focus. Our main activities will be aligned with the areas of strength covered by our four research clusters, but will be complemented by the emerging activity of the new talent that has reinforced them. Thus, the department remains distinguished for its work in polymer chemistry (new appointments: <u>Becer</u>, <u>Wilson</u>) and materials chemistry (new appointments: <u>Días</u>, Jenner) and computational chemistry (new appointments: <u>Maurer</u>, <u>Sosso</u>, <u>Bartók-Pártay</u>, <u>Stansfeld</u>). Our research in these areas will accordingly remain internationally leading throughout the next REF cycle. Of our other recent appointments, <u>Greenhalgh</u> (appointed 2020) works on catalysis using organo-chalcogen compounds; <u>Ward</u> (appointed as HoD, 2017) strengthens coordination / supramolecular chemistry.

Our funding portfolio diversity – [UKRI (41%), EU (33%), industry (15%) and charities (5%) (Sept2013 – Aug2020) are all well represented; section 3] – is a particular strength which will help us to retain a leading position in a challenging external funding environment. With our expanded research portfolio and rebalanced staff age profile, we are very well placed to remain at the forefront of UK chemistry.

Our future research will also include:

REF2021

- New CDTs. Chemistry participates in the £4M EPSRC "HETSYS" CDT (2019-2027), a Maths/Physics/Chemistry/Engineering collaboration. Further, the University committed to support, from 2019, Warwick/Industry-funded CDTs in 'Analytical Science' and 'Diamond Science and Technology', capitalising on £2M of commitments from industry for each CDT to support PhD studentship intakes during 2019-2024 (section 1.4).
- **Ongoing BBSRC and MRC DTPs**, led by SLS and WMS respectively, have significant Chemistry involvement and provide studentships in the life sciences area of our portfolio.
- Further internationalisation of our research partnerships: in addition to numerous individual links supported by Newton/GCRF funding (£1.3M since 2014; section 4), the ongoing **Monash-Warwick Alliance** (REF5a, 2.12.1) will continue to engender excellent collaborative work between the two institutions (section 4).
- Continuing vigorous recruitment of, and support for, ECF applicants in areas aligned with our research priorities (section 2). We have further successes for the new REF cycle [Karasulu, EPSRC-ECF (computational materials), from 11/2020; <u>Palacio-Lozano</u>, Leverhulme ECF (mass spectrometry) from 5/2021].
- Led by Shipman from Chemistry, a major expansion of STEM provision is being planned under the auspices of the 'STEM Grand Challenge' (REF5a, 4.2) - a key priority in the university's 'Excellence with Purpose Strategy' to 2030. A new Science Precinct will provide space for growth, including completely new physical infrastructure for Chemistry, and is being designed to maximise possibilities for interaction between departments in terms of co-location of labs and capabilities where appropriate, proximity of staff with shared interests, and spaces such as 'incubator labs' to allow partnerships with industry to flourish - facilitating and improving what we already do well. New staff hires, based on the additional capacity and improved collaborative opportunities associated with this infrastructure, will be particularly targeted towards interdisciplinary challenges. Accordingly preparation for this facility – in terms of staff appointments and research development transcending traditional subject boundaries – is already part of Chemistry's research strategy for the next REF cycle. These plans demonstrate the University's longterm vision and commitment to interdisciplinary scientific research with industry engagement (REF5a, 2.1, 4.1). The project, currently at RIBA stage 1 design, should be delivered within the next REF cycle and will likely constitute the university's largest ever capital spend.

1.4 Strategic aims for impact: this REF cycle and beyond

Developing real-world impact from our research to address global societal problems has always been embedded in our culture. A vigorous institution-level action plan (REF5a, 2.6, 2.7) ensures the effective generation of impact from our research, with substantial recent strengthening of our impact-supporting processes both university-wide and departmentally.

We enjoy excellent and responsive central administrative support and institutional funding to facilitate impact development. New institutional support mechanisms include appointment of Research Impact Managers and Research Impact Co-ordinators, dedicated to promoting impact development, who are integrated into the department, attending Research Committee meetings and working closely with academic staff. Other resources include an on-line 'Impact Resource Bank'; faculty-wide training sessions, and Impact Acceleration funding. The new 'Impact Leave' scheme – above and beyond normal 'Study Leave' – prioritises cases for leave based on developing impact opportunities: <u>Haddleton</u>, 2017/18; <u>Gibson</u>, 2018/19; <u>Unwin</u>, 2019/20; <u>Fox</u>, 2019/20 had 'Impact Leave' specifically to develop translational aspects of their work. These



new processes have boosted significantly impact development during this REF cycle, contributing to our Case Studies, and this will continue.

Since REF2014 we have developed a greater focus on promoting impact as a key consideration for recruitment, annual review and promotion processes. Impact is high on the agenda at the department's Research and Executive committees: we foster a culture in which *all* faculty are aware of impact possibilities and can pursue them with central advice and support. Senior academics <u>Unwin</u> and <u>Walton</u> (with extensive industry collaborations) are the department's 'Impact Champions' who work with staff, with the help of our Research Impact Manager and Coordinator, to identify impact opportunities and the best methods to exploit and develop possibilities.

Economic/business impact from our work is created by (a) working directly with established business and industry, and (b) exploitation of inventions through spin-out and licensing. We also generate societal impact *via* extensive research-based outreach and public engagement (section 4). These routes to achieving impact rely on specific mechanisms, as follows.

(a) Working with established businesses and industry. We have generated a consistent industry-based research income averaging £1.3M per year by working with 55 businesses who have partly or wholly funded a quarter of our PhD studentships since 2014. PhD funding mechanisms include CDT studentships (see below), iCASE awards, and Warwick Collaborative Postgraduate Research Scholarships (WCPRS) which provide matched funding to support industry contributions to studentships.

The establishment of EPSRC-funded CDTs (2014-2022) in Molecular Analytical Sciences (MAS), and Diamond Science and Technology, have significantly increased commercial engagement by our academics, enabling many academics to secure their first funded interactions with industry. These CDTs are industry-facing and require an industry contribution of ≥£40k per studentship: sponsors include Bruker, Corbion, AZ, Syngenta, DSTL, Lubrizol, Pfizer, De Beers, Element Six, Newport SpectraPhysics, JM, and AWE.

The University has supported additional CDTs in Polymer Chemistry (2014-2022); Analytical Science (2019-2024); and Diamond Science and Technology (2019-2024) in recognition of the strong business links and associated funding streams in these areas. The Polymer Chemistry CDT has been outstandingly successful, with industry co-funding of 42 PhD students totalling £2.2M from partners including Unilever, Lubrizol, AZ, DSM, Syngenta, Hempel, Dulux, CSIRO, Merck, Altana and Infineum.

Industrial partnerships have flourished through our five Royal Society Industry Fellowships since 2014: <u>Stavros</u> (2020, with Lubrizol); <u>Gibson</u> (2019, with GE Healthcare); <u>Scott</u> (2017, with Infineum); <u>Walton</u> (2015, with JM); and <u>Macpherson</u> (2014, with Element6). Two of these (<u>Scott</u>, <u>Macpherson</u>) led directly to Impact Case Studies. Five RSIFs during this REF cycle in a department of our size is exceptional and clearly indicates the scope and quality of our interactions with industry partners.

Other mechanisms for promoting industry collaborations include:

• Regular **faculty-wide networking events** such as 'Industry Days' (five since 2017) unite academics having marketable skills and industry representatives with problems to solve. They focus on how our academic research can benefit the activities of the affiliate



company, and facilitating the funding and collaboration mechanisms that underpin these symbioses. Links with Infineum, Lubrizol and De La Rue have benefited from these events.

