Institution: University of Bristol
Unit of Assessment: 8: Chemistry
1. Unit context and structure, research and impact strategy

The School of Chemistry at Bristol is one of the largest, most globally engaged, and vibrant departments in the UK. It leads within a world-class enabling eco-system of cross-disciplinary research institutes, industrial partnerships, entrepreneurial incubators and physical infrastructure. Our continued success and scientific identity are built on the intellectual quality, energy and enthusiasm of our staff and students; broad-ranging academic strength across the entire discipline; entrepreneurial culture; awareness of global impact and environment; and a collaborative, supportive, and diverse science environment that pervades the entire School.

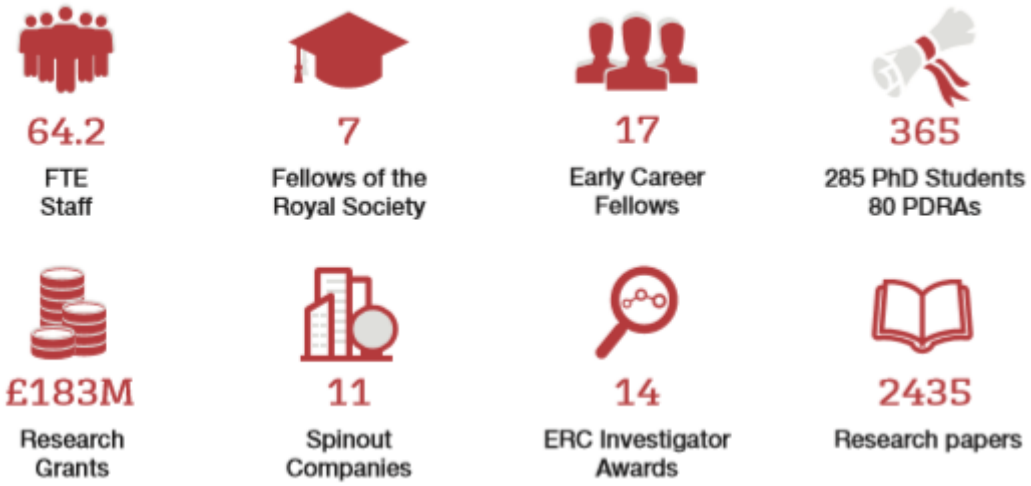

Figure 1.1 Bristol Chemistry REF2021 Submission [all references to people in this figure are current headcounts]

Our goal is to make fundamental and transformative contributions to the discipline, providing leadership and innovation in the field and high-quality training for the next generation of leaders in science. We are at the centre of national and global initiatives, including antimicrobial resistance, climate change, synthetic biology and digital chemistry. Following REF2014, we renewed our research strategy and restructured our research groupings into more focused Themes. We refreshed our leadership, improved the diversity of our appointments (including recruiting our first female Head of School), and substantially expanded our entrepreneurship and translation activities as well as producing significant global social and policy impacts.

The strength, depth and diversity of our School, and the success of our focus on intellectual excellence, impact, collaboration and collegiality, is shown by a selection of highlights in the REF period:

- *People* - Our world-leading staff include seven Fellows of the Royal Society (FRS), with at least one in every research Theme. Five are in post (**Aggarwal, Ashfold, Evershed, Mann, Orr-Ewing**), one retired in 2017 (**Simpson**) and one moved to a prestigious Canada Research Chair in 2019 (**Manners**). We also have 4 Members of the Academia Europaea and 10 RS Wolfson Research Merit Awardees.

- *Impact* - Substantial impact activities include the spinout of 11 companies from academic staff and another 2 from our students, *e.g.* Ziylo (**A. Davis**), which was bought by Novo Nordisk in a deal worth up to US$800M (awarded Global University Venturing Exit of the Year 2019) – generating up to £39M for the University. A new company Carbometrics, spun out as part of the deal, could yield as much again. The creation of Ziylo led our chemists to independently establish UnitDX, a deep tech incubator in central Bristol which has already supported a community of 57 companies in biomedical and other chemically-based disciplines (£40M of investment by December 2020).
- *Funding* - £183M of research grants awarded (Principal Investigator (PI) and Co-Investigator (CoI)) and £13.6M of investment in our equipment base. These include major grant successes such as 7 European Research Council (ERC) Advanced Investigator Grants, 4 ERC Consolidator Grants, 3 ERC Starter Grants, 2 Horizon2020 Future and Emerging Technologies (H2020 FET), 2 Biotechnology and Biological Sciences Research Council Strategic Longer and Larger Grants (BBSRC sLOLA), 1 Engineering and Physical Sciences Research Council (EPSRC) National Consortium and 2 EPSRC Programme Grants.
- *Diversity* - Our strong commitment to Equality, Diversity and Inclusion (EDI) is evidenced throughout this submission. There are 11 female staff (*cf* 5 in 2014) across every career-stage, including 2 females in our 4-strong senior leadership team (*cf* 1 in REF2014), 3 female professors (*cf* 1 in REF2014), and 7 female early career researchers (ECRs) (*cf* 3 in REF2014) and 6 staff from ethnic minorities (*cf* 3 in 2014). We have hosted 66 independent early career fellows (19 female) in the School during the REF period, with 17 included in our REF submission.
- *Covid-19 Response* - A key example is the Bristol Aerosol Research Centre (**Bzdek**, **Cotterell**, **Reid**) which is leading Covid-19 projects to inform the Scientific Advisory Group for Emergencies (SAGE) and UK Chief Medical Officers, with **Reid** sitting on the Department for Environment, Food & Rural Affairs (DEFRA) Environmental Transmission and Department for Digital, Culture, Media and Sport (DCMS)/Public Health England (PHE) Advisory sub-groups of SAGE. A further £1M of funded programs of research across the School are centred around the Covid-19 virus, treatments and transmission.
- *Training* - We lead and partner in 11 Centres for Doctoral Training (CDT) (14 in the REF period) spanning every Research Theme in the School. Our success in developing the next generation of chemists is exemplified by our award-winning Chemical Synthesis CDT which has run continuously since 2009 (funded to 2028) and published over 225 research papers in that time.
- *Prizes and Awards* - Over 40 leading International and UK awards for our staff; including: International Union of Pure and Applied Chemistry (IUPAC) Distinguished Women in Chemistry/Chemical Engineering Award (**Willis**), RS Davy Medals (**Aggarwal FRS**, **Mann FRS**), RS Wolfson awards (**Manby**, **Raven**, **Woolfson**), Phillip Leverhulme awards (**Glowacki**, **Bower**), American Chemical Society (ACS) Cope Scholar Award (**Aggarwal FRS**), Humboldt Research Award (**Aggarwal FRS**, **Woolfson**), Prix Franco-Britannique, Société Française de Chimie (**Clayden**), Herbert P. Broida Prize of the American Physical Society (**Ashfold FRS**), Yamada-Koga Award (**Aggarwal FRS**), JMT Medal (**Mulholland**), ACS Pimentel Award (**Shallcross**).

Research Strategy and Objectives

A root-and-branch review of our research areas in 2014 identified the need to encourage greater interdisciplinarity, impact-focus, and agility to address global challenges and enhance our impact and innovation environment, while maintaining the breadth of expertise and critical mass required for excellence across chemical science. We reconfigured into 5 Research Themes (previously 9) that define key focus areas and link to the wider research landscape through University Research Institutes and external partnerships. This approach provides flexibility to shape the direction of emerging research areas and respond to new initiatives such as those in minimal biology, interactive VR, machine learning and robotic synthesis, as well as addressing global challenges such as air pollution, climate change, Covid-19 pandemic response and antimicrobial resistance. These streamlined and focused Themes enabled us to map a new research agenda to provide leadership in Digital Chemistry (developing and applying digital tools for chemical science) and Global Change (developing and applying chemical science for emerging global challenges). These scientific ambitions align with our parallel impact strategy to encourage a culture of entrepreneurship and societal impact (see *Impact Strategy and Objectives*) enabled by the evolution of new infrastructures within the University, wider City of Bristol and the South West.

Overview: Our core research strategy is to enable individual excellence and a critical mass of expertise and resources while preserving our collegial and collaborative environment, and build partnerships in interfacial and challenge-led areas. Our priorities and objectives are:

- International intellectual and scholarly leadership in our core Research Themes and partner disciplines, with overarching ambitions in Digital Chemistry and Global Change.
- Supporting delivery of impact in areas of global and national importance such as air pollution, climate change, sustainability, Covid-19, and antimicrobial resistance.
- Expanding our culture of entrepreneurship, providing our researchers with tools and opportunities to translate their research into solutions of value to industry and society.
- Providing an inclusive, diverse, collaborative and interdisciplinary research environment which nurtures future leaders in the discipline.
- Growing our outstanding infrastructure and equipment base to integrate strongly with our Research Themes.

Research Structure

The five new Research Themes which emerged from our 2014 review are: **Chemical and Synthetic Biology**; **Computational Chemistry**, **Theory and Dynamics**; **Environment and Energy**; **Functional Molecules and Materials**; and **Synthesis and Catalysis**. Research strategy is developed and overseen by the Research Committee, comprising the Research Director, Theme Leads, Infrastructure Lead, Industry Lead, ECR Representative, Impact Lead and School Industry Partnership Manager (a post created through dividends from the Ziylo sale).

