Institution: University of Sheffield
Unit of Assessment: B-08 Chemistry
1. Unit context and structure, research and impact strategy

The goal of the Department of Chemistry in Sheffield is to discover new chemistry for a better life and a sustainable future. Our research addresses fundamental problems, and our outward-facing ethos ensures that we tackle important challenges at the interfaces of chemistry with biology, healthcare, physics, and engineering. The University of Sheffield provides an outstanding environment for such interdisciplinary research, and much of our research work is closely aligned with the Faculty of Science priorities in 'Nanoscience and Nanotechnology', 'The Process of Life', and 'A Sustainable World'.

We aim to:

- Conduct world-class research at the forefront of chemical knowledge.
- Build strong collaborations at the boundaries between chemistry and other disciplines, locally, nationally, and internationally.
- Achieve impact through translation of knowledge into industrial applications, improvements in healthcare, quality of life, and public understanding of science.
- Embrace equality, diversity, and inclusion (EDI) and hence enable every member of the department to fulfil their potential.

In the assessment period, we have built on our strong performance in REF2014:

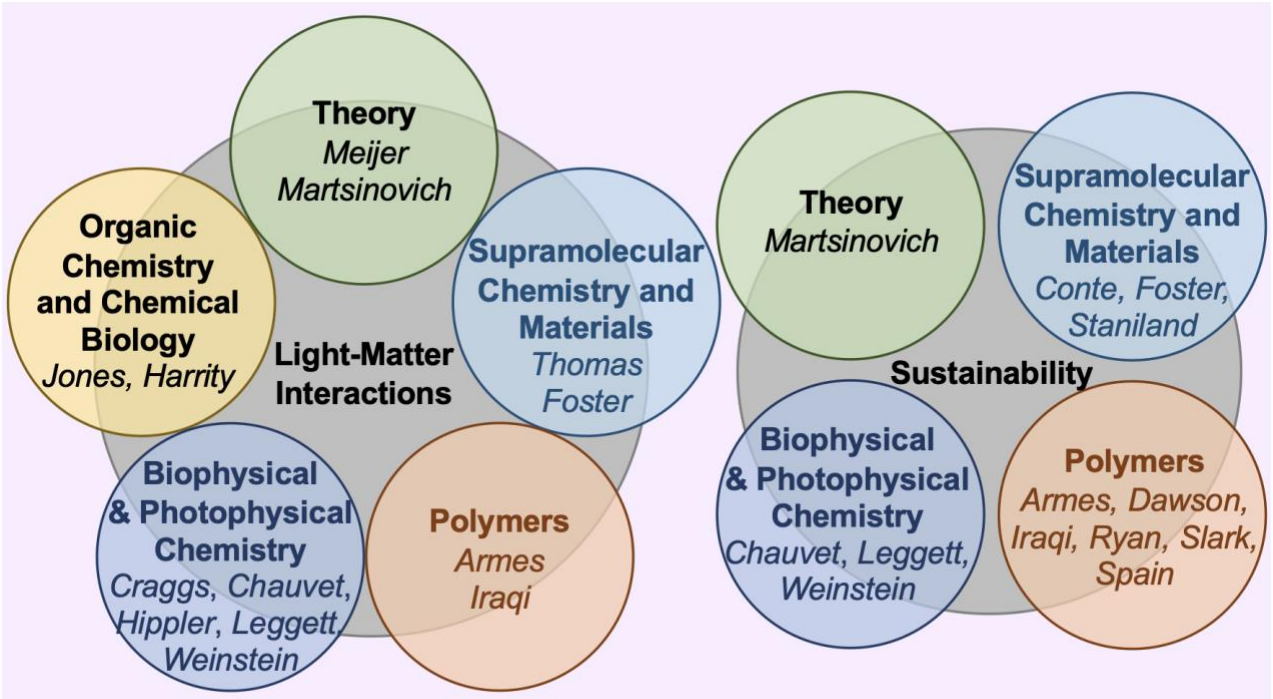
- **World-class research:** Since 2014, *Armes* has been elected FRS and various staff have won RSC prizes and awards, e.g. *Armes*: Interdisciplinary Prize, *Harrity*: Bader Award, *Staniland*: Harrison-Meldola Medal, and *Weinstein*: Chemical Dynamics Award. Our staff have contributed as PI or Co-I to 26 grants with award values of >£1M e.g. *Leggett* £7.3M 'Molecular Photonic Breadboards' (EPSRC).
- **Strong collaborations:** The Polymer Centre led by *Armes* remains a powerhouse for interdisciplinary work involving >50 individual research groups in Sheffield. Additionally, *Ryan* has established the philanthropically funded ***Grantham Centre for Sustainable Futures***, (£8.7M). *Weinstein* established the Porter Lab as a global force in ultra-fast spectroscopy, with partners across four continents, including the USA, Germany, Switzerland, Japan, Australia and India. *Craggs* played a leading role in an international consortium of 20 groups that defined data standards for single-molecule FRET measurements. *Leggett* led an EPSRC Grand Challenge Network that drafted a 'Roadmap for Biological Physics' which EPSRC used as the foundation for its strategy in soft matter research.
- **Impact:** The Grantham Centre drives work with international impact ranging from the manufacture of sustainable plastics to developing hydroponic farming systems within refugee camps in the Middle East. *Ryan* has served on the science advisory boards of Unilever and SCJohnson; the appointment of *Slark* on an EPSRC Manufacturing