- Similarly the Polymer Club (launched 2013) promotes interactions between Warwick's polymer science community and ≈50 international companies with regular industry / academic meeting days. Benefits include access to scientific infrastructure and expertise, including contract work; participation in new collaborative research and teaching ventures; and access to future employees with polymer and colloid chemistry expertise.
- Embedding staff from industry in research groups. <u>Macpherson</u> (Hach), <u>Scott</u> (Interface Polymers Ltd.), <u>Fox</u> (RxCelerate) and <u>Barrow</u> (Hyundai) all have long-term visitors from industrial collaborators working in their groups on translational aspects of their research projects. This provides seamless translation of research outcomes into the business partner's development and exploitation processes: extending such interactions wherever possible is part of our ongoing research strategy.
- The Chemistry department markets its specialist analytical and synthetic services to a range of (mostly industry-based) clients through *Warwick Scientific Services* (WSS). This has generated £1.4M of contract analysis, and short-term R&D contracts for Chemistry since Jan 2014. Small-scale interactions initiated *via* WSS have pump-primed longer-term collaborations with industry including funded PhDs (Unilever, Lubrizol) and PDRAs (Infineum).
- Visits of researchers to industry for secondments / placements using a range of mechanisms: Knowledge Transfer Partnership secondments; 26 Marie Curie ESRs all with secondments; >40 UKRI Impact Acceleration Account secondments; studentship placements *via* CASE awards and other industry-funded PhDs.

(b) Exploitation of inventions through spinouts and licensing. The Department works closely with Warwick's technology transfer arm, Warwick Ventures (REF5a, 2.8) on all aspects of technology transfer and innovation. This REF cycle, 135 patents were filed from Chemistry (including 48 joint with industry) with 8 proceeding to the national stage. Five spinout companies have been formed: *Interface Polymers Ltd* (Scott, Nov2013; see Impact Case Study); *Medherant Ltd* (Haddleton, Dec2013; see Impact Case Study), *Verdel instruments* (O'Connor, Sept2015), *Erebagen* (Challis, July2020) and *4D-Medicine* (July2020, shared with Birmingham using IP from Dove developed at Warwick) – see Section 4.2.

Early-stage impact development is supported by EPSRC and BBSRC Impact Acceleration Accounts and BBSRC Flexible Talent Mobility Awards (31 EPSRC IAA Awards totalling £618k: 9 BBSRC IAA and Flexible Talent Mobility awards totalling £174k). Further, the Warwick Impact Fund (REF5a, 2.7) provides a fast-response mechanism to help translate promising research into impact with grants of ≤£50k; Chemistry staff have won £578k in WIF grants since 2014. Honorary visiting academic appointees from industry have advised on developing impact from our work including: <u>Khoshdel (ex Unilever)</u> working with the polymer chemistry groups; <u>Blasco</u> (Lubrizol Global Skin Care manager) supporting translational aspects of work on sunscreen photophysics (PI <u>Stavros</u>); <u>Lewtas</u> (*ex* Exxon and Infineum) working with <u>Scott</u> on establishment of Interface Polymers Ltd; <u>Hanna-Brown</u> (Technology/innovation lead at Pfizer) worked with <u>Unwin</u> on establishing the MAS CDT, and provides teaching.

With improved institutional-level support and department-based processes, new compounds, materials and methodology from Warwick Chemistry have had worldwide impact, as our Impact Case Studies and many additional examples show. Our four REF2021 Case Studies relate to



transdermal drug delivery using wearable polymer patches (<u>Haddleton</u>); new materials to facilitate manufacturing with polymers (<u>Scott</u>); use of electrochemical sensing and analysis methods for applications from water quality monitoring to medical diagnostics (<u>Macpherson</u>); and a multifunctional scanning electrochemical probe microscopy platform that has been commercialised, sold and used globally (<u>Unwin</u>). These have socioeconomic impact in the areas of healthcare, diagnostics, environmental analysis, energy technologies, corrosion science and manufacturing; additional examples from our developing impact 'pipeline' are in section 4.

2. People

Staff changes this REF cycle. The impact of our new staff appointments has been transformative: 30% of the department's permanent T&R academic staff (including fixed-term ECFs, 40% of our independent researchers) have been appointed since 2017. This expansion, principally at early-career level (Section 1), and the associated areas for academic appointment, resulted from department-wide consultation during the Strategy Renewal. In March 2017 we had no Assistant Professors; by March 2020 we had eleven new Assistant Professor appointments (four of them proleptic following award of major fellowships), plus two more senior appointments (<u>Stansfeld</u> and <u>Ward</u>). Some senior staff departed for promotions / significant new roles elsewhere (see below).

To complement these academic staff appointments, we have also appointed fixed-term research fellows (ECFs). A rigorous internal sift procedure ensures that we support only applicants whom we believe – after a selection process comparable to that used for Assistant Professors – to be appropriate candidates for permanent academic positions in the future, and whose expertise matches our strategic priorities. The appointments of <u>Senn</u> (2017), <u>Wilson</u> (2019), <u>Pike</u> (2019) and <u>Jenner</u> (2020) to proleptic Assistant Professorships, following award of RS-URFs (<u>Senn</u>, <u>Wilson</u>, <u>Pike</u>) and a BBSRC-FLF (<u>Jenner</u>), precisely validate this strategy. Other ECF appointments are <u>Barry</u> (2014, Leverhulme ECF, medicinal chemistry – now Professor at Bradford), <u>Menon</u> (2017, WISB Career Development Fellow, chemical biology); <u>Bentley</u> (2018, Ramsay fellowship, electrochemistry); <u>Alberti</u> (2018, Leverhulme ECF, chemical biology); <u>Whale</u> (2019, Leverhulme ECF, ice nucleation); and <u>Kang</u> (2020, Leverhulme ECF, electrochemistry).

This rebalancing of our age profile (16/48 of our REF-submitted staff are Assistant Professors or ECFs) associated with our expansion will provide continuity throughout the next REF cycle and a strong platform for future excellence. Of the staff submitted most are on 100% FTE contracts apart from those with temporary reductions due to parental responsibilities; 5 are fixed-term ECFs.

T&R Staffing strategy; staff development: Our recruitment processes facilitate our research strategy by:

(i) Matching academic disciplines for recruitment to our research priorities, in order to (a) strengthen areas of established excellence; (b) increase interdisciplinary research by fostering links across academic disciplines; and (c) develop new research activities linked to current societal problems and industrial needs (section 1.2).

(ii) Focussing on attracting outstanding early-career staff to maintain a balanced age profile and thereby provide succession planning for key research areas, following institutional strategy (REF5a, 3.1).

(iii) Supporting early-career staff with generous start-up resources, free access to our outstanding facilities, and priority access to institutional funding streams.

These tactics drive our continuing mission to deliver world-class, impactful research. We expect new appointees to develop into accomplished leaders, and we provide strong support to enable this. New Assistant Professors benefit from low teaching / admin workloads (ramping up to a full load after 3y). Start-up packages include a PhD studentship with consumables support; £20k for discretionary spend plus significant equipment items by agreement; free access to department and RTP facilities; and a structured probationary programme lasting for up to 5y. Annual targets and performance goals are agreed with the HoD. Mentoring is considered key to academic career progression: new appointees are allocated a senior colleague as mentor who provides advice on matters including establishing a group, preparing grants, and teaching.

Equally important is the way in which the department has a culture of embracing new appointees and finding opportunities to collaborate, an ethos which facilitates the exceptional career progress of younger staff. This is illustrated by some younger members of our current professoriate: *e.g.* <u>Gibson</u> (Assistant Professor, 2012; Professor, 2016): <u>Lewandowski</u> (Assistant Professor, 2011; Professor, 2019); Habershon (Assistant Professor, 2012; Professor, 2020). The success of senior colleagues who moved this REF cycle further illustrates this: <u>O'Reilly</u>, <u>Dove, Taylor</u> and <u>Troisi</u> (all appointed as ECFs) left as full professors, with <u>O'Reilly</u> (HoD, Birmingham), <u>Jones</u> (Provost, Birmingham), <u>Taylor</u> (Professor of Chemical Education / Pro-Dean, Leeds) and <u>Rodger</u> (HoD, Macquarrie) taking senior managerial roles elsewhere following successful periods at Warwick.