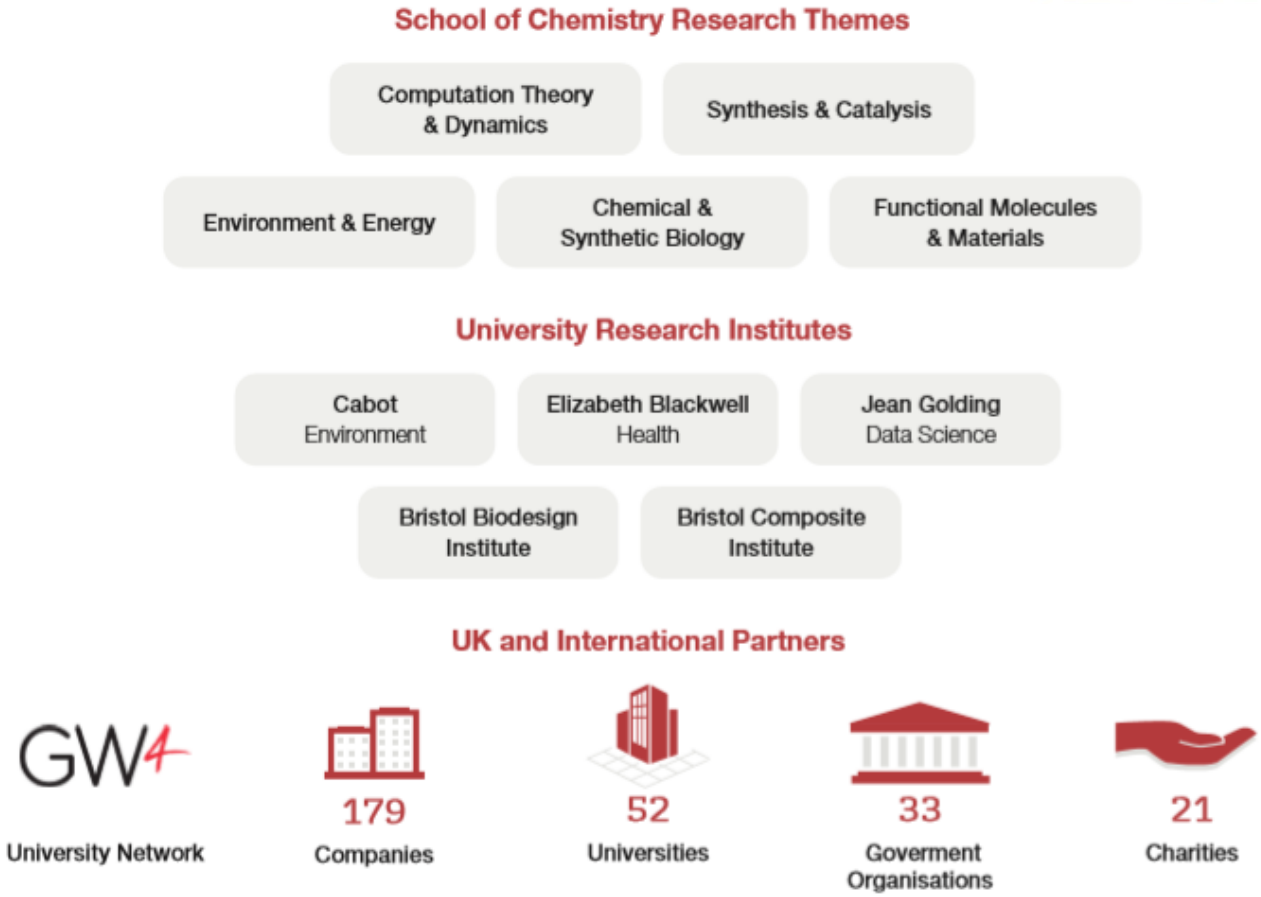

Figure 1.2: School of Chemistry Research Environment

Our Research Themes (described below) are designed to be at the frontiers of the discipline with most staff being members of more than one theme. The Theme Leads provide strategic oversight, identifying blue skies and impact-focused topics that cut across activities, which can form the nucleus for large-scale initiatives, *e.g.* recent examples include 'eco-formulation' and 'digital synthesis'. Theme leads also coordinate large-scale project and equipment bids, postgraduate researcher (PGR) training and seminar programmes. They advise the School Executive Board on academic staff recruitment, including attracting research fellows into our early career pipeline which has underpinned our substantial improvements in diversity over the REF period.

Integration into wider research infrastructures: Our Themes are strongly integrated with the multidisciplinary University Research Institutes (URIs; see Institutional-level Environment Statement (REF5a) focusing on Environment (Cabot Institute), Data Science (Jean Golding Institute (JGI)) and Health (Elizabeth Blackwell Institute (EBI)), supported by Specialist Research Institutes (SRIs), *e.g.* the Bristol BioDesign Institute (co-lead **Woolfson**, Chemistry and Biochemistry) and the Bristol Composites Institute (Engineering and Physics), and institution-wide programmes, *e.g.* BristolAMR antimicrobial resistance network (led by **Mulholland**) and Advanced Computing Research Centre. Our leadership in these pan-university bodies ensures the School influences and aligns with University of Bristol (UoB) strategy and enables us to seize cross-disciplinary opportunities rapidly and effectively. This is channelled outward through the GW4 grouping of research-intensive universities in the South West (Bristol, Cardiff, Bath and Exeter). Theme descriptions and Section 4 provide further detail on our leadership and integration into national and international research infrastructures.

NOTE: *In theme descriptions, numbers of academic staff and ECR/postdoctoral research associate (PDRA)/PhDs are* **current** *values. Academic staff are counted for every Theme to which they contribute, but ECR/PDRA/currently enrolled PhDs and other metrics are assigned to their most closely aligned Theme and counted only once.*

Chemical and Synthetic Biology (CSB) Theme (Lead: Crump)

Figure 1.3: Chemical and Synthetic Biology Theme

This interdisciplinary Theme is underpinned by strong links to the University's Elizabeth Blackwell Institute, and leads cross-University programmes, such as the Bristol BioDesign Institute and BristolBridge antimicrobial resistance project. It is closely allied with the Schools of Biochemistry and Biological Sciences in the Life Sciences Faculty, strengthened by joint appointments (**Parmeggiani**, **Woolfson**). Successes over the REF period include:

- Establishing the UK's first Max Planck Institute (MPI) in physical/biological sciences (**Mann FRS/Woolfson**). The Max Planck Centre for Minimal Biology is hosted in Chemistry and led in partnership with Biochemistry (Berger) and leading scientists at MPIs in Heidelberg, Mainz and Munich. It creates international partnerships addressing the most challenging questions in minimal biology and biodesign, advancing the future of health and medicine, *e.g.* a US$2M US/UK partnership (National Science Foundation/BBSRC) to probe cell morphogenesis.
- Major collaborative programmes, including the BBSRC/EPSRC-funded BrisSynBio Synthetic Biology Research Centre (**Woolfson** PI; **Crump**, **Mulholland**, **Simpson FRS**, **Willis**, CoIs; £15M, 2014–2021, >170 research papers; 9 patents (3 for Chemistry), 4 spinout companies (2 for Chemistry)); Global Challenges Research Fund and Healthcare/Impact Partnerships to develop the next generation of bio-inspired carbon dot probes for rapid bacterial detection (**Galan** PI, £1.6M); BBSRC sLOLA grants in natural

products with high value (**Mulholland** CoI with Manchester, £3M) and agrochemical leads (**Willis** CoI with Warwick, £3.5M).

- Developing the next generation of bio-science experts through partnership in two major CDTs: SynBio CDT (Bristol, Oxford, Warwick, industry and public partners); BBSRC South West Biosciences Doctoral Training Partnership (SWBio DTP) (led by Bristol, with GW4 partner Universities).
- Two spinout companies: **Glaia** (**Galan**, 2019) develops nanotechnologies for agriculture to increase crop yields and allow crops to be farmed outside their traditional growing regions; **Rosa Biotech** (**Woolfson**, 2019) exploits α-helical barrel technology in biosensing and medical diagnostics, and won the Health Award at the Royal Society of Chemistry's Emerging Technologies Competition (2019).

Research Highlights: Defining the nature of the catalytic ferryl species in a heme enzyme, thus resolving >40 years of debate on the identity of this intermediate (*Science* 2014); Identifying a bona fide natural Diels-Alderase in the biosynthesis of the antibiotic abyssomycin (*J. Am. Chem. Soc.* 2016); Demonstration and the first mechanistic interpretation of heme as an activator of cardiac K_{ATP} ion channels (*PNAS* 2016); Design and construction of entirely new protein structures - α-helical barrels (*Science* 2014) and miniproteins (*Nat. Chem. Biol.* 2017); Resolving a long-standing issue of whether or not the α-helix dipole truly stabilises protein structures - it does not (*Nat. Chem. Biol.* 2015); Controlling intracellular uptake and organelle localization using glycan-coated nanoparticles, with implications for targeted drug delivery systems (*Angew. Chem. Int. Ed.* 2014); Showing that artificial foldamers will insert into vesicle membranes and respond to stimulation by light (*Science* 2016) and ligand binding (*Nat. Chem.* 2017).

Computational Chemistry, Theory and Dynamics (CTD) Theme (Lead: Orr-Ewing FRS)
The CTD Theme focuses on using fundamental theory and advanced experimental techniques to investigate, predict and understand dynamics and reactivity in molecular and materials science. It links substantially into all Themes in the School, and more widely in the University, *e.g.* Physics, Biological Sciences, Biochemistry, and the Cabot, JGI, EBI, and BioDesign Institutes. The Theme works closely with industry including Oracle, BP, Dow Chemicals, Janssen Pharmaceuticals, Amgen, Element 6, Hyundai, Bridgestone and AWE. Researchers are exceptionally well-served with world-leading equipment including ultrafast laser laboratories, a unique and pioneering VR suite, and University Advanced Computing Research Centre High Performance Computing (HPC) resources and specialist Research Software Engineers (led by **Woods**). Theme members are also major users of large-scale national and international equipment infrastructures, UK Tier 1 and 2 HPC Facilities and international beamlines (see Section 3).

Figure 1.4: Computational Chemistry, Theory and Dynamics Theme.

Successes over the REF period include:

- Leading major grants: ERC Advanced Grant (**Orr-Ewing FRS**, €2.5M); 4 EPSRC Catalysis Hub grants (**Mulholland** (CoI), £14M total) EU FET-Open grant (**Oliver** (CoI), €4.9M with Warwick and EU partners); ERC Consolidator Grants (**Glowacki**, €2.0M; Royall – joint appointment in UoA9, €2.0M); EPSRC Programme Grants (**Ashfold FRS**, £4.6M; **Glowacki** (CoI), £4.1M with Maths).
- Developing the next generation by hosting 4 RS/UKRI-funded ECR Fellows in the REF period (**Bourne-Worster**, **Glowacki**, **Oliver**, **Rigby**) and the Bristol hub of the EPSRC Theory and Modelling in Chemical Sciences CDT (Oxford, Bristol, Southampton) which has trained 81 students and is partnered with 20 international companies.
- 3 spinout companies: **Entos** (**Manby**, 2020) is commercialising electronic structure and dynamics software, attracting substantial Silicon Valley venture capital (confidential value, but has built a team of 17 scientists/engineers) with a multi-million dollar grant from Schmidt Futures to develop "Envision", a platform for chemical discovery and education; **ArtSci** (**Glowacki**, 2018) is a not-for-profit company commercialising an open-source, multi-person interactive molecular dynamics virtual reality (VR) software framework - 'Narupa'; **Dynamerse** (**Bennie**, 2019) creates interactive dynamic simulation environments for industry – winning the Creator Fund Challenger 2020 award (beating 400 other start-up companies from UK universities).