Fellowship expands our industry-facing activities; and the award of a prestigious DSM Materials Science Award to *Armes* reflects his sustained world-class impact.

- **Embracing EDI:** In 2015 we were awarded an Athena SWAN Silver Award, which was retained in 2020. Six staff have been promoted to personal chairs since 2014, and half of our female staff are now professors, reflecting our continuing determination to foster EDI among staff at all levels.

We have appointed 10 new staff in the assessment period to realise our research goals and to lay the foundation for sustained excellence and growth beyond 2021. The University has invested to develop our staff profile, and also to replace Hunter and Ward (now at Cambridge and Warwick, respectively) and retiring staff (e.g. Pickup). Two appointments (*Foster* and *Slark*) were made following award of competitive fellowships. Our recent appointees have published outstanding papers and achieved substantial success in grant capture. The combined achievements of these new staff, together with the continued success of established staff, provide a strong foundation for continued strength in Chemistry at Sheffield.

We have made multi-million-pound investments in major infrastructure to facilitate world-class research, including the Porter Lab (£2.2M), new equipment to support chemical analysis (£2.2M), and state-of-the-art instrumentation for small-angle X-ray scattering and surface analysis (total £2.5M). These developments will enhance an already vibrant, forward-looking department, and provide a foundation for future success.



Box 1. Work on light-matter interactions and sustainability involves many Research Groups.

1.1 Research structure

Since REF2014, we have refocussed our research organisation. The five new research groups (details **§1.2)** provide support and mentoring for staff with cognate research expertise. However, many staff collaborate widely within the Department, with academic partners in Sheffield and external to the University, with industry and with other external organisations (see **§4**). Consequently, the Department also supports four strong cross-cutting research themes (**§1.4)**: 'nanomaterials', 'the chemistry-biology interface', 'light-matter interactions' and 'sustainability' (for

examples, see **Box 1**), reflecting the success of our 2014 strategy for interdisciplinary research. For example, work at the chemistry/biology interface (previously focussed on a single group) has now expanded to involve all research groups.

Each group has a head, assisted by a junior member of staff as deputy head, to facilitate succession planning. While the group heads are appointed for their research leadership, they also provide line management to group members across all areas of their work (including teaching and leadership) as part of the Department's new matrix management strategy. Group heads form part of the Research Committee, which advises the Departmental Executive on the strategic direction of research in the Department and also ensures that research conforms to the University's Policy on Good Research and Innovation Principles.

1.2 Research objectives

Our *research groups* reflect our core areas of disciplinary excellence and underpin our *four cross-cutting interdisciplinary themes* (**§1.4**). The strategic recruitment of 10 staff since REF2014 has both deepened our core expertise and further enhanced our strong cross-cutting interdisciplinary themes.