Demonstrating awareness of impact considerations is an explicit part of the recruitment process for new academics and is embedded into our selection procedures (REF5a, 2.6). During their first 2y, new staff complete the teaching training programme 'Academic and Professional Practice for Teaching Excellence' (APPTE), leading to 'Fellow of the Higher Education Academy' status; they also attend workshops on areas such as grant writing and research team management. Satisfactory completion of probation (100% success rate this REF cycle) comes with promotion to Associate Professor. Although the formal probationary period is 5y, highperforming staff often meet criteria for promotion sooner (*e.g.* <u>Becer</u>, 2y; <u>Gibson</u>, <u>Senn</u>, <u>Maurer</u>, 3y; <u>Chaplin</u>, <u>Notman</u>, 4y).

A workload allocation model allows T&R staff space to flourish whilst maintaining their teaching/research balance: this is facilitated by a team of eight teaching specialists with permanent contracts (from laboratory demonstrators to Associate Professors) who take a high proportion of the more routine teaching associated with *e.g.* teaching laboratories, as well as leading pedagogical developments, ensuring that research priorities can be met whilst providing an optimum UG learning environment (REF5a, 3.2). Our study leave programme provides teaching/admin relief for a year to those with time-consuming challenges, following the university principle that academic staff can apply for study leave every seventh year, with priority given to those with plans for (i) impact development, (ii) new research projects, and (iii) major grant applications.

Academic staff career development. As well as our collaborative and supportive ethos, effective internal processes strengthen our strong track record of staff development. A department promotions committee reviews and feeds back on promotion applications annually. Although promotion is self-driven, this panel proactively identifies strong performers early and



encourages them to apply to ensure equality of opportunity. Recently the university clarified the promotions criteria, with the four categories of *research and scholarship*; *teaching and learning*; *impact, outreach and engagement*; and *collegiality, leadership and management* being explicitly considered and scored separately, allowing appropriate recognition for all types of contribution (REF5a; 3.3). During this REF cycle we promoted <u>Tosin</u>, <u>Notman</u>, <u>Corre</u>, <u>Becer</u>, <u>Senn</u> and <u>Maurer</u> to Associate Professor following completion of probation; <u>Dixon</u>, <u>Marsh</u>, <u>Chaplin</u>, <u>Hatton</u>, <u>Stavros</u> and <u>Rourke</u> to Reader; <u>Bon</u>, <u>Gibson</u>, <u>Costantini</u>, <u>Stavros</u>, <u>Lewandowski</u>, <u>Hatton</u>, <u>Blindauer</u>, <u>Habershon</u> and <u>Clark</u> (T-only) to Professor.

Research fellows. We apply the same considerations around choice of field, potential links to other departments, quality of candidates, and awareness of impact to appointment of ECFs as we do to Assistant Professors, on the basis that we expect them to become competitive for Assistant Professor posts. We therefore sift fellowship applicants carefully, and consequently there is an excellent conversion rate of ECFs to permanent appointments, with *all* recent RS-URFs progressing to Assistant Professorships. The career trajectories of two recent appointees (<u>Wilson</u>: postdoc, to Leverhulme ECF, to RS-URF, to Assistant Professor; and <u>Jenner</u>: postdoc, to Leverhulme ECF, to Assistant Professor) illustrates the development opportunities given to our ECFs and the recruitment 'pipeline' provided by the fellowship schemes.

With support provided from the initial application stage, Fellowship applicants enjoy coaching from potential hosts, mentors and the HoD; and *via* mock interview panels comprising current Fellows and senior academics, with administrative support for the whole process (*e.g.* help with costings; detailed feedback on application drafts). Our ECFs benefit from the same academic networking opportunities, free facilities access, and access to the University's skills development courses, as our permanent academic staff. All ECFs have a senior academic staff mentor: the department Postdoctoral Society (PSoC), and a faculty-wide ECF support network, provide social and networking opportunities. ECFs enjoy career development opportunities beyond their research including teaching, outreach and public engagement, and representation on relevant department committees (*e.g.* Safety; Wellbeing and Diversity).

Postdoctoral research assistants are supported by structures that meet or exceed the principles of the EC Charter for Researchers and Code of Conduct for the Recruitment of Researchers, and the UK Concordat to Support the Career Development of Researchers. Career progress is monitored *via* annual review meetings with the PI, plus 1:1 meetings with the HoD on arrival and four months before contract end. Structure is provided by the 'Certificate in Transferable Skills in Science' for Postdoctoral Researchers. Resources available include mentoring schemes, careers consultations, and an annual 'Warwick Postdoctoral Science Symposium' with invited lectures from ECRs; courses provided by the Learning & Development Centre (LDC) covering impact and public engagement; and training on impact awareness for all ECRs is provided *via* the Research Fellows Forum.

Additionally, peer-group support for RAs and ECFs comes from PSoC (the Postdoctoral Society of Chemistry): formed in 2018 and managed entirely by postdocs, with department financial support, it provides a supportive environment for all ECRs. PSoC is extremely active in welcoming and providing practical advice to ECRs who are new to the UK; organising networking and social opportunities; promoting ED&I issues amongst our ECR community (see later) and providing them with a voice in the department; and organising training events through the Research Fellows forum – covering *e.g.* grant writing, patent law, science communication, and (recently) several career development webinars during the COVID-19 lockdown.

Since 2014, 219 postdocs have worked in the department: the geographical distribution (*ca.* 30% international, 30% EU, 40% UK) indicates the attractiveness of the department to researchers globally. The quality of the training and the supportive environment mean that our postdocs have an excellent track record of progressing to additional postdocs, industry jobs, independent fellowships or academic positions. Postdoc alumni this REF cycle contribute substantially to chemistry academia worldwide, with *ca.* 20% now in independent academic posts: in China (x13, including four full professorships), USA, Canada, Australia, India, Brazil, Switzerland [ETH Zurich (full professor)], EU countries (including France, Portugal, Italy, Spain, Germany, Austria, Belgium, Poland); and UK institutions [including UCL, Bradford (full professor), Leeds, Nottingham, Warwick, Loughborough, OU]. Some postdoc alumni in industry facilitate ongoing collaborations [*e.g.* our Platform Agreement with Lubrizol (section 4); <u>Macpherson</u>'s Impact Case Study involving Hach; <u>O'Connor</u>'s FTICR-MS instrument development with Bruker].

Training and supervision of PGR students. Average PhD graduations during the REF2021 cycle (43 p.a.) are up from 31 p.a. last cycle. PGR recruitment has grown in line with our new staff appointments (average enrolments of 51 across this REF cycle, with 57 in 2019/20), reflecting our successes in winning PhD funding *via* industry and CDTs, leading to an average PGR population of ≈170 at any time. The group is ethnically diverse (with 2019/20 enrolments at 47% BAME – compared to 26% in 2013/14). The average 60:40 (male:female) gender balance since REF2014 matches the sector average. PGR students declaring a disability, typically 8% in Chemistry, are supported *via* a needs assessment made by the Student Support disabilities team.

PhD training and support (REF5a, 3.9, 3.10) allows students to integrate fully into the department's culture. Induction on project-specific technical, analytical and research issues is followed by an RCUK-compliant PG Certificate in Transferable Skills in Science (PGCTSS). Structured to complement the students' research programmes, it provides researchers with the skills needed to be effective from the start of their studies whilst equipping them with the personal and professional transferable skills necessary for their next career stage. Accordingly PGCTSS provides an integrated package covering both research-specific training modules and a broader programme of soft skills, all integrated into our graduate school reporting/continuation requirements. Soft-skills modules include 'Science Communication and Impact', 'Academic Scientific Writing', 'Decision-making and Leadership', 'Business, Innovation and Commercialisation' and 'Research Ethics and Practice'. Students' future employability is addressed with training in CV writing and interview skills. All PGCTSS courses provide networking opportunities, with several delivered jointly with other universities (Bristol, Cambridge, Imperial, Oxford, Southampton).