Research Highlights: Computational discovery of ultra-fast energy dissipation mechanisms in collisions of atoms with graphene (*Science* 2019); Pioneering VR tools for interactive molecular dynamics simulations (*Sci. Adv.* 2018); Computational and spectroscopic stereochemical molecular structure elucidation from 128 possible diastereomers each with >6 million potential conformations (*Nature* 2017); Combining ultrafast infrared (IR) spectroscopy with atomistic simulations to unravel the dynamics and energy dissipation mechanisms of exothermic reactions in strongly interacting solvents (*Science* 2015). Femtosecond to microsecond transient absorption spectroscopies observing reactive intermediates participating in multi-step photoredox catalytic cycles, for sustainable organic photocatalyst design (*J. Am. Chem. Soc.* 2018; *Nat. Commun.* 2019).

Environment and Energy (E^2) Theme (Lead: Briscoe)

The E^2 Theme leads our ambitions in Global Change, conducting world-leading research addressing Earth system chemistry (climate change, air quality, nutrient cycling) and developing new materials to generate clean energy and enhance food production. Theme members are deeply engaged with the Cabot and Elizabeth Blackwell University Research Institutes as well as UK and international governmental and non-governmental organisations such as the US Environmental Protection Agency (EPA), Intergovernmental Panel on Climate Change (IPCC), World Meteorological Organization (WMO), Department for Business, Energy & Industrial Strategy (BEIS), and Historic England.

Figure 1.5: Environment and Energy Theme

Successes from the REF period include:

- Developing the next generation by leading the new EPSRC Aerosol Sciences CDT (**Reid**, Bristol, Bath, Cambridge, Hertfordshire, Imperial, Leeds, Manchester) in a multidisciplinary collaboration with 50 industrial and public-sector partners, and substantial ECR success with 5 Royal Society and Natural Environment Research Council (NERC) independent fellowships (**Bzdek**, **Cotterell**, **Lloyd**, **Naafs**, **Roffet-Salque**) and an ERC Starter Grant (€2.3M, **Bzdek**).
- Driving international policy agendas in Global Change, *e.g.* the Atmospheric Chemistry Research Group (**O'Doherty**, **Rigby**, **Shallcross**) are founding members of the NASA-funded AGAGE (Advanced Global Atmospheric Gases Experiment), lead the WMO 2018 Assessment of Ozone depletion and chapters of the IPCC 2019 climate change report, as well as informing UK, USA, Thailand and South African governments on policy concerning greenhouse gases and air quality.
- Leading major multidisciplinary grants, including the Bristol Radiocarbon Accelerator Mass Spectrometer (BRAMS) (**Evershed FRS**, £1.9M) investment for organic geochemistry analysis across Archaeology, Chemistry and Earth Sciences; Photovoltaic Technology based on Earth Abundant Materials (PVTEAM) (**Fermin**, PI, £2.0M) which partnered 12 companies and universities including Tata, Johnson Matthey, and Pilkington focusing on sustainable thin-film photovoltaic technologies.

Research Highlights: Revealing the palaeoecological range of honey bees and their exploitation by pre-historic farmers (*Nature* 2015); Demonstrating that terrestrial temperatures in past elevated CO_2 worlds were much higher than previously thought, suggesting increased land warming due to anthropogenic climate change in the next century (*Nat. Geoscience* 2018); Identifying global increases in emissions of the banned ozone depleting substance, CFC-11, pinpointing eastern China as the primary source of the rise (*Nature* 2018; *Nature* 2019); Exposing the significant role of surfactants in cloud formation, radiative forcing and hence climate change (*PNAS*, 2020).

Synthesis & Catalysis (S&C) Theme (Lead: Aggarwal FRS)

Bristol is the UK's leading academic centre for chemical synthesis research, and this Theme spans the development and application of methods for the construction of molecular targets from ligands and catalysts to natural products, functional materials and biomimetic molecules.

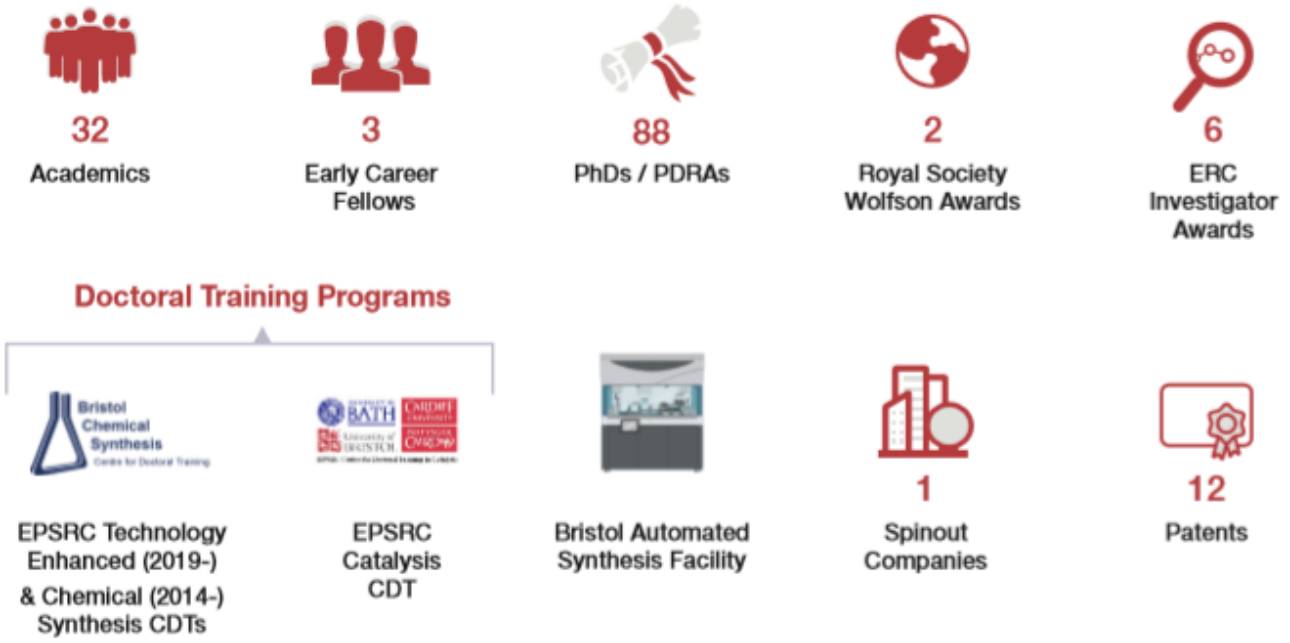

Figure 1.7: Synthesis and Catalysis Theme

Strengths in molecular synthesis underpin activity across the School, particularly in synthetic biology and biological and materials chemistry. New technologies for synthesis are a focus, particularly automated synthesis, flow chemistry, photochemistry, electrochemistry and biocatalysis. Activity is centred in the purpose-built Synthetic Chemistry Building, accommodating ~200 laboratory-based researchers and incorporating a dedicated and technician-supported instrument suite comprising GC, LC and TLC-MS reaction monitoring, reaction automation and purification capabilities. Successes over the REF period include:

- Leading (**Aggarwal FRS**/**Booker-Milburn**/**Clayden**) the UK's longest-running EPSRC-funded CDT (2009-). The latest evolution, the Technology-Enhanced Chemical Synthesis CDT (2019-2028), integrates machine learning, automation and other emerging digital and experimental technologies to enable chemical synthesis. Through this and our partnership in the EPSRC Catalysis CDT (2014-2023) we have trained over 80 PGRs during the REF period.
- 8 Major Individual Investigator awards (2 ERC Advanced grants (**Aggarwal FRS**, **Clayden**), 2 ERC Consolidator grants (**Bower**, **Galan**), 2 ERC Starter grants (**Bower**, **Lennox**), 2 RS Wolfson Research Merit Awards (**Aggarwal FRS**, **Clayden**).
- Major investments in Digital Chemistry, including the Bristol Automated Synthesis Facility which is capable of 128 parallel reactions (–70°C to 140°C, inert atmosphere, solid handling, automated purification; £750k, EPSRC) and VR laboratories which underpin the CDT and research programmes across the Theme.
- Commercialisation and enterprise success with 12 patents and technology transfer applications, *e.g.* Innosyn and Merck scale-up of **Aggarwal**'s decarboxylative borylation chemistry and spinout company Photodiversity (**Booker-Milburn**, 2015) applying high-throughput flow photochemistry to provide complex, sp^3-rich scaffold libraries to pharmaceutical and agrochemical industries.

Research Highlights: A modular approach to the synthesis of molecules designed to adopt linear/helical shapes through iterative homologation of boronic esters (*Nature* 2014; *Nat. Chem.* 2019); Exploiting conformational preferences to deliver a general and practical way to make new families of modified alpha-arylated amino acids (*Nature* 2018); Developing iron-based catalysts to

replace less abundant metals in cross-couplings (*Nat. Catal.* 2018); Coordination of Pd(0) to phosphine-modified block copolymer micelles induces inter-micelle cross-linking (*Nat. Commun.* 2016); Atom-economic catalytic methods for selective carbohydrate synthesis (*J. Am. Chem. Soc.* 2017; *Angew. Chem*. 2017); Elucidation of the mechanism of the most active homogeneous MeOH dehydrogenation catalyst known (*J. Am. Chem. Soc.* 2016); Using flow X-ray absorption spectroscopy to reveal the mechanism of iron-catalysed Negishi cross-coupling (*Nat. Catal.* 2019); Unique biocatalytic C-H functionalisation building heterocycles from a non-activated methyl group (*Nat. Catal.* 2018); The first sp^3 C-H bond activation based on metal-free ambient temperature photoredox catalysis (*Nature* 2020).