Following REF2014, we prioritised research at the chemistry-biology interface. Consequently, biological problems now motivate an increasing proportion of our activities across all research groups. In particular, we have created two foci of research excellence by differentiating between *biophysical chemistry* (including spectroscopy, biophysics and energy transfer in biological systems) and classical *chemical biology* (which is combined with organic chemistry to create a more tightly focused unit).

Biophysical and Photophysical Chemistry (Head: Weinstein)

To drive success in this new group we established the Porter Lab (**§1.4)** under the leadership of *Weinstein*, who uses ultra-fast methods to investigate the dynamics of electron and energy transfer processes (*Science* 2014). To further build strength we appointed *Chauvet*, a spectroscopist with broad interests in ultra-fast techniques (*Science* 2017) and their application to biological systems (NE/T010924/1, NERC, £794k with *Martsinovich*), complementing the work of *Hippler*. *Chauvet's* work on energy transfer in photosynthesis (EPSRC EP/R045305/1) complements that of *Leggett* (*Nano Lett.* 2016, programme grant EP/I012060). *Craggs* was appointed to establish expertise in single-molecule Förster resonance energy transfer (FRET) methods for single-molecule analysis. He has played a leading role in a major international multi-laboratory study (*Nat. Methods* 2018, **§1.4**). In the next five years, we will build on this critical mass by developing new programmes in polaritonics (with JClark, Lidzey and Tartakovskii, Physics) and quantum optics (programme grant EP/T012455 2020-25, *Leggett*).

Organic Chemistry and Chemical Biology (Head: D.Williams)

This aim of this group is to drive work at the interface between organic synthesis and biological chemistry. *Partridge* was appointed to build strength in catalysis and to complement existing strength in synthetic chemistry (*Coldham, Harrity*). *Harrity* drives the application of synthetic methodology to the design of cancer drugs with Skerry, Oncology (Wellcome, £2.95M; £2M follow-up grant), while *Chen* (*Nat. Chem. Bio.* 2014) focuses on drug discovery, and *Jones* collaborates with Foster (Biology) on anti-microbial resistance (e.g. £1M MRC grant). *N.Williams* leads in physical organic chemistry, exploring the fundamentals of non-covalent interactions (*Nat. Chem.* 2016 and a £2.2m EPSRC grant with Hunter, Cambridge and *Leggett*), and signal transduction in membrane systems (*Nat. Chem.* 2017 and *JACS* 2017). *D.Williams* studies nucleic acid chemistry,

including a particularly fruitful collaboration with Patel (LMB, Cambridge) on alcohol-induced cross-link repair (*Nature* 2020). In the next five years we will expand work on drug discovery (e.g. spin-out *Modulus Oncology, Harrity* **§1.4**) while continuing to invest in the fundamentals of synthetic and biological chemistry.

Polymers (Head: Ryan)

This established area of international excellence was further strengthened by the appointment of *Spain* (drug delivery, biomaterials), complementing the work of *Parnell* (biologically-inspired materials). To build on *Ryan's* leadership in sustainability (**§1.4**) we appointed *Dawson* (microporous polymers for energy applications) and *Slark* (EPSRC Industry Fellow, £1.5M). *Armes'* continued leadership in polymer chemistry has been recognised by his election to FRS (2014), his ERC Advanced Investigator grant (2013-2018), and his current EPSRC Particle Technology Fellowship. Over this assessment period he has established polymerisation-induced self-assembly (PISA) as an important field within polymer science (e.g. *JACS* 2017, 2019). This work, in collaboration with *Mykhaylyk* and *Ryan*, has been underpinned by major investment in SAXS instrumentation (**§3.2**). The ***Polymer Centre*** (Director *Armes*), is central to our strategy to maintain strength in interdisciplinary research, with >50 members across the Faculties of Science, Engineering, Medicine, Dentistry & Health, and the Advanced Manufacturing Research Centre, and research ranging from the development of new chemistry, theories and measurement techniques through to applications in healthcare, energy, transport and consumer goods. The Polymer Centre remains important in our planning for the next five years, when we will prioritise further expansion of work on sustainability and continued enhancement of links with manufacturing.