Research students also have access to courses from the Graduate School, Student Careers and Skills service, Institute of Advanced Study, and the LDC. All PhD students are encouraged to participate in either UG laboratory teaching or outreach activities; a bespoke laboratory demonstrating course is delivered with the LDC. Access to such courses and information is *via* the Warwick *SkillsForge* portal, where students (and supervisors) document and track their skills development. Individual PGR students have an academic advisory committee that reviews progress / continuation reports at key stages. Employability statistics are excellent (latest graduate outcomes survey: 91% in work of whom 97% 'highly skilled', including recent PhD alumni in academic positions in China (x5), Thailand, Brunei, Nigeria, US, UK).



Undergraduate students make valuable contributions to our research, not just through finalyear projects but also university-funded summer internships (URSS: Undergraduate Research Support Scheme) which regularly funds 20-30 students in Chemistry. <u>Haddleton</u>'s Impact Case Study with Medherant arose from a URSS project (2014).

Supporting equality, diversity and inclusion (REF5a, 3.4). ED&I considerations are integrated into the terms of reference of, and discussions at, key committees (*e.g.* Executive; Research; Education; Promotions) and inform all considerations of workload allocation, support for study leave, internal funding, and selection of REF outputs. We have held an **Athena SWAN Silver award** continuously since 2010.

We established in 2018 a 'Wellbeing and Diversity' group (<u>Dixon</u>, chair, with representation from staff and student groups) which considers work/life balance issues associated with the Athena SWAN agenda alongside broader ED&I issues, and develops an annual action plan in response to the 'staff satisfaction' survey. This led directly to *e.g.* the annual 'demystifying promotions' workshop and establishment of our 'core hours' policy (below). The Executive Committee reviews implementation of ED&I principles in all areas of departmental business, and includes the 'Wellbeing and Diversity' group Chair.

Given our staff profile when our Strategy Renewal concluded, gender and age diversity were priorities. Our previous top-heavy age profile has been comprehensively addressed. To aid gender diversity, all recruitment committees / interview panels must have an appropriate gender balance; job adverts are scrutinised by the 'Wellbeing and Diversity' group chair (<u>Dixon</u>) to ensure that language is appropriately inclusive, and we ensure female representation on shortlists for academic posts (extending deadlines and re-advertising if necessary). Focussing on these recruitment principles saw appointment of two female assistant professors in 2019 (<u>Brinkert, Bartók-Pártay</u>).

We encourage women, at all levels, into leadership roles, recognising their value as role models. The department established (2018) a Chemistry Women's Network for female staff and PhD students, with mentoring available outside the formal process for probationary academics. We ensure that female staff or speakers are represented at department-run events, including conferences, and are particularly alert to the opportunity that our seminar programme offers to promote female academics at all career stages, with 30% female invited speakers this REF cycle.

Consistent with our Athena Swan Silver status, our flexible working policy applies to all staff. Examples include:

- new parents can work part-time, with return to full-time work guaranteed later (*e.g.* <u>Notman</u>, <u>Senn</u>)
- phased return to full-time work after parental leave with practical support as required; (a
 dedicated breastfeeding / lactation room is well used)
- rearranging administrative responsibilities to accommodate parental leave (*e.g.* <u>Senn</u>, <u>Greenhalgh</u>)
- scheduling department meetings during 'core hours' (10am-4pm) to allow all staff to participate
- encouraging non-standard working patterns (compressed hours, working from home *etc.*) to support people with caring responsibilities



• ensuring that opportunities such as study leave or conference travel funding are equally available to all staff.

Chemistry department members have led several initiatives, now embedded university-wide, designed around issues raised by women to help them develop into scientific leaders. These include:

- The student-led 'Women in Science' programme (*e.g.* Nov2019, a one-day event 'Women in Science Success Stories' open to all staff, ECRs and PGRs).
- Warwick Conference Support Fund: provides financial support to cover care responsibilities associated with conference attendance, including covering childcare costs for invited external seminar speakers to enable them to visit.
- Annual 'Demystifying the Promotions Process' workshops which, along with reform of the promotion criteria (REF5a, 3.3), have resulted in chemistry applications for promotion (and successful outcomes) doubling recently, with 24 promotions during 2017-20 *vs.* 10 during 2014-17.

The department has expanded ED&I activities to create as inclusive an environment as possible, recognising the well-known benefits of diversity in innovation and scholarship.

- The 'Wellbeing and Diversity group' has:
 - organised workshops during the 2020 lockdown, facilitated by an external consultant, on 'Positive Behaviours' and 'New Ways of Working', to establish a set of core expected behaviours, and reflect on policies and practices in the Department
 - started monitoring all aspects of recruitment processes to ensure fairness
 - extended the Chemistry Women's Network (originally solely for academics) to ECRs and PhD students.
- PSoC, supported by the Wellbeing and Diversity group, champions ED&I issues particularly among the ECR community, conscious of the particular challenges facing early-career staff in academia. Initiatives include:
 - organisation of symposia celebrating accomplishments of our female academics as part of International Women's Day
 - organisation during 2019/20 of the seminar series 'Breaking Barriers' (supported by an RSC grant to <u>Rogers</u>, a Senior Research Fellow) which showcased LGBT, ethnic minority, or disabled academics representing the wealth of diversity in academia
 - organisation of a Black History Month symposium
 - working with the department to raise awareness of mental health issues facing students and staff, including arranging Mental Health First Aid training for ECRs.
- We have strong role models from the LGBTUA+ community:
 - In 2016 <u>Bon</u> started and was inaugural chair of the university's LGBTUA+ taskforce, a body of staff and students which makes recommendations to the University D&I Committee. He contributes to the LGBTUA+ community in science through his senior tutor role and media interviews, *e.g.* the LGBTSTEM and 500QueerScientists initiatives.
 - In 2016 PhD student <u>Jaggers</u> launched the University's first Role Models Guide, a collection of profiles of LGBTUA+ students, staff and alumni who shared their experiences of Warwick. <u>Jaggers</u>, who conceived this project and was principal author, participated in the 2015 Stonewall Young Leaders Programme.



The increasing diversity of our PGR student body led to formation in 2020 of a Black Students Society, initiated and led by PGR student <u>Kariuki</u> with support from the department and student ChemSoc, with a remit to make recommendations to the department that will help recruitment, integration and academic performance of BAME students.

3. Income, infrastructure and facilities

3.1 Grant income. Our average annual grant income this REF cycle is £8.1M, plus £736k inkind facilities use, with strong performers across all four research clusters. New staff (appointed 2017-2020) have been notably successful at winning major fellowships (see below) allowing us to maintain a strong income performance despite the lowering of our age profile – vindicating our research strategy.

Our grant-winning success provides clear evidence that our research and staff recruitment strategies are working. It is enabled by *both* (i) the quality of the people we attract, with the associated mentoring and development opportunities; and (ii) the ongoing excellence of our established staff. The departmental and wider university's culture of collaboration across disciplines, focus on research areas aligning with societal needs (*cf.* the GRPs), and ready access to outstanding facilities, also support our research income – much of which involves cross-department collaborations within Warwick (especially WMG, Physics, Engineering, SLS, Medicine) and between institutions (section 4). Grant income success also reflects the administrative support, rigorous internal peer-review, and mock interviews that we provide.