Functional Molecules and Materials (FMM) Theme (Lead: Patil)

The FMM Theme addresses interdisciplinary research challenges based on the development and application of new materials, spanning physical and biological sciences and engineering. Reflecting this breadth, the Theme membership extends over the Schools of Chemistry, Mathematics, Physics, Biochemistry and Mechanical Engineering, *e.g.* **Royall** (UoA 9) and **Fox** (UoA 8) are both joint appointments in Chemistry and Physics. The FMM theme is strongly integrated into University centres: for example, leading the Centres for Protolife Research (**Li**, **Mann FRS**) and Organised Matter Research (**Davis**, **Mann FRS**, **Patil**), and through close engagement with the Bristol Composite Centre and Interface Analysis Centre. Wider Theme links include the National Composites Centre, Advanced Composites Centre Specialist Research Institute, the Nanoscience and Quantum Information Centre, and the Bristol Robotics Laboratory.

Figure 1.6: Functional Molecules and Materials Theme

Successes from the REF period include:

- Five spinout companies: Ziylo (**A. Davis**, 2014) based on a breakthrough in glucose receptor development; Carbometrics (**A. Davis**, 2018) is developing new glucose sensor chemistry in market-leading continuous glucose monitors; Advanced Diamond X Ltd (**Fox**, 2018) provides commercial synthesis of ultra-high purity diamonds for materials applications; Eutomic Ltd (**Hall**, 2018) offers magnetic control of polymorphs for pharmaceutical and agrochemical applications; Arkenlight PLC (**Fox**, 2020) is commercialising diamond-based nuclear battery technologies.
- Co-leading (with Physics) the EPSRC Bristol Centre for Functional Nanomaterials (BCFN) CDT (£4.6M, 2014-2022) which now operates as a fully industrially funded programme, and partnering in the EPSRC Diamond CDT (2014-19, led by Warwick).
- Major grant awards in materials characterisation and control, *e.g.* MagnaPharm (**Hall**, €2.9M, EU FET-OPEN) to direct pharmaceutical polymorphism through crystallising in high magnetic fields; Establishing the world-leading and UK-unique NanoESCA Facility (**Fox**, £1.96M, EPSRC), possessing extraordinary surface sensitivity for energy-filtered Photoemission Electron Microscopy (PEEM) and micro-ARPES (Angle Resolved Photoemission Spectroscopy, 19 nm lateral resolution, 20meV energy resolution), for characterising electronic properties of nano-structured and two-dimensional materials.

Research Highlights: First demonstration of the micro-crucible mechanism of nanowire growth (*Science* 2014); Predicting a new class of non-sticky gels (*PNAS* 2020); Design and construction of protocells that exhibit novel functions (*Nat. Chem.* 2014), autonomic motility (*Nat. Chem.* 2018) and can be programmed for artificial phagocytosis (*Nat. Mater.* 2017), predatory behaviour (*Nat. Chem.* 2017), prototissue assembly (*Nat. Mater.* 2018) and chemical computation (*Nat. Nanotechn.* 2019). Demonstrating that simple inorganic salts control the porosities, pore size distributions and functionality of growing cross-linked conjugated microporous polymers (*Angew. Chem. Int. Ed.* 2019); Creating the best synthetic receptor for glucose, capable of outstanding affinity and selectivity in water – the most challenging of solvents (*Nat. Chem.* 2019); Designing anion carriers capable of operating in live cell membranes, implying potential for treating channelopathies such as cystic fibrosis (*Nat. Chem.* 2016).

Impact Strategy and Objectives

Our Impact strategy encourages a culture of entrepreneurship and policy impact across our School, enabled by supporting infrastructures that allow colleagues to identify and leverage the impact opportunities created by their research. Our School Industry Partnership manager leads our industry engagement, supported by the Faculty Science Partnership Office, to develop strategic partnerships with key companies who span our Research Themes. Key enabling structures within the University are Research and Enterprise Development (RED) team, who support commercialisation through spinouts and protection of intellectual property, and the PolicyBristol and Public Engagement teams who provide expertise and funding for policy and societal impacts (see REF5a). We also promote impact through external partnerships such as the award-winning UnitDX (lab-based) and SETSquared (non-lab based) incubators, as well as the Science Creates and Spin Up Science enterprises, that provide infrastructure, expertise and venture capital support for innovators (see REF5a).

Commercial Impact success: Establishing 11 spinout companies over the REF period, including the phenomenally successful Ziylo exit in 2018, is no accident. We have driven this forward by reinvesting income from spinouts and external partners into impact priorities, *e.g.* establishing a Royal Society of Edinburgh (RSE) Enterprise Fellow (**Bennie**) to develop interactive VR for catalysis that led to the spinout of Dynamerse; using the School's share of Ziylo income to fund: (i) an Industrial Partnership Manager to engage and enhance links and collaborations (ii) a Lecturer in Innovation in Education and (iii) a number of targeted PhD and PDRA posts in the School. We make significant use of Impact Acceleration Accounts (IAA), with 33 projects (£1.07M) funded to support commercialisation, knowledge transfer secondments, and early career researcher kickstarter grants alongside more exploratory projects. An exemplar of this is the world's first commercialisation of optical tweezers funded by an IAA knowledge transfer partnership in 2014 between **Reid** and BIRAL Ltd that has led to £1M of sales to date. Four of our successful spinout companies have developed from IAA support, *e.g.* ArkenLight (**Fox**) developed from two IAA projects to explore diamond and nanodiamond dynodes, and Glaia (**Galan**) from IAA-funded investigations of fluorescent carbon dots for rapid detection of bacteria. Our School worked with 179 companies in project sponsorship, consultancies, knowledge-transfer programmes and commercial research agreements and hosted 9 industrial professors during the REF period to maximise opportunities to identify and exploit current commercial challenges that our research can address. The entrepreneurial successes of our staff and student role models such as **Destecroix** (PhD graduate, Ziylo co-founder) have embedded this same culture into our student cohort, with 2 further spinout companies created by our students over the REF period (Anaphite, **Burrows**; Albotherm, **Allington**). We reinforce this commercial focus for postgraduates and undergraduates

by providing entrepreneurship/IP training and career mentoring opportunities for them (see Section 2).

Policy Impact Success: We work closely with PolicyBristol to bring together academic, policymaker and practitioner expertise to enhance the impact of our research by influencing policy at the local, national and international level. This is exemplified by our Impact Case Study "*Aerosol science informs clinical and public health policy on COVID-19 transmission*" which describes the contribution of the Bristol Aerosol Research Centre to informing the UK Chief Medical Officers, SAGE and the Department of Digital, Culture, Media and Sport about the risks of Covid-19 airborne transmission in medical procedures (*e.g.* anaesthesia, intubation/extubation, ventilation and dentistry) and the performing arts (*e.g.* singing and woodwind performance). Similarly, our Atmospheric Chemistry Research Group (**Shallcross, Rigby, O'Doherty**) contribute to and lead reports for the IPCC and WMO (both United Nations bodies). They have also worked with international governmental agencies (US EPA, Thai Pollution Control Department, UK Meteorological Office and BEIS, South African Weather Service, and health agencies in Laos and Vietnam), to enable policy change based on improved scientific data, *e.g.* informing decision-making which accelerated Thailand's implementation of EURO 6 emissions standards to 2022 from 2028.

Collegiality, collaboration and partnerships: Interdisciplinarity is a defining characteristic of our research, and a focus for our strategy over the REF period. This is demonstrated by joint appointments, *e.g.* with Biochemistry (**Parmeggiani**, **Woolfson**); Computer Science (**Glowacki**); Physics (**Fox**, **Royall**), and leadership of interdisciplinary endeavours, *e.g.* Max Planck Centre for Minimal Biology (**Mann FRS, Woolfson**) and BristolBridge (**Mulholland**). As an example, the latter brought together over 200 researchers across five Faculties to address antimicrobial resistance leveraging £3.8m in follow-on funds (including winning the Longitude Prize) to establish the now self-sustaining Bristol AMR cross-faculty research community, which has a £15.4M funding base and is a Research Strand of the Elizabeth Blackwell Institute. Section 4 describes further examples of leadership across disciplines, including founding of BrisSynBio and the Bristol Biodesign Institute (**Woolfson**, Berger (Biochemistry)) and chairing Steering Groups of the UK Catalysis Hub and UK central counterparties (CCP) (**Mulholland**) and CCP5 (**Allan**).

Open Science: Bristol Chemistry is committed to Open Science (see REF5a). We firmly believe that a culture of transparency and openness ensures effective communication and dissemination as well as the highest quality science. **Woods** leads the UK Research Software Engineering community where the default position is open-source projects with open data. In software our School leads in open-licence practices, with examples including Narupa (**Glowacki**), PGOPHER (**Western**), BioSimSpace (**Mulholland**, **Woods**), Elfin (**Parmeggiani**), IMPRESSION (**Butts**, **Glowacki**); SCORER, BUDE and CC+ (**Woolfson**). Staff are also involved in Open Data initiatives, including a community commitment (*J. Chem. Inf. Model.*, 2020) led by **Mulholland** to share data and models on Covid-19 targets, and NMReData (**Butts**) which aims to provide greater transparency and quality in reported spectroscopic data. All our research outputs and published datasets are made open access via our institutional repository (PURE) and Research Data Storage Facility.