Supramolecular Chemistry and Materials (Head: Thomas)

We appointed *Foster* to work on metal-organic nanosheets (MONs), broadening cross-cutting work in nanomaterials (**§1.4**) and complementing existing strength in metal-organic framework materials (MOFs), e.g. *Brammer,* who studies the fundamental chemistry of MOFs (*Nat. Chem.* 2017) and intermolecular interactions (*Chem. Sci.* 2017). *Staniland* was appointed to further strengthen work on nanomaterials, bringing expertise in biologically-inspired design (*PNAS* 2014) and synthetic biology (*Nat. Commun.* 2019). *Thomas* designs functional molecular architectures that bind to biomolecules, with wide-ranging applications from cell biology (*JACS* 2017) to treating antimicrobial resistance (*ACS Nano* 2019). Work on inorganic materials is focussed on applications in catalysis (*Conte* and *Haynes*, *Angew. Chem.* 2018) and energetic materials (*Portius*). In the next five years, we will expand work on nanomaterials and the fundamental chemistry of MOFs (multi-centre EPSRC grant 2020-23, *Brammer*), and develop translational pathways for *Thomas's* work on antimicrobial resistance with recent seed-funding for a spin-out.

Theory (Head: Meijer)

Following the retirement of *Pickup*, we expanded the group by appointing *Martsinovich* and *Hill*. *Martsinovich* studies materials and interfaces and enhances interdisciplinary work on sustainability and light-matter interactions (**§1.4**); with *Chauvet* and colleagues in bioscience she recently received a £794k NERC grant to investigate the dynamics of phosphates in soil. *Hill* addresses the fundamentals of chemical theory, particularly electronic structure. Currently, he is developing machine-learning methods for basis set development for many-atom systems (EPSRC EP/T027134). *Fowler* also focuses on fundamental problems, in particular graph theoretical approaches to conductivity and aromaticity (*JCP* 2015). *Clarke* uses theory to study polymer materials. *Meijer* studies chemical dynamics (*JACS* 2017), develops theory to support ultra-fast spectroscopy with *Weinstein* (*Nat. Chem.* 2017) and studies light-matter interactions. In the next

five years we aim to expand theory further to exploit opportunities for new work at the chemistry-biology interface.

1.3 Impact

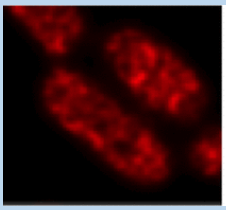
***Strategy*:** Building on our REF2014 strategy to maximise societal relevance, we aim to embed non-academic impact in our projects. At the project formulation stage, the Departmental Impact Lead and the Faculty knowledge exchange (KE) team support academic staff in identifying partners, to ensure that an impact strategy is embedded from the start. Key stakeholders are consulted to maximise explicit relevance to non-academic agendas. Once potentially impactful research has been completed, we support staff to disseminate results to non-academic audiences to enhance its impact. For example, we host dissemination events, and support staff involvement as advisors to SMEs, and secondment to companies (e.g. *Coldham*, Liverpool Chirochem). The departmental Workload Allocation Model is used to relieve staff of teaching and administrative commitments to pursue impact-related activities (e.g. *Ryan* has a 50% appointment to Grantham Centre).

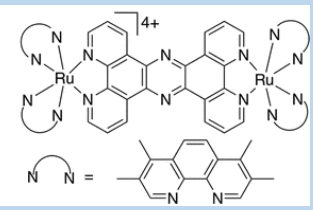
***Industrial impact*:** Central to this strategy is the Polymer Centre (**§1.4)**. Both *Armes* and *Ryan* have extensive portfolios of industrial collaborations and long track records of driving policy change more broadly. For example, *Ryan* has served on the Science Advisory boards of Unilever, SCJohnson and STFC. Moreover, his EPSRC Prosperity Partnership with AkzoNobel is an excellent example of translating fundamental research into economic impact (detail **§3.1(b)**). *Armes* was awarded the biennial €50,000 DSM Materials Science Award in 2016, the only UK scientist to have received this prize. He is involved in two of our three impact case studies. Our Chemistry with a Year in Industry degree has further enhanced interactions with industrial partners, evidenced by our *Inkjet Pigments* impact case study, which was initiated following an undergraduate student placement. The student was shortlisted for a 2015 National Undergraduate Employability award after nomination by her company employer.