Our strong industry interactions (55 industry funders this REF cycle, £1.3M p.a.) underpin our partly or wholly industry-funded PhD studentships (*ca.* 25%) as well as smaller projects through WSS. Major industry sponsors include Infineum (£1.8M this REF cycle) and Unilever (£772k); other regular partners Syngenta (natural product discovery, synthetic biology; £474k this REF cycle) and Lubrizol (physical chemistry, materials, polymers; £1.0M) have 'platform agreements' with the university which formalise IP arrangements in exchange for regular funding. Indeed, Lubrizol fund more PhD studentships at Warwick than at any other UK university.

Grants (excluding fellowships) of total value >£1M this cycle:

- £10.5M BBSRC-EPSRC Multidisciplinary Research Centre in Synthetic Biology (>£1M to Chemistry: <u>Challis</u>, Col; 2014-2021)
- £8M BBSRC-EPSRC 1GHz solid-state NMR instrument (Lewandowski, Col; 2018)
- Eur6.7M EU-H2020 grant 'ZELCOR' (Bugg, Col; 2016; 18 partners)
- £5.4M EPSRC programme grant (<u>Unwin</u>, Col; 2018; 8 computational / experimental groups)
- Eur4.9M FET-OPEN EU grant 'BoostCrop' (Stavros, PI; 2018; 14 partners)
- Eur4.1M, H2020 ITN (Becer, PI; 2019; 12 partners)
- £4M H2020 (O'Connor, PI; 2017) FTICR-MS network grant 10 partners
- £3.5M Innovate UK grant 'Chemo-enzymatic synthesis of speciality glycans' (<u>Gibson</u>, Col; 2015 – 12 partners)
- £3.5M BBSRC strategic 'Lola' award (Challis, PI; 2013; with £500k from Syngenta)
- £2.4M BBSRC-EPSRC grant for UK high-field ss-NMR facility (Lewandowski, Col; 2020)
- £2.1M BBSRC/FAPESP grant on Lignin valorization (Bugg, PI; 2017; 3 UK, 1 Brazil partners).
- £2M EPSRC 'Underpinning multi-user equipment' (Shipman, Col; 2017)



- £1.2M MRC iCASE program in Biomedical Technologies 12 studentships (<u>Gibson</u>, PI; 2017)
- £1.2M EU grant, 'EUTOPIA' Science and Innovation Fellowships (<u>Scott</u>, PI; 2020; see section 4.1)
- £1M EPSRC responsive-mode grant (<u>Habershon</u>, PI; 2019; with UCL and Birmingham)
- £1M EPSRC 'Core capability' equipment (Shipman, PI; 2014)

Other grant successes include:

- Numerous personal fellowships: 3 ERC Starter grants (<u>Gibson, Chaplin, Lewandowski</u>, 2014); 5 ERC Consolidator grants (<u>Troisi</u>, 2014 [moved]; <u>Perrier</u>, 2015; <u>O'Reilly</u>, 2015 [moved]; <u>Dove</u>, 2016 [moved]; <u>Gibson</u>, 2020); 3 RS-URFs (<u>Senn</u>, 2017; <u>Wilson</u>, 2018; Pike, <u>2019</u>); 2 RS-URF extensions (<u>Chaplin</u>, 2016; <u>Notman</u>, 2019); 2 EPSRC-ECFs (<u>Hatton</u>, 2015; Bartók-Pártay, <u>2020</u>); UKRI-FLF (<u>Maurer</u>, 2019); RS Leverhulme Senior Fellowship (<u>Stavros</u>, 2016); BBSRC-FLF (<u>Jenner</u>, 2018); 5 RS Industry Fellowships (<u>Macpherson</u>, 2014; <u>Walton</u>, 2015; <u>Scott</u>, 2017; <u>Gibson</u>, 2019; <u>Stavros</u>, 2020).
- Other ECR fellowships: 6 Leverhulme Trust (<u>Barry</u>, 2014; <u>Wilson</u>, 2016; <u>Jenner</u>, 2017; <u>Alberti</u>, 2018; <u>Whale</u>, 2019; <u>Kang</u>, 2020); Ramsay fellowship (<u>Bentley</u>, 2018).
- Six MSCA ITN / EJDs (<u>Becer</u> as PI; <u>Ward</u>, <u>Gibson</u>, <u>Unwin</u> (x2), <u>Dove</u> [moved] as Co-Is) providing 11 PhD studentships.
- 17 MSCA-IF postdoctoral fellows since 2014.
- Leadership of a successful CDT (Molecular and Analytical Sciences, from 2014); key contributions to others (Diamond, from 2014; Synbio, from 2014; HETSYS, from 2019).
- Participation in other PhD studentship programmes including (i) the Midlands Integrative Biosciences Training Partnership (MIBTP), a BBSRC-funded DTP spanning 5 universities (2020-28); (ii) NERC 'CENTA', a CDT spanning several Midlands universities encompassing environment / ecology themes (2014-22); and (iii) the Interdisciplinary Biomedical Research (IBR) MRC DTP.

3.2 Infrastructure, facilities

Chemistry's research is accommodated in three buildings. The original (and regularly refurbished) 1960's C-block, houses most synthetic chemistry; the newer 'G-block' accommodates computational and some physical chemistry; the newest Molecular and Analytical Sciences building (2011) accommodates several synthesis groups, solid-state materials research, and many shared analytical facilities such as XRD, EM and high-field NMR. The university is now committed to, and has started detailed planning of, a new science precinct to include new buildings for Chemistry, Physics and Engineering (section 1.3).

The department is exceptionally well-equipped with world-class instrumental and analytical facilities: maintaining and continually improving these is a deliberate strategy that drives world-leading science. Capital investments have come partly from the university *via* Research Technology Platforms (see below), and partly from EPSRC/BBSRC equipment grants.

NMR: 8 solution instruments (2 with cryogenic probes) from 300-700 MHz, with one new (500 MHz with ¹³C-optimised cryoprobe) and three with magnet or console upgrades since 2014 (investment £1.4M). Additionally, the UK National Research Facility for High-Field Solid-state NMR includes 11 instruments up to 850 MHz, supporting research from battery materials to membrane-bound proteins; this was recently supplemented by the UK's first 1 GHz instrument (EPSRC, £8M, plus £1M institutional support) led jointly by Chemistry/Physics.

MS: 20 instruments cover all types of ionisation, mass analysers and detection methods. Since 2014 we have installed 8 new instruments (GC-MS, LC-MS/MS x2, Q-TOF x2, MALDI-TOF/TOF x2, ICP-MS), value > \pm 2M. A Nov2020 £3.1M EPSRC grant (plus £0.5M institutional support) for a new FTICR-MS (PI <u>O'Connor</u>) brings spend on new MS equipment to > \pm 5M since 2014.

Other major equipment items are grouped into centrally-managed *Research Technology Platforms* (RTPs) which lie outside department silos and are accessible to all university researchers and external partners from industry. Maintaining world-class infrastructure *via* the RTPs is a core part of the university's research and impact strategy (REF5a, 4.3). The RTPs in X-ray diffraction, Electron Microscopy, High-Performance Computing, Spectroscopy, and Polymer Characterisation benefit Chemistry substantially; two of these [Polymer Characterisation (<u>Haddleton</u>), X-ray Diffraction (<u>Walton</u>)] are hosted and led from Chemistry.

Investment this REF cycle which benefits chemistry includes:

- Microscopy, £2.6M (3 SEM, 3 TEM, 2 AFM, 2 optical systems)
- X-ray Diffraction, £2.2M (two single-crystal instruments with twin Cu/Mo sources, two high-resolution and five other powder diffraction instruments; a SAXS facility; an X-ray spectrometer system)
- Polymer characterisation, £0.7M (GPC/SEC, thermal analysis, particle sizing)
- Scientific Computing, £8.5M [two high-performance clusters with 2300 and 3500 cores, plus access to a *Tier 2 HPC centre* (HPCMidlands+, 15,000 cores) through a collaborative award to Warwick and six regional partners
- Spectroscopy, £0.5M (Raman, IR microscopes, fluorescence).