Future Research Directions

We have a clear vision for our future research direction, with strong support from the University which is investing in the development of Digital Chemistry and Global Change as the unifying elements in our research strategy. We believe that Digital Chemistry, broadly defined as the application and development of digital tools in chemical science, will transform our discipline over the next decade. Our commitment to this is demonstrated by ~£3.0M of funding (EPSRC, BBSRC, RSE, BP, University) in the last two years. This has included automated synthesis robotics integrated with predictive quantum chemistry and machine learning techniques (**Butts/Aggarwal FRS**), as well as equipment and fellowships for VR development and translation (**Bennie**, **Glowacki**, **Mulholland**, **Allan**) and new computing and data storage infrastructure (**Fey**). This is on top of £20M of University investment ring-fenced for HPC facilities over the next decade. Similarly, our ambitions in Global Change see chemical science as a crucial element in solving the increasingly global challenges of our modern world, particularly climate and sustainability. Activity will be driven through our existing Atmospheric Chemistry and Aerosol centres as well as new initiatives such as Eco^3-formulation (Lead: **Briscoe**) which targets cross-disciplinary and industrial engagement in formulation, chemical synthesis, catalysis and functional materials to reduce environmental impact. The School's strategic focus on innovation, translation and industrial partnerships will be enhanced by opportunities provided by the University/Bristol City Council partnership to create the Temple Quarter Enterprise zone in Bristol city centre (2020-), one part of which is a recent £1.5M UKRI award to enable University partnership in expansion of UnitDX, with laboratory capacity set to treble in 2021. We have also recently created an Entrepreneur-in-Residence role (Phil Bates, formerly Oracle), funded by the Royal Society – this will focus on a translational remit linked to Digital Chemistry and will provide in-house specialism to support our staff in commercialising and spinning out their research. These impact-focused initiatives coupled to our forward-looking research programs will ensure we are well placed to continue our success into the future.

2. People

Demographics, Staffing Strategy and Staff Development

The School currently has 63 permanent academic staff comprising 32 Professors, 6 Readers, 5 Senior Lecturers, 4 Lecturers, with 9 core-funded Research Fellows and 7 Teaching Fellows (2 Professorial) who support research and teaching activities respectively. We also host 17 independent research fellows, all submitted to REF, three of whom hold proleptic Lectureships. We are proud that we have substantially improved our diversity profile since REF2014, especially with women in key leadership roles across our senior leadership team (50% female) and decision-making committees (>30% female/transgender/BAME membership in Research, Teaching and EDI Committees).

Staffing and diversity strategy: Our core staffing strategy is to build an inclusive, supportive environment within a world-leading research infrastructure that attracts and retains a diverse community of the very highest intellectual quality. We ensure that succession planning and recruitment processes take three factors into account: research excellence, maintaining a breadth of expertise across our Research Themes, and equality of opportunity. We have balanced strategic appointments at professorial level (**Clayden** in Synthesis & Catalysis; **Raven** in Chemical and Synthetic Biology) with attracting, and making permanent appointments (proleptic where needed) from a strong early career pipeline of leading independent Research Fellows across all our Research Themes (**Bzdek**, **Fey**, **Glowacki**, **Lennox**, **Naafs**, **Oliver**,and **Rigby**). This emphasis on

strength in depth and our early career pipeline is also delivering an improving gender profile since REF2014, roughly doubling BAME and female representation across all career levels (Figure 2.1) and a well-balanced age profile (average age **45**). Similarly, our commitment to the long-term support of our staff is reflected in low numbers of fixed-term positions, all arising from externally funded fellowships (14%). These diversity improvements are especially noteworthy given limited opportunities to recruit during the REF period, with low turnover of permanent academic staff (only 6 leaving) in that time – our staff rarely want to leave our strong and collegiate research environment.

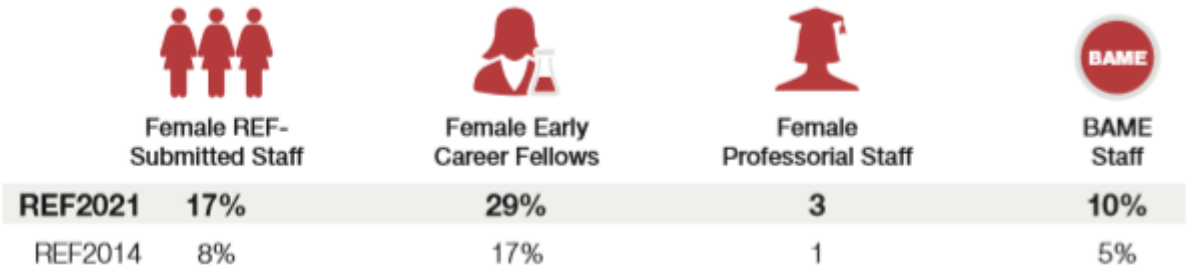

Figure 2.1: Chemistry staff diversity

Over the next REF period we will build on this strategy, targeting mid-level professorial appointments in our focus areas of Digital Chemistry and Global Change, while maintaining our strong early career pipeline, using proleptic appointments to ensure excellence across the breadth of our Research Themes and prioritising diversity in all recruitment processes.

Developing a high quality and diverse early career pipeline: Our long-term future success is built on our talent development strategy: identifying, attracting, and nurturing the best and brightest minds. Our research strength, infrastructure and collegial environment ensure that we are an attractive School for early career staff to undertake their independent fellowships.
ECRs are proactively identified and engaged in discussions around their future ambitions and directions. In cases where there is a good science match on both sides, a senior mentor is appointed, and candidates are encouraged to apply for independent fellowships. We work closely with fellowship applicants and the University's RED team to prepare them for the application and interview processes, including mock interviews with panels of senior staff. Once in post, they are embedded within Research Themes that provide vibrant and intellectually stimulating environments, with support and mentorship by senior colleagues within those themes. Our Staff Review and Development process (see below) provides a structure for ECRs to build their long-term science plans with full support from their mentor and Theme leaders. The School strategically invests in talent development, providing ECRs with independent research lab space, prioritising requests for PhD studentships, funding new equipment to support grant proposals, prioritising their applications to competitive funding calls, and covering costs for access to instrument Facilities. We also ensure very minimal teaching loads through our Workload Allocation Model, to support them in launching successful research programmes.

Clear evidence of the success of this strategy and our ability to attract leading ECRs from across the globe to Bristol is that we hosted a total of 66 independent fellows in the REF period, funded from a wide range of grant agencies (29% female, 70% international). This included 8 RS URFs, 2 RS Dorothy Hodgkin Fellows, 1 EPSRC Early Career Fellow, 2 NERC IRFs, 7 RS Newton Fellows,

39 EU Marie Curie Fellows, 1 Royal Commission for the Exhibition of 1851 Fellow, 1 RSE Enterprise Fellow, and 1 EPSRC Research Software Engineering Fellow.

Successes of our early career staff: Our successful mentoring of our ECRs is evident in their major grant successes, notably 3 ERC Starter grants during the REF period. Similarly, of the 14 ECRs in our previous REF2014 submission, four have already been promoted to Professor in Bristol (**Galan, Royall, Bower, Rigby**), three to Reader/Senior Lecturer (**Glowacki**, **Fey** and **van Der Kamp** (now in Biochemistry)) and six have taken academic appointments elsewhere (**Tew**/Oxford, **Hudson**/British Columbia, **Bonet**/Hull, **Zheng**/Northwest, **Grubb**/Fort Lewis, **Leitao**/Auckland). All of this demonstrates the excellence of academic training and support that we offer through our talent development strategy.

Staff departures: We take enormous pride in the achievements of staff who excel with us, and the strength of our support and environment that allows them to continue to succeed in their discipline elsewhere. During the REF census period, four permanent academic staff left us, each of them to prestigious roles in other institutions: **Bower** (to Regius Research Chair, Liverpool, 2020), **Harvey** (to Head of Quantum and Physical Chemistry, Leuven, 2014), **Manners FRS** (to Canada Research Chair, Victoria, 2019) and **Wass** (to Director of Catalysis Institute, Cardiff, 2018). In addition, **Simpson FRS** retired to an Emeritus Senior Research Fellowship (2017) and **Pancost** moved to Head of Earth Sciences in Bristol (2018).

Visiting scholars: We typically host ~30 visiting scientists within the School at any time, as well as 4 Visiting Professors who are appointed on a fixed-term but renewable basis and work with staff on collaborative research topics and deliver postgraduate courses. We have also hosted 9 leading international scholars through the University's Benjamin Meaker Visiting Professorship scheme during the REF period. Through our named lectureships, and the largest annual 1-day chemistry symposium in Europe (Bristol Synthesis Meeting), we attract the highest quality of scientific presentations to Chemistry, including 3 Nobel Laureates (Arnold, Levitt, Feringa).

Staff development and line management: Our core aim is to create an environment in which all staff can flourish in their chosen field. Annual staff review and development is undertaken for all core-funded members of staff by our 3 Section Heads (who are line managed in turn by the Head of School) and by PIs for grant-funded research staff. Workloads are managed by an agreed Workload Allocation Model that ensures committed time for research activities, plus balancing of teaching and other roles across all members of the School. We ensure excellent employment practices which include positive action in equality, diversity and inclusion (see '*Equality and Diversity*' below) and support flexible working for all staff. Leadership and advice in this are provided by the School EDI Committee which contributes to higher-level decision-making through our School Executive Board and the Faculty-of-Science and University EDI Committees. The vital importance of supporting women at key career transition points is fully recognised by the School, which has established the Women-in-Science Mentoring Scheme particularly targeted at PGRs, PDRAs and ECRs with the aim of providing a supportive environment for individuals and to encourage women to pursue careers in science.

Promotions: All promotion cases proceed through University processes from an annual open call to all staff, with a specific Faculty steer to line managers to encourage diversity in applications for promotion. The School ensures support for all staff through an additional internal Promotion Committee (Senior Leadership Team, 50% female representation) who check that no staff are

overlooked and provide personalised guidance on all applications prior to submission. Promotion applications are considered at a Faculty Committee, led by the Dean, which makes formal recommendations to the University Promotions Committee where final decisions are made. Both committees consider the submitted CV, letters from external assessors and any individual circumstances (including, for example, career breaks and caring responsibilities). Evidence successful guidance of candidates through this process is 22 staff promotions since REF2014, including 11 to Professor and 11 to Associate Professor (formerly Reader/Senior Lecturer).