Since 2014, our work with industrial partners has grown significantly. In addition to major joint research grants, CASE-type PhD studentships are a particularly important means to build and maintain strong industrial links. For example, *Armes* leads the Centre for Doctoral Training (CDT) in 'Polymers, Soft Matter and Colloids' that supports 50 CASE-type research projects, each with at least £40k of industrial cash per studentship. The CDT has facilitated ECR engagement with multiple industrial partners, including *Dawson*, *Mykhaylyk*, *Spain*, *Foster,* and *Partridge*. Furthermore, the Faculty provides up to 50% of the cost of joint studentships with an industrial partner.

***SMEs*:** We work with a wide range of external partners and we strategically target different types of stakeholder as projects develop along an impact pipeline. The Faculty has a team dedicated to supporting technology transfer, including business development, and supports development of collaborative academic research through KE grants co-funded by industry. For example, *Craggs* acted as a project partner for Thorlabs and Cairn Research; *Iraqi* worked with local SME Ossila on a KE project focused on the scale-up of nanomaterials production; *Thomas* has worked with Lumicks plc to develop probes for single-molecule imaging of nucleic acids; and *Weinstein* has worked with StoliCatalysts as part of a KE project funded by the University. Additionally, staff are encouraged to exploit opportunities to spin companies out and to work with SMEs. Redbrick Molecular was established by *Jones* with a University investment of £225k. It provides compound libraries for the drug discovery industry. Redbrick has sponsored two PhD studentships and two EPSRC grants, and has provided placements for three Sheffield PhD students and one PDRA in the assessment period. *Coldham* has commercialised his compounds with Liverpool Chirochem,

and *Harrity* is spinning out a company based on his collaboration with Skerry (**§4.2**). During this assessment period we have received 20 Impact Accelerator Account (IAA) awards worth £486k, providing a foundation for maximising impact over the next five years.





Kirsty Smitten PhD 2016 – 2020
Forbes 30 under 30 Europe list 2020
Nova Prize winner for Chemistry 2018

Smitten et al, *ACS Nano* **2019**, *13*, 5, 5133.

Box 2. Work by Kirsty Smitten, supervised by Jim Thomas, yielded potent new antimicrobial leads. With University knowledge exchange funding, a patent has been filed (PCT/GB2020/050875) and Kirsty is now establishing a start-up company to commercialise the work.

Impact on society: Important societal challenges motivate much of our research, and in some cases have led to international impact. For example, *Thomas* led a joint project with Foster (Molecular Biology and Biotechnology department, Sheffield) that uncovered promising new antimicrobial agents. The work received widespread media coverage (**Box 2**), with a CBS camera crew visiting Sheffield to make a short film (broadcast 05/07/19).

Through his Grantham Centre work, *Ryan* has had widespread impact both locally and internationally (see **§4.2**). He is a regular guest on BBC radio and has collaborated extensively on environmental issues with artists of national renown, such as Helen Storey and Simon Armitage. His collaboration with Armitage 'In Praise of Air' was widely reported in the national media.

1.4. Interdisciplinary research

Strategy: Much of the most exciting research in chemistry now lies at the intersection with other disciplines. Our research groups (**§1.2**) provide the foundation that underpins our **four cross-cutting interdisciplinary** themes, all of which have been supported strategically by recent appointments. Our recruitment strategy has targeted the appointment of early-career researchers (ECRs) who are expected to lead our expansion of interdisciplinary research (**§1.2**). The following are examples of particularly impactful activities in the assessment period:

- ***Nanomaterials*** was identified as a key theme in 2014; *Staniland* (biologically-inspired nanomaterials) and *Foster* (2D materials) were appointed to complement the expertise of *Armes* and *Leggett* (Faculty research theme lead in nanomaterials), and have established

well-funded research programmes. Additionally, we have significantly expanded work in two areas (chemistry-biology interface and light-matter interactions) and developed a new cross-cutting priority in sustainability.