A vital part of the department's research strategy is to provide free-at-the-point-of-use RTP access (cost: £0.6M annually) – there is no barrier to accessing world-leading facilities for any department researcher. These facilities support both our fundamental research and impact activities: all four Impact Case Studies for REF2021 (and other emerging impact examples, section 4) benefited from the quality of, and ease of access to, RTP facilities.

Other facilities:

- The Warwick Centre for Ultrafast spectroscopy (2017). A £1.5M ultrafast laser spectroscopy facility (<u>Stavros</u>, PI), £620k EPSRC grant + UoW and industry support, comprises four beamlines spanning the UV/Vis to far-IR regions with femtosecondtimescale excitation; already it has >50 user groups worldwide and >30 publications including JACS and Nat. Chem.
- Warwick Analytical Sciences Centre integrates analytical research across several departments. It has facilitated the successful Molecular and Analytical Sciences CDT, a Marie Curie IDP, our MSc programmes in Analytical Science, and allowed interactions with industry. A £950k EPSRC grant (2020; joint Physics/Chemistry) will ensure that this remains cutting-edge.
- The *Chemical Biology Research Facility*, housing much of the CSSB cluster, is a purpose-built laboratory/office complex (extended in 2016) with dedicated technician support. It is among the best facilities in the world for research at the Chemistry/Biology interface and includes, apart from lab/instrument space, a spacious cold room; dedicated laboratories for growth of BHSL 1 and 2 microorganisms; radiochemistry laboratory; dark room.

Research is exceptionally well-supported with our professional support staff team expanding in line with academic staff numbers (22 technical, 24 administrative: 30% increase since REF2014). Restructuring the 'core technician' team has allowed each research cluster to have the responsive, dedicated support (with appropriate expertise) that it needs. Skilled technician colleagues with specific expertise in areas such as electronics, mechanical work and glassblowing – with dedicated workshop facilities – are intimately involved in equipment design and development. Experienced instrumentation specialists for NMR, MS and X-ray crystallography (at levels equivalent to assistant / associate professor) make equally important scientific contributions: overall our research support staff are co-authors on >150 papers since 2014. Recognising the importance of contributions from technical staff, a clearer career development pathway (up to Professorial level) has been developed (REF5a, 3.3).

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

4.1 Research collaborations, networks, partnerships

We are an outward-facing department, taking a leading role in many interdisciplinary and useroriented activities: our interactions with industry and other users of our research are as important as our core disciplinary excellence, and the collaborative nature of our research (section 1) is illustrated as much by our collection of partnerships as by our grant portfolio.

Many flagship collaborations, networks and partnerships are illustrated by the list of major grants (Section 3.1). Some are collaborations between departments within Warwick (*e.g.* WISB; MAS and HETSYS CDTs; IBR DTP). Others are shared with multiple institutions, including the 'Diamond' and 'Synbio' CDTs; MIBTP; numerous EU networks; UKRI sLoLa and Program grants; EPSRC ss-NMR national facility. The new Euro10M EUTOPIA programme, a partnership of six EU universities, provides opportunities for co-tutelle PhDs, postdoc fellows and researcher mobility (REF5a, 2.12.1). The international scope of our collaborations is shown by publication numbers (2014-2020) involving overseas partners (Australia, 415; USA 187; China 158; Germany, 127; France, 100; out of >1900 publications involving 68 other countries).

A continuing major academic partnership is the **Monash-Warwick Alliance (MWA)** (REF5a, 2.12.1). This institution-level cooperation in research and teaching is spearheaded by strong chemistry-based collaborations in polymer science and structural biology, supported by joint appointments during the REF period (<u>Perrier</u>, <u>Challis</u> from Warwick; <u>Chan</u>, <u>Davis</u> from Monash). The collaboration has generated >360 joint publications out of >1900 for the department (2014-20) including <u>Haddleton</u>, 55; <u>Perrier</u>, 92; <u>Wilson</u>, 42; <u>Challis</u>, 18. The collaboration has led to substantial grants for Warwick PIs in Australia, *e.g.* <u>Perrier</u> [AU\$2M from Australian Research Council (ARC) since 2014]. Particularly notable is participation of staff in major projects including ARC Centres of Excellence [*Innovations in Peptide and Protein Science*, AU\$35M, <u>Challis</u> co-PI, 2020-27; *Convergent Bio-Nano Science* &Technology, <u>Haddleton</u> (Partner Investigator), AU\$30M, 2014-21; *Electromaterials Science*, Unwin (Partner Investigator) \$25M 2014-21], and the new (2021) major initiative *Tackling Antimicrobial Resistance*, *ca*. AU\$2M (<u>Challis</u>, Col).

Our range of international partnerships involving visiting appointments or other external funding is extensive. Several staff have held visiting professorships overseas: <u>Haddleton</u> (Soochow, China, 2014-2017); <u>Walton</u> (Sao Paolo, Brazil, 2014-2017); <u>Bon</u> (Tasmania and Lyon, 2014);



<u>Sadler</u> [Universities of Hong Kong (2012-2015), Zhengzhou (2017-19) and Anhui (2017-20)]. Others have collaborations with partners in developing countries supported by GCRF or Newton Institutional Links funding (<u>Challis</u>, Philippines; <u>Ward</u>, Egypt; <u>Walton</u>, Indonesia; <u>Barrow</u>, Colombia); or funding agencies in Brazil (<u>Bugg</u>, <u>Walton</u>).

We likewise benefit from *incoming* visiting academics or industrialists (*ca.* 50 this cycle with 32 currently active, Section 1.4) who work with specific research groups, some funded by fellowships from our Institute for Advanced Studies. We attract world-leading academics to deliver annual named lectures [*e.g.* Warwick Polymer lecture, <u>Hawker</u> (USA), 2018; Warwick Chemical Biology lecture, <u>Craik</u> (Aus), 2019; Warwick Catalysis lecture, <u>Reek</u> (Netherlands), 2019; Warwick Structural Biology lecture, <u>Strynadka</u> (Canada), 2020].

Industry collaborations are core to both our research and impact strategies (sections 1.3, 1.4), with many multi-grant collaborations. Aspects of our industry interactions which deserve reemphasising include the five RS Industry Fellowships since 2014; 'platform' sponsorship agreements with Lubrizol and Syngenta (section 3.1); and the growing numbers of industry partners with staff embedded in our research groups. Our industry interactions include partnerships with instrument manufacturers, *e.g.* <u>O'Connor</u> (Verdel; hardware for 2D mass spectrometry); <u>Barrow</u> (Bruker and Exxon; MS analysis software), <u>Macpherson</u> (Hach; water analytics – Impact Case Study) and <u>Unwin</u> (BioLogic; scanning electrochemical probe microscopy – Impact Case Study). Of the permanent academic staff in this submission, 26/41 (63%) have had industry funding since 2014: these ongoing interactions will ensure future collaborations with a wide range of industrial partners.

4.2 Broader contributions to research base, economy and society

Prizes and awards: The quality of our staff, and the support we provide, are reflected in external awards and other recognition indicators, distributed across all research clusters and career stages.