Equality, Diversity and Inclusion

Our strategy for Equality, Diversity and Inclusion is coordinated through the School's EDI Committee (Chair: **Manby**; with constituencies across the School) and EDI considerations are applied throughout all decision-making processes in the School. The EDI Chair sits on the School Executive Board and EDI is a standing (usually opening) item in our 3 monthly School Assemblies. We have made huge strides in EDI since our Athena Swan Bronze award renewal in 2018. In the past two years we have become recognised as a beacon of excellent practice in EDI across the institution, with our strategies and practice to improve diversity being disseminated by the Faculty of Science and the University EDI Oversight Group. Innovations to foster an inclusive environment have included:

- Putting EDI front-and-centre at staff events, *e.g.* introducing a 15-minute inclusion item in all School Assemblies with presentations on Privilege, Microaggressions and Being LGBT+ in a University – a practice that is now disseminated across the Faculty of Science.
- Leading high profile EDI activities such as:
  - *Being-BAME-in-STEM (Science, Technology, Engineering and Mathematics)* events (now University-wide) that are aimed at better understanding BAME inclusion and equality and developing strategies for improvement.
  - Working with City Academy in Bristol to help BAME students experience and be inspired by university-based science.
  - The Red Heroes Project (@RedHeroes_Chem) to address period poverty across our School community.
- Scheduling research seminars and committees in family-friendly hours and active balancing of EDI when selecting speakers.
- Establishing prominent displays across the School highlighting:
  - Diverse early career Inspirational Bristol Scientists and BAME students who have made outstanding contributions in the University and to society.
  - Our support mechanisms for all members of our School community, *e.g.* against bullying and harassment.
  - LGBT+ with a flag in our main foyer and promotion of gender pronoun ID badges, widely worn around the School and in teaching activities.
- Actively managing uptake and compliance with EDI training for all academic staff (currently >98% uptake), mandatory Partnership Working and Sexual Harassment workshops and an established EDI Code of Conduct for School events, visitors, and off-site activities.

Equality of research support: We pride ourselves on ensuring equal and inclusive research support to all our researchers in the SoC through all stages of academic progression, with a positive working environment, including flexible and part-time work. Home working by academics is supported by line managers and two of our REF-submitted staff work part-time (three over the REF

period). Our research support decisions prioritise ECRs and researchers who are re-establishing themselves after career or funding breaks, *e.g.* financial support for co-funding grant applications, prioritising these groups for studentship support and ring-fenced budgets to cover their use of our central instrument Facilities so that these become 'free-at-point-of-use' for these supported researchers.

EDI Summary: The inclusive environment we have built is reflected in positive diversity statistics. We are submitting around twice as many female and ethnic minority researchers to REF2021 as REF2014. This improvement is driven primarily by attracting a diversity of staff through our early career pipeline, and then successfully supporting and retaining them within this positive and inclusive environment. For example, all but two of our female REF-submitted staff started as ECRs in the School. In the post-Covid era we intend to continue supporting hybrid home/campus working for all staff who wish to take advantage of this. Our consistent EDI improvements have genuinely changed the culture and behaviours of the entire School, and we are determined to build on these successes to create even greater diversity in the future.

Research Students

Our Graduate School (Director: **Hall**) is one of the largest in UK chemistry, with 285 PhD and 15 research Masters students currently enrolled (43% female, 20% minority ethnic) and 352 graduated during the REF period. It operates within the Bristol Doctoral College, which is the coordinating centre for sharing good practice across the University. We place substantial emphasis on maintaining this strength and scale in our postgraduate community which underpins our research success.

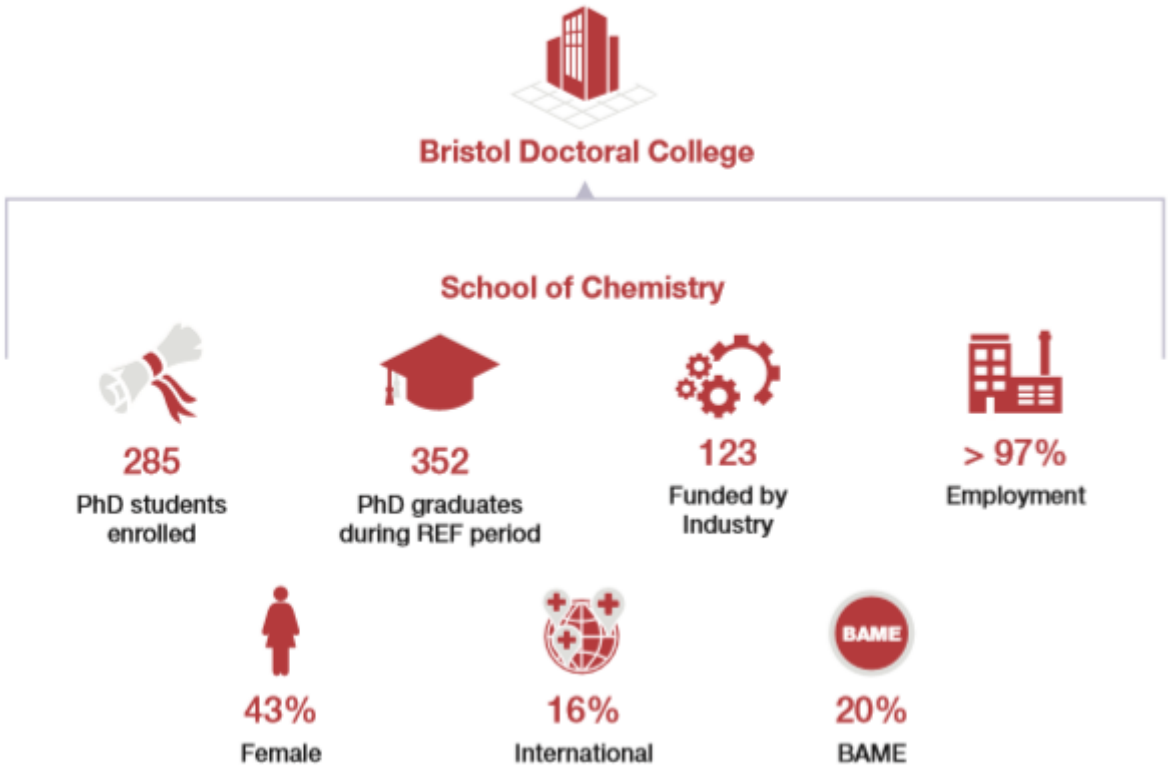

Figure 2.2: Chemistry Postgraduate Research

The School of Chemistry currently leads or partners in 11 Research Council doctoral training programmes (14 over the REF period), testifying to the breadth and depth of the science undertaken in the School. We currently:

- **Lead four EPSRC CDTs**: (2019-) Technology Enhanced Chemical Synthesis (£6.6M) and Aerosol Science (£6.8M); (2014-) Chemical Synthesis (£5.3M) BCFN (£4.6M) with Physics.
- **Partner in five EPSRC CDTs**: (2014- and 2019-) Theory and Modelling in the Chemical Sciences (with Oxford and Southampton); Composites Science, Engineering and Manufacturing and Advanced Composites for Innovation and Science (both with Engineering at Bristol); Catalysis (with Cardiff and Bath); Diamond Science and Technology (with eight other UK universities).
- **Partner in three BBSRC/NERC CDTs**: BBSRC SWBio Doctoral Training Partnership (2015- and 2020-, with GW4); BBRSC/EPSRC SynBio CDT (2014-, with Oxford and Warwick); NERC GW4+ Doctoral Training Partnership (2014-, with GW4 universities).

The quality of the research training and career development that our postgraduates receive is demonstrated in our REF-submitted papers: 63% include one or more Bristol PhD students as authors. Our PhD students have obtained substantial recognition of their excellence in science and its communication, including a Springer thesis prize, six Japan Society for the Promotion of Science (JSPS) Fellowships, a Houses of Parliament STEM for Britain gold medal, and dozens of prizes awarded for their presentations at national and international meetings.

Postgraduate recruitment: We recruit from around 400 high quality applications every year and diversity (20% BAME, 43% female) is considered at every step by our Graduate Recruitment team (2 female, 2 male) with PGR applications reviewed by at least three academic staff who all receive Unconscious Bias training. Our gender profile is strong, being above the 2017 Royal Society of Chemistry (RSC) reported national average in Chemistry and has been at this level throughout the REF period. Funding for our PGRs comes from Research Councils/CDTs (55%, including substantial industry contributions), direct industry support (20%) overseas scholarships (8%), EU (8%), and University and other sources (9%). Chemistry staff also co-supervised >100 PGRs in other Schools and Faculties (not counted in this submission), e.g via SWBio DTP, NERC and MRC GW4 DTPs.

Entrepreneurship: The seismic shift in our entrepreneurial culture since REF2014 is also reflected in our postgraduate training. For example, we run Business Modelling Workshops, covering commercialisation of a discovery through to pitching a Company in a 'Dragons Den' type event. One of the judging panellists was so impressed by a winning team that they are now working together on a commercial launch. Our Technology Enhanced Chemical Synthesis (TECS) CDT partners with UnitDX to provide week-long events for our students to establish business networks and support them to define their own career paths by launching start-up companies. The success of these strategies is demonstrated by two of our postgraduate researchers launching their own start-up companies and around 30 more going into careers in start-up companies immediately after graduating – including **Dr Andy Chapman** who was awarded the 2020 RSC “Rising Star in Industry” prize for his work in spinouts.

Postgraduate support: To ensure a diversity of academic and pastoral support, all students are supported by a team of four academic staff. Academic and pastoral support are primarily provided by the Supervisor through regular one-to-one meetings (typically weekly or fortnightly), with a

pastoral point of contact provided by an independent second supervisor who is explicitly outside the research project. Academic progress is supported by annual progress monitoring via written report and interview involving two independently appointed staff with detailed feedback afterward, including student responses through our online records system. All supervisor, assessor/interviewer and student comments are read by the Graduate School Director and the Faculty Graduate Dean who can initiate action, *e.g.* three-month Enhanced Academic Support, where unaddressed concerns are identified.