Becer:	2019 RSC Macro Group Young Researcher medal.
Bentley:	2020 ISE Early Career Analytical Electrochemistry Prize.
Brinkert:	2020 Russian Academy of Sciences/COSPAR Zeldovich medal.
<u>Challis</u> :	2017 RSC Interdisciplinary Prize.
<u>Chaplin</u> :	2015 RSC Harrison-Meldola Memorial Prize.
<u>Gibson</u> :	2018 ACS Macromolecules/Biomacromolecules Young Investigator Award;
	2015 RSC Dextra Carbohydrate Group Medal;
	2015 Polymers for Advanced Technologies 'Young Talent' Award.
<u>Lewandowski</u> :	2016 RSC Marlow medal;
	2015 ISMAR Abragam Prize.
Macpherson:	2019 RSC Geoffrey Barker Medal;
	2017 Royal Society Innovation Award.
Perrier:	2019 Macro Group medal;
	2014 IUPAC/Samsung Young Polymer Scientist award;
	2014 ACS Macromolecules/Biomacromolecules Young Investigator Award.
Rogers:	2020 RSC 'Inspiration and Industry' Award (for Schools work).
Sadler:	2014 EPSRC 'Recognising Inspirational Scientists and Engineers' award.
	2016 Journal of Organometallic Chemistry 'Bioorganometallic Chemistry' award.
<u>Scott</u> :	2016 RSC Emerging Technologies prize.
<u>Unwin</u> :	2019 ACS Electrochemistry Award (only 2nd non-US recipient in 30y);



2018 Society of Electroanalytical Chemistry's Charles N. Reilley Award (1st UK recipient in 35y);
2017 International Society of Electrochemistry Prize for Experimental Electrochemistry.
2016 RSC Supramolecular Chemistry award

<u>Ward</u>: 2016 RSC Supramolecular Chemistry award.

Other esteem indicators:

- Four Wolfson Merit Awards: <u>Haddleton</u> (2011-16), <u>Challis</u> (2013-18), <u>Perrier</u> (2014-19), <u>Unwin</u> (2017-22).
- <u>Haddleton</u>: Clarivate Analytics 'Highly Cited' researcher (2018).
- <u>Sadler</u>: Fellowship of European Academy of Sciences; Honorary Fellowships of Chinese Chemical Society and Indian Chemical Society (all 2019)

Major personal fellowships: See section 3.

Institutional lectures: The >500 invited department seminars or institute-level lectures (55% overseas) delivered by staff this REF cycle include several prominent named lectureships and invited lecture tours.

- Named lectureships: <u>Challis</u> (Illinois, 2017; McGill, 2018; UC Berkeley, 2020; Oxford, 2020); <u>Unwin</u> (Cincinnati, 2019; Colorado State, 2019); <u>Sadler</u> (Oxford, 2016; SUSTech, China, 2017; USTC-China, 2019); <u>Haddleton</u> (Dutch Chemical Society, 2015; North Carolina, 2017).
- Invited lecture tours: <u>Bon</u> (China and East Asia, 2015, 2017, 2019); <u>Challis</u> (China, 2015, 2017; North America, 2018, 2020; Australia/NZ, 2018), <u>Haddleton</u> (China, 2014, 2015, 2017; Romania, 2017; India, 2019); <u>O'Connor</u> (China, 2018); <u>Perrier</u> (China, 2017); <u>Sadler</u> (Switzerland, 2014; Czech republic, 2015; China, 2017; India, 2019); <u>Unwin</u> (Canada, 2015; Australia, 2015; USA, 2019); <u>Walton</u> (Indonesia, 2017; Brazil, 2018; China, 2019); <u>Wills</u> (China, 2016).

Conference lectures: Of the >670 invited conference lectures delivered this REF cycle, >75% were at overseas/international meetings, including numerous plenary/keynote invitations. 12 staff have given \geq 20 invited conference lectures; 25 have given \geq 10, including some recently appointed colleagues (<u>Maurer, Brinkert, Wilson</u>).

Societal impact of research: our developing 'pipeline'. Beyond the Impact Case Studies, applications are emerging from all research clusters in other ways following our impact-development strategy. These examples, with contributions to healthcare, environment, catalysis, manufacturing, and sustainable energy generation, constitute an impressive pipeline of developing impact.

Synthesis and Catalysis:

- A new drug discovery platform 'MagicTag[™] provided a lead compound for adenocarcinoma treatment, passing phase 2 clinical trials with ValiSeek (<u>Marsh</u>).
- Development of light-activated anti-cancer metallo-drugs (Sadler) with AngloAmerican.



- <u>Fox</u> works closely with drug development companies (Epsilon3Bio, STXPharma, RxCelerate), providing lead compounds and synthesis expertise to their multi-£M investments, with compounds reaching phase 1 (2020) and phase 2 (2014) clinical trials.
- Macrocyclic peptides as drug candidates (<u>Shipman</u>) patent pending with Nanna Therapeutics.
- Commercialisation by JM, and additional patent with GoldenKeys (China), of asymmetric transfer hydrogenation catalysts (<u>Wills</u>).

Chemical, Structural, Synthetic Biology:

- The spinout Erebagen (July2020), supported by Innovate UK ICURe/BBSRC funding, will develop a synthetic biology platform for creation of novel natural product libraries (Challis).
- Development of a bioengineered library of antibiotics targeting *Acinetobacter baumannii* (WHO 'critical priority' pathogen) (European / US patents) (<u>Challis</u>).
- Collaboration with Biome Bioplastics, supported by BBSRC, EPSRC and Innovate UK grants, generating feedstock for bioplastic synthesis *via* lignin degradation (Bugg).

Materials and Polymers:

- New polymers for delivery of chemotherapeutic drugs (<u>Perrier</u>) featured in the 'Stand Up To Cancer' campaign (CRUK/Channel4, 2018).
- The new (Oct2020) spinout 'Cryologyx' markets cryopreservatives for cell and tissue cold-storage for medical use under a licensing agreement with GE healthcare (<u>Gibson</u>).
- <u>Gibson</u> has developed a cheap, rapid diagnostic tool for COVID-19, currently at the spinout stage (glycandx.com).
- New heterogeneous catalysts for electrocatalysis and cleaner air patents pending with JM (<u>Walton</u>).

Measurement and Modelling:

- Mass spectrometric analysis of polluting oil residues in Canada, *via* the government agency 'Environment and Climate Change Canada' (<u>Barrow</u>). The underpinning software is being tested further by ExxonMobil; Bruker Daltonics want to license it for use in their FTICR-MS instruments.
- Understanding mechanisms of photo-protection with sunscreens, and development of a THz 'skinometer' to improve skin cancer prevention and treatment, with Lubrizol (<u>Stavros</u>).
- The spinout 'Verdel Instruments' develops and markets hardware for 2-D mass spectrometry (<u>O'Connor</u>).

Beyond research, our extensive contributions to the chemistry community, nationally and internationally, include:

• Journal editorships: <u>Becer</u> (European Polymer Journal, 2018-); <u>Bugg</u> (Bioorganic Chemistry, 2013-18); Haddleton (Polymer Chemistry, 2009-17); <u>Ward</u> (RSC Advances, 2011-18).