Postgraduate research skills, careers and professional training: Alongside training in research techniques, we enable all our students to build a portfolio of skills of value in their research programmes and future careers. We integrate best practices from our CDTs and the Bristol Doctoral College (BDC) into our development programme for the whole postgraduate cohort. PGRs participate in safety, professional development, personal development planning, well-being and entrepreneurship courses delivered by external experts. Core research skills are developed through the BDC, with courses on responsible research, research planning, time management, leadership, networking, presentation skills, and professional and career development. The Bristol Futures programme offers wider-scope personal development courses such as sustainability, innovation and global citizenship to all researchers. Within the School, postgraduates are also given tailored training in teaching and many join our outreach and public engagement activities as STEM Ambassadors (147 since 2014). Specific careers support within the School is provided by an academic Careers Lead and the Faculty of Science specialist careers team with regular events promoting careers opportunities and training, *e.g.* careers fairs, alumni and industry careers presentations, supplemented by the central Bristol *mycareers* online portal with webinars, online courses and opportunities to engage with alumni mentors. Consequently, our postgraduate cohort has excellent careers outcomes with 97% in employment 3 months after graduation (32% to PDRA positions)

3. Income, infrastructure and facilities

Research Income and Strategies

Our core strategy as described in Section 1 aims to build and maintain world-leading research programmes which requires leadership and engagement in national and international agendas that align with the scientific excellence in our Research Themes. To achieve this, we commit substantial time and energy to building relationships with key organisations and funders that allow us to shape and exploit national and regional investment agendas. Our success is reflected in our research income of £183M (£83M as PIs) over the REF period, with examples of partnerships and infrastructures that enable this being:

- *International interdisciplinary research partnerships*. In Global Change, **Rigby** and **O'Doherty** lead two NERC Highlight projects (DARE-UK and Moya-UK) and are partners in the NASA-supported Advanced Global Atmospheric Gases Experiment (AGAGE) programme that monitors global gas emissions.
- *UK and regional partner organisations* such as the GW4 network, entrepreneurial incubators (SetSquared, UnitDX) and over 280 different organisations, comprising 179 companies, 33 different governmental partners (8 international), 21 charitable institutions and 52 other UK and international universities.
- *Collaborative research programmes in thematic areas*. Our 509 funded research programmes have included 2 EPSRC programme grants (**Ashfold FRS** PI and **Glowacki**,

CoI); 2 EU FET grants (**Hall** PI and **Oliver** CoI); EPSRC National Consortia (**Reid**, CoI); and 2 BBSRC sLOLA grants (**Willis** CoI, **Mulholland** CoI).

Research Infrastructure and Facilities

A 5-year strategic planning process is the basis of our world-class research infrastructure and estate (Figure 3.1), with an annual programme of major improvements to underpin our current and future ambitions.

Figure 3.1 School infrastructure and investment

Estate: Chemistry is housed in a single purpose-built site, newly built or entirely refurbished to world-leading standards in a rolling capital programme over the last 20 years. Our site provides a total available laboratory area of 6870m^2 (370 fume cupboards) and out-of-lab office space for all PDRA and PGR researchers. It hosts an in-house Chemistry library, refurbished in 2017 to house 80 computers and >150 private study spaces. We entered REF2014 with an outstanding Estate base which underpinned the breadth of our research needs and consequently we have focused new Estate investments (**£2.2M**) during this REF period on emerging priorities:

- Digital Chemistry (VR labs, HPC, automated robotic synthesis and laser facilities).
- Global Change (atmospheric and materials chemistry laboratory refurbishments).
- PhD training (Training hubs for two new CDTs).
- Strategic appointments (chemical biology laboratory repurposing).
- EDI support (accessible showers, gender neutral toilet facilities, disability signage).

School researchers also use facilities based in the Life Sciences and NanoScience & Quantum Information buildings, which offer state-of-the-art analysis capabilities for researchers in biological chemistry/synthetic biology and materials chemistry and our NanoESCA Facility.

Equipment infrastructure and investment: Our buildings are equipped with **£36.2M** of world-class, state-of-the-art scientific instrumentation and infrastructure, and dedicated mechanical, electronic and glassblowing workshops, all supported by 36 FTE research technical professionals and dedicated research fellows. Our 5-year equipment planning process maximises leverage from substantial institutional cash support (£2.3M) for equipment bids. Since REF2014 we have invested a total of **£13.6M** into our equipment base, including: **NMR spectroscopy** (£3.4M, BBSRC/EPSRC/MRC/UoB) including a dedicated 700MHz 1.7mm microcryoprobe system, 600MHz and 500MHz ^{1}H and ^{13}C cryoprobes and 500/600MHz metabolomics spectrometers, supporting synthesis, catalysis, functional molecules, biological chemistry and synthetic biology; **Materials Characterisation** (£4.4M EPSRC/UoB) including the UK-unique NanoESCA Facility, 200keV High resolution FEG and EELS/energy-filtered TEMs and a dual microfocus single crystal X-ray diffractometer, supporting functional materials and energy research; **Radioisotope accelerator MS** (£1.9M BBSRC/NERC/UoB) - the UK's most ultra-compact high-precision

accelerator MS providing compound-specific ^{14}C analysis for our world-leading organic geochemistry research cluster; **Ultrafast laser spectroscopy** (£450k, ERC/EPSRC/UoB) enabling femtosecond to nanosecond studies of photochemical reactions in the gas-phase and solution, coherent 2D vibrational and electronic spectroscopy, and ultrafast microscopy, supporting our cluster of excellence in ultrafast laser spectroscopy; **Automated Synthesis Robotics** (£750k EPSRC/UoB) capable of running dozens of parallel and serial reactions across a wide temperature range, under inert conditions and with photochemical capabilities to support synthesis and catalysis.

Central Facilities: Much of the University's equipment base is housed in Chemistry, which hosts 7 major shared instrument Facilities. These are underpinned by a team of 13 FTE dedicated research technical professionals and led by academic Directors. The strategic decision to centralise these core capabilities means that we can underpin our entire research portfolio and catalyse shared activities across the University with a long-term financial model that also future-proofs our equipment base. These Facilities, with a user-base of ~400 researchers, are recognised as centres of best practice in UoB for equipment support, training, sharing and sustainability. Training and career progression of our specialist Facility staff is crucial and we work with the GW4 Technical and Infrastructure and Knowledge (TIK) Group to ensure effective support structures and development for our research technical professionals.

The **NMR** Facility comprises 12 high-field instruments (300-700 MHz) serving both physical and life sciences; The **Chemical and Biological Mass Spectrometry** Facility and complementary NERC **Life Sciences Mass Spectrometry** Facility together comprise 18 systems, including the UK's first GC-Orbitrap installed in 2018; The **Chemical Imaging** Facility (8 Scanning Electron Microscope (EM)/Transmission EM/Atomic Force Microscopy instruments) offers characterisation of chemical systems, high-speed imaging and physical properties measurements, and coordinates with complementary Interface Analysis Centre and Wolfson Bioimaging suites for materials and bio-oriented imaging applications respectively; The **X-ray diffraction** Facility comprises four instruments for single-crystal and powder diffractometry, including recent investments in micro-focus sources and variable temperature powder analysis; The **Bristol Radiocarbon Accelerator Mass Spectrometry** Facility is a newly established state-of-the-art resource specialising in methods for radiocarbon determinations of gases, solids and dissolved organics from diverse environmental matrices including atmospheres, soils and waters; The **NanoESCA Surface Analysis** Facility is a UK-unique multi-platform capability combining PEEM, high-resolution X-ray Photoelectron Spectroscopy (XPS) and Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED).

Facilities supporting Themes: Our School also hosts specialist clusters of UoB and UKRI-funded instruments supporting Theme needs with pooled research technical professionals and underpinned by financial support from the School. Examples of these include analytical suites for chemical and biological synthesis (React-IR, 10 LC/GC-MS, biosuite, peptide synthesis, biophysical characterisation) and materials (DSC, ELS, BET, TGA), automated synthesis robotics, soft matter analysis suite, atmospheric chemistry sensor arrays (UK and international), aerosol science instrumentation and ultrafast-laser laboratories. These suites form strong links to wider University Facilities, for example our dedicated 400-core Chemistry computational cluster acts to triage our researcher's substantial use of the University's central 'BlueCrystal' 16000 CPU, 150 GPU High Performance Computing Facility and other HPC Facilities, *e.g.* BlueGem and BluePebble. These in turn filter engagement with GW4 Isambard and Isambard II (Tier 2) and

Archer (Tier 1) UK HPC systems. The University's commitment to centralised facilities to support our science is evidenced by a **£20M** ring-fenced budget for HPC over the next decade.

National and international Facilities: Our world-leading teams, particularly in ultrafast laser spectroscopy and materials chemistry, are significant users of beam time on major international research facilities (~£7.6M in-kind over the REF period), including: ISIS/Diamond (UK), Institut Laue-Langevin (France), Deutsches Elektronen-Synchrotron (DESY-Flash, Germany), Paul Scherrer Institut Light Source (Switzerland), Dalian Coherent Light Source (China), Heinz Maier-Leibnitz Zentrum (Germany), Free-Electron Laser Facility (FERMI, Italy), Central Laser Facility (UK), Berkeley Advanced Light Source (USA), SLAC Accelerator (USA). Our researchers also lead programmes making substantial use of Tier 1 and 2 national HPC, *e.g.* HECBioSim (Chair: **Mulholland**) was allocated 1.07M kAU on ARCHER (6.6M CPU hours, £570k in-kind value).

Equality focus: One of the key drivers behind our strategy for centralised and Theme-level Facilities is to ensure world-leading techniques are accessible for all our researchers, especially ECRs or those re-establishing their research careers who therefore do not need to procure and maintain their own entire instrument base. As highlighted in '*Equality of Research Support*' above, we provide funding to minimise the cost of Facility access for these groups. Equality in supporting large infrastructure bids is also underpinned by institutional mechanisms such as feedback and mentoring from senior academics in the Faculty of Science and mock panel interviews for all applicants.

Impact focus: The scale and quality of our core facilities and infrastructure enhance our interactions with industry, Research Councils UK strategic priorities and underpinning of the UK R&D base. External demand for our Facilities has risen sharply with over 60 companies requesting bespoke access. These cover the spectrum from University start-ups (*e.g.* HelloBio, Photodiversity, Ziylo, UnitDX, ArtSci, Rosa Biotech, Glaia, Carbometrics, Pertinax) through small and medium-sized enterprises (SMEs) (*e.g.* CatSci, Anaphite, Isca Biochemicals, Barden Corporation) to global corporations (*e.g.* Mars, BP, Oracle, Hyundai). The impact-focus, infrastructure and expertise available in Bristol were key drivers for members of our School (co-founders of Ziylo) to spin out the deep tech incubator UnitDX in 2017 to establish an extensive innovation hub in Bristol. Their first facility has supported 57 companies, which themselves have generated 125 jobs and collectively raised over £40M to date. A University-wide service-level agreement with UnitDX enables all companies in the incubator to access our world-leading Facilities and expertise with minimal barriers. This is fully described in our accompanying Impact Case Study.