•	Other journal EB memberships / Associate Editorships: <u>Blindauer</u> (x2), <u>Bugg</u> , <u>Challis</u> (x4), <u>Gibson</u> (x5, including <i>Biomacromolecules</i>), <u>Lewandowski</u> , <u>Maurer</u> (x2), <u>Perrier</u> , <u>Sadler</u> (x4, including <i>Organometallics</i>), <u>Scott</u> , <u>Stavros</u> , <u>Unwin</u> (x6, including <i>Langmuir</i>), <u>Ward</u> , <u>Wills</u> ; 13 Advisory Board memberships.
•	<i>Book editorships</i> : <u>Bon</u> (RSC Soft Matter series, 2015); <u>Walton</u> (RSC Inorganic Materials series, 2017-).
•	 Learned society committees: <u>Barrow</u> (British Mass Spectrometry Society, Committee member, 2015-; Education officer, 2018-). <u>Blindauer</u> (Society for Biological Inorganic Chemistry council, 2015-19; RSC Inorganic Biochemistry group committee, 2012-). <u>Bon</u> (Chair, International Polymer Colloids Group, 2014-15). <u>Dixon</u> (Trustee and Treasurer, British Biophysical Society, 2018-20; Secretary, RSC Biophysical Chemistry group, 2007-17). <u>Gibson</u> (Chair, RSC Carbohydrate group, 2017-19). <u>Habershon</u> (RSC Faraday Division council, 2018-; secretary / treasurer, RSC Theoretical Chemistry group, 2018-). <u>Haddleton</u> (RSC Publishing Board, 2017-). <u>Lewandowski</u> (RSC Faraday Division awards committee, 2016-18). <u>O'Connor</u> (British Mass Spectrometry Society executive committee: member, 2015-18; trustee and treasurer, 2018-) <u>Tosin</u> (RSC Chemical Biology and Bioorganic group committee: member 2015-20, Chair 2020-). <u>Unwin</u> (ACS Electrochemistry Award panel, 2019-; Society of Electroanalytical Chemistry Awards panel (2019-); UK Blavatnik Awards Jury for Chemistry (2017-20); Chair for Experimental Electrochemistry Prize panel (2020-). <u>Ward</u> (RSC Dalton division awards committee, 2018-20).
•	Conference organisation: Staff at all levels participate in conference organisation with ≈80 conferences worldwide benefiting from our involvement. Major contributions (Organising Committee Chair level) include: <u>Bartók-Pártay</u> (Psi-K conference, Lausanne, 2020) <u>Blindauer</u> (RSC Dalton Meeting, Warwick, 2016). <u>Bon</u> (International Polymer Colloids Group Meeting, New Hampshire, 2015). <u>Bugg</u> (Annual ESBOC symposia, Wales, 2014-18). <u>Challis</u> (RSC 'Directing Biosynthesis' conferences, 2015, 2017, 2020; Innes-Boskovic Summer Schools in 'Applied Molecular Microbiology', Croatia, 2018 and 2020). <u>Corre</u> (RSC Chemistry and Biology of Natural Products annual symposia, 2014-17). <u>Costantini</u> (Summer schools 'Nanoscience at Surfaces', Cambridge, 2016, 2018; IOP International Symposia on surface science, 2017, 2018) <u>Dixon</u> (RSC Faraday Joint Interest group conference, Warwick 2017). <u>Gibson</u> (RSC Carbohydrate group 100 th Anniversary meeting, 2016). <u>Habershon</u> (Faraday Discussion 'Quantum Effects in Complex Systems', Warwick, 2019; 'Quantum Effects on Condensed Phase Systems' series, USA, 2015, 2017, 2019). <u>Haddleton</u> (Warwick Polymer Chemistry meeting, 2016). <u>O'Connor</u> (European FTMS biennial meetings, 2014-2020).



Perrier (IUPAC Macro conference, Cairns, 2018). Shipman (RSC Organic Division meeting, Warwick, 2019). Sosso / Maurer (RSC Faraday meeting 'Computational Molecular Science', UK, 2019). Stavros (RSC Spectroscopy and Dynamics meetings, 2016 and 2020). Unwin [RSC Faraday Discussions (York, 2016; Bath, 2018); Symposia 'Single Nanoparticle Electrochemistry', Pittcon, Chicago, 2017 and 'Single Entity Electrochemistry', ISE Meeting, Bologna, 2018]. Other significant contributions: Brinkert: Member, UK Space Exploration advisory committee (2020-). Bugg: Co-Director, BBSRC-funded 'Lignocellulosic Biorefinery Network' (2015-19). Challis: Expert Committee Member, Novo Nordisk Foundation Challenge Program (2016); Expert Committee Member, Canada Foundation for Innovations 2020 funding competition. Gibson: ERC Consolidator grant panel member (2016-18). Lewandowski: Executive committees, EPSRC National Solid-State NMR facility (2020-), MRC Collaborative Computational Project for NMR (2019-). O'Connor: Chair/organiser of British Mass Spectrometry Society 'vision committee' to develop 5/10/20y roadmap for EPSRC. Rogers: Member, RSC Members Communities Board (2018-2020). Sadler: Chair, Royal Society Summer Science Exhibition Committee (2013-19); Vicechair, RS Public Engagement Committee (2013-2019). Scott: Chair, Advisory Board, EPSRC/RSC National Chemical Database Service (2013-2017). Tosin: MC member, EU-COST action CM1407. Expert witness work: Bon (Recictel, 2017); Haddleton (Olaplex, 2018); Becer (Hogan Lovells, 2018); Scott (Hogan Lovells, 2019); Perrier (Lubrizol 2018-19). Membership of RS funding panels (Newton fellowships, International Exchanges, etc.): Notman, Corre, Scott, Bon, Chaplin.

Research-based outreach & public engagement. Our strong outreach and public engagement events showcase our research to the general public and schoolchildren.

Schools-based events: We are renowned for bringing our research to schoolchildren *via* outreach activities. Our outreach lead <u>Barker</u> was shortlisted for a THES national award (2017); his work led to development of a broader institutional Widening Participation initiative in which he has been embedded in a local school since 2019. Together with our team of laboratory tutors (who have specific outreach responsibilities), and many academic staff, *>50000 schoolchildren have been reached by our schools-based events this REF cycle* with events varying from making slime (primary school children) to research-focussed presentations to senior students on machine learning (<u>Sosso</u>), drug development (<u>Fox</u>), antibiotics (<u>Jenner</u>, <u>Corre</u>), lasers (<u>Stavros</u>), electrochemistry (<u>Macpherson</u>) and 'elements of life' (<u>Sadler</u>). We hosted an RSC Education Coordinator (2015-20) and participated in the 'Spectroscopy in a Suitcase' programme. <u>Rogers</u> manages the Chem-BAM website (2017-20) – a hub for research-led outreach activities – and led the 'ChemBox2017' project (joint with Birmingham) which provides training and equipment for research-led activities to ten West Midlands schools where >250 students have enjoyed workshops on subjects including 'biopolymers for cancer' and 'chemistry of light'.



We have also hosted many *incoming* schools groups with >3500 visitors undertaking experiments in our teaching laboratories. The student ChemSoc has organised since 2016 an 'Annual Conference on Research in Natural Sciences' (ACORNS), which brings \approx 200 sixth formers from the region to hear talks from \approx 20 academics. Several academics have provided research-focussed workshops for school children as part of large grants: *e.g.* <u>Challis</u> (BBSRC sLoLa project), annual groups of six A-level pupils to examine natural product discovery; <u>Hatton</u> (EPSRC fellowship), workshops (2017, 2019) for groups of 35 y9/10 children, making simple solar cells using fruit-based dyes; <u>Stavros</u> (EPSRC grant for WCUS), one-day event 'Improving the world with lasers' for year 7-10 children (2019). We have provided *ca.* 20 individual research internships (*e.g.* Nuffield research placements) for sixth-formers.

Public engagement activities: These have taken many forms with colleagues using research as the basis of events from local 'Pint of Science' or 'Café Scientifique' lectures (<u>Sosso</u> x3, <u>Bon</u> x2, <u>Corre</u>, <u>O'Connor</u>; ≈50 attendees) and a Warwick Christmas lecture (<u>Sosso</u>, 2018; 1000 attendees) to national-level events like the Sept2019 British Science Festival, held at UoW (128 events, 16k attendees), involving presentations from <u>Ward</u>, <u>Hatton</u>, <u>Macpherson</u>, <u>Bugg</u>, <u>Sadler</u> and <u>Notman</u>. Week-long Royal Society Summer Science Exhibition exhibits were provided by <u>Macpherson</u> ('Diamond is More than Just a Gemstone', 2016, >12k visitors) and <u>Sadler</u> ('In your element - A periodic table for life', 2019, >5k visitors): <u>Sadler</u> has given his 'Periodic Table' talk in schools all over the world. Other examples: <u>Bon</u> (RSC Materials Outreach lecturer 2015-16); <u>Gibson</u> (Cheltenham Science Festival, 2015); <u>Barrow</u> (British Museum, 2018); <u>Macpherson</u> ('Science Lates', London Science Museum, 2015). <u>Unwin</u> hosted Leverhulme-Trust funded 'artist in residence' <u>Courtney</u> (2016) who helped researchers to develop artworks from chemistry research images which were used at public events in Coventry (Earlsdon Festival; Herbert gallery).