Environmental sustainability: This is a core value at Bristol, and high on our agenda for actions, with the University declaring a climate emergency in 2019. This is underpinned by £2M/annum of capital investment and campus-wide sustainability initiatives (*e.g.* Green Labs, Let's Eco Sort It). The School has invested in a series of large-scale sustainability projects (£0.7M) including improvements to lighting, compressed air infrastructure, drying cabinets, ultra-low temperature freezers. These have reduced our consumption of electricity by 17%, equivalent to 1M tonnes of CO_2 emissions, despite concomitant expansion in the School. Similarly, a new central liquid nitrogen facility has reduced losses and delivered substantial cost reductions (~£120k *pa* saving) and switching water-cooled turbomolecular vacuum pumps for air-cooled systems has eliminated our largest source of water use. Crucially, these investments include projects that do not fully recover their costs but have major environmental benefits (*e.g.* electricity reductions, recycling).

We are currently scoping a helium gas recovery and reliquification operation (through the School of Physics) for our NMR Facility which will recover >3000 litres/annum of this finite resource.

Financial sustainability: The financial sustainability of our Estate and infrastructure is crucial for our long-term future. The costs of our major equipment Facilities and their research technical professional staffing are sustained through TRAC-compliant charging, which recovers running costs directly from research and teaching users. We successfully recover >90% of these >£1M/annum costs, with the remaining 10% being committed to free access for pump-priming, supporting diversity considerations for ECRs and post-career break staff, and international student support. Our financial model future-proofs our Estate and infrastructure, supported by ~£100k/annum industrial income streams to these Facilities.

Future plans: The recent transformation in entrepreneurial culture in Bristol and the associated infrastructure and incubator space will bring positive and reciprocal benefits to the School's physical and non-physical infrastructures. The new £300M Temple Quarter University Enterprise Zone focuses on digital, business and social innovation and anchors a new innovation district including the Engine Shed and UnitDX. The University's partnership in the coming UnitDX expansion will provide new state-of-the-art space for spinout companies in artificial intelligence, smart energy, agri-food and clean growth aligned with our School Research Themes and strategic priority areas of Digital Chemistry and Global Change. We are working closely to integrate our theme-level and major Facilities into this evolving infrastructure to maximise the opportunity for researchers across the School and University.

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

Collaboration is at the heart of our research and is increasingly conducted in large inter- and multi-disciplinary teams. Indeed, 88% of our REF-submitted publications are collaborative, 60% include international collaborators as co-authors, 53% have co-authors from another UK academic department and 37% are with industry. Our global reach is illustrated in Figure 4.1, showing our research links to organisations in >130 locations worldwide.

Figure 4.1 Chemistry collaborations (bubble size represents the number of organisations)

Interactions and leadership with key research users, audiences and beneficiaries: We are engaged in >100 national and international networks and partnerships, covering all the School's Research Themes. Many cases of our leadership have been highlighted throughout Sections 1 and 2 of this document and further examples include: **Butts** (Co-founder of UKMRM and ConnectNMR NMR networks; President, SMASH NMR conference), **Reid** (President, UK and Ireland Aerosol Society); **Eastoe** (Coordinator, International Consortium on New Low Surface Energy Materials); **Fermin** (Chair, PVTEAM Consortium); **Woods** (Chair, UK Research Software Engineering network). The School has also established networks with other universities to cement research relationships. International examples include: Jilin University, China (**Li**, **Mann FRS**, **Faul**), Rhodes University, South Africa (**Shallcross**) and Dalian Institute of Chemical Physics (**Ashfold FRS**).

Wider contributions to economy, society and industry: Our five Impact Case Studies demonstrate the breadth of our impact globally, encompassing climate change, commerce, sustainability, cultural heritage, and Covid-19 policy impact in health and culture. We are especially proud of our societal impacts, exemplified by our massive Outreach programme (see *Engaging with diverse communities and public*, below) which has partnered to engage over a quarter of a million members of the public internationally in the REF period. Similarly, our Atmospheric Chemistry Research Group has made major societal contributions around greenhouse gas emissions inventories and modelling being used by the IPCC, with impacts on global climate change initiatives, which has led to prosecution and closure of factories in China breaking ozone-depleting CFC emissions bans.

Commercially, staff have obtained 27 patents during the REF period. Our 11 spinout/startup companies established by School staff during the current REF period (Figure 4.2) target diverse goals from non-profit open access software development (ArtSci) to improved crop production (Glaia) and medical diagnostics (Rosa Biotech). Our work with 179 companies, ranging from SMEs to global conglomerates, creates mutually beneficial outcomes in fundamental research as well as translational and knowledge transfer opportunities for our partners. This is reflected in **£8.5M** industrial support for PDRA-based research over the REF period, and **£3M** to support PhD studentships and undergraduate research projects across companies as diverse as: Airbus, AstraZeneca, Bayer, BP, Bridgestone, Bristol Water, CatSci, Chiesi, Codexis, Cresset, Croda, Dextra, Dow, Dr Reddy's, EcoEgg, Edwards, Element Six, Eli-Lily, Evotec, GSK, Heptares, HyphaDiscovery, Hyundai, Imerys/FiberLean, Infineum, Janssen, Johnson Matthey, Lucite, Merck, Novartis, Novo Nordisk, Nutrica, Oracle, Procter & Gamble, Pfizer, Prozomix, Sasol, Solvay, Syngenta, Toyota, UCB and Victrex.

Figure 4.2: Spinout companies established by Chemistry staff

Engaging with diverse communities and the public: We believe we have the most active public engagement programme of any UK Chemistry department. Led by Mr Tim Harrison, it has run over 650 events over the REF period and engaged >175,000 UK school students, teachers and members of the public. Many of our >650 Outreach activities (school visits, public lectures, published resources, laboratory experience days) centre around research activity in atmospheric chemistry and climate change. Our partnership with the Primary Science Teaching Trust has developed the STEM/Science Trails program which has trained teachers in ~25% (>5000) of UK primary schools to investigate local pollution and family travel habits, leading to Schools changing their travel-to-school policies and parental engagement with their children's education. Our team has delivered training to international partners who have engaged >75,000 members of the public, such as the Sci Bono Discover Centre (South Africa) and the South West Australian "Old Ways, New Ways" program to enable genuine and measurable impacts on awareness of climate science in disadvantaged communities such as the South African Townships and the First Peoples of Australia. **Shallcross** is an internationally recognised leader in this activity as President of the Royal Society of Chemistry Education Division, Director of the Primary Science Teaching Trust, Convenor of the Education Forum, and winner of the 2017 RSC Nyholm Prize and 2020 ACS Pimentel Award.

Wider influence, contributions and recognition: Our substantial influence and recognition across international research communities is illustrated by numerous Fellowships of academic and professional societies, *e.g.* FRS, Academia Europaea, FRS(Edinburgh), FRS(South Africa), Royal Societies of Chemistry, Meteorology and Biology, Institute of Physics and two honorary doctorates. Our staff hold visiting professorships in 6 international institutions, memberships of 16 University, governmental and industry Advisory Boards, and serve on over 50 committees of professional societies including 2 RSC Division Presidents (**Raven**, **Shallcross**). Staff have received 46 major international, ACS and RSC awards and prizes during the REF period, including 2 Royal Society Davy Medals (**Mann FRS** 2016; **Aggarwal FRS** 2019), RSE Sir James Black Medal (**Simpson FRS** 2016), 10 Royal Society Wolfson Merit Award and 2 Philip Leverhulme Awards (**Glowacki** and **Bower**, 2016). School staff have given >750 keynote, plenary or invited talks worldwide (not including invited UK seminars) and led 21 international conferences including chairing 5 Gordon Research Conferences.

We play a full part in the leadership of international, EU and UK grant awarding bodies including: Physical Sciences Panel Hong Kong RAE (**Ashfold FRS**, **Orr-Ewing FRS**), ERC Advanced Grant Committee (**Aggarwal FRS**, **Raven**), Italian Research and University Evaluation Agency (**Eastoe**) Irish Research Council Outer Board (**Eastoe**), EPSRC Science, Technology and Engineering Board (**Mulholland**) and Strategic Advisory Teams (**Booker-Milburn**, **Butts**, **Mulholland**, **Woods**), BBSRC Transformative Research Technologies Panel Chair (**Woolfson**), BBSRC Appointments Board (**Mulholland**), UK Synthetic Biology Leadership Council (**Woolfson**), NERC/BBSRC Individual Merit Promotion Committee (**Evershed**), EPSRC ARCHER Resource Allocation Panel Chair (**Mulholland**), EPSRC UK Catalysis Hub Steering Committee Chair (**Mulholland**) and Science and Technology Facilities Council (STFC) Physical Sciences and Engineering Advisory Panel (**Orr-Ewing FRS**).

Co-operation and collaboration in PGR training: We are proud of our national leadership around doctoral training and discuss this fully elsewhere in this document, with the full list of 11 CDTs in which we are currently engaged given in Section 2. This leadership is recognised nationally by the high demand for our CDT leaders, *e.g.* **Booker-Milburn** and **Raven** have served on six CDT Advisory Boards (Nottingham (Chair), Oxfordx2, Imperial College London, Cardiff and Cambridge).

Looking to the Future

Our School has a deeply embedded culture for intellectual and scholarly excellence that thrives on new ideas and opportunities, and is creating economic, entrepreneurial and societal impact worldwide. We have outlined in this statement a clear vision for our future research activities, with a focus on digital enabling technologies (Digital Chemistry) and global challenges (Global Change), and we have strong support from the Faculty and University to deliver this. Our impact priorities are entrepreneurship and addressing global challenges, supported and enabled by outstanding Bristol infrastructure and organisations. Our ambitious and energised staff cohort will be further strengthened by targeting investments in strategic priorities at professorial level and by ensuring a continuing strong early career pipeline across the breadth of our research portfolio. We are excited about the future research directions and impact-focus of our School and confident that our thriving, supportive, diverse and stimulating environment will continue to be a place where world-leading scientists can excel.