- ***The Chemistry-Biology Interface*:** Many members of the department enjoy fruitful collaborations with bioscientists. *Craggs*, *Thomas* and *D.Williams* are active in the Sheffield Institute for Nucleic Acids, which investigates the role of nucleic acids in health and disease. Similarly, *Jones*, *Weinstein*, *Thomas* and *Craggs* make important contributions to the £7M Imagine:Life initiative, led by Hobbs (Physics) which focuses on the development of imaging technologies in the life sciences. *Leggett* established (with Hobbs) and led (2013-2016) the EPSRC Grand Challenge Network on Understanding the Physics of Life. He drafted a 'Roadmap for Biological Physics' for EPSRC that shaped its priorities in biological physics and soft matter.

- ***Light-Matter Interactions*:** The Porter Lab was established with a £1.36M EPSRC grant plus £0.8M institutional investment to create a world-class facility for interdisciplinary research in light-matter interactions. The appointments of *Chauvet* (ultra-fast spectroscopy of biomolecules) and *Craggs* (single-molecule measurements on biomolecules) significantly broadened our activities at the chemistry-biology interface, complementing *Leggett*'s work on nanophotonics and nanofabrication and the theory work of *Martsinovich* (materials and interfaces) and *Meijer* (dynamics). We have built strong collaborations with other Sheffield departments including Physics (e.g. Cadby, J. Clark, Hobbs, Tartakovski), Biology (Foster, Hunter, Kelly, Smyth, Williamson) and Medicine (Bryant, Lambert).

- ***Sustainability*:** The return of *Ryan* to academic research after serving as Faculty Vice-President was the catalyst for a major new initiative in sustainability. This underpinning theme now runs through every research group. He directs the Grantham Centre, which supports doctoral training (**§1.4**) and is an important nexus for interdisciplinary collaboration across the University in sustainability. He has received multiple large research grants focused on the sustainable production of polymeric materials (**§4.2**). *Ryan*'s 'Circular Economy' EPSRC grant (*Plastics: Redefining Single-Use*; £1.01M) combines the skills and capabilities of 37 social scientists, scientists, engineers, medics, and arts and humanities academics (including *Armes*, *Slark*, *Spain* and *Mykhaylyk* in Chemistry) and stakeholders drawn from industry, policy and the third sector, to address specific needs for the plastics supply chain. The appointment of *Slark* via a £1.5M EPSRC Professorial Fellowship further boosts our activity in sustainability, which also includes recent appointees *Chauvet*, *Conte*, *Dawson*, *Foster*, *Martsinovich*, *Spain,* and *Staniland*.

Interdisciplinary research training is greatly enhanced by our leading roles in interdisciplinary CDTs. *Armes* leads the £7.1M EPSRC CDT in Polymers, Soft Matter and Colloids, CDT-PSC (**§2.2**). Its 50 PhD students are spread across 27 research groups and are co-supervised by 19 supervisors. Every student spends six months on secondment working on-site with their industrial sponsor: this enriches the interdisciplinary nature of their scientific training while providing real-world work experience. *Leggett* was the Sheffield lead academic for the CDT in Molecular-Scale Engineering (2011-2018), which embedded interdisciplinary research training by requiring every PhD student to have at least two supervisors from different disciplines. The Grantham Centre trains its student cohorts using the same CDT model. Four staff have also been involved in the Sheffield E-Futures CDT. Numerical data on PGR students are provided in **§2.2**.

***Large awards for interdisciplinary research*:** Various large grants awarded to members of the Department have supported our interdisciplinary research. For example, *Chauvet* and *Martsinovich*

were awarded £794k (NE/T010924/1, NERC) for an ambitious collaborative project with Cameron (Animal and Plant Sciences) and NSF-funded US collaborators (Kansas, Texas and Alabama) which aims to develop new methods for measuring and modelling the distribution of phosphate in soils. *Leggett* has led two EPSRC Programme Grants (Low-Dimensional Chemistry, £4M, 2011-16 and Molecular Photonic Breadboards, £7.3M, 2020-25), each involving collaboration at the biology/chemistry/physics interface. *Meijer* collaborated with Blakey (Mechanical Engineering, now at Birmingham) on three EU grants (CleanSKY2 programme) focused on auto-oxidation of jet fuels (total £1.7M) with Rolls-Royce as an industrial partner.

During the next five years we will:

- prioritise developing proposals for large interdisciplinary collaborative projects;
- consolidate strong work at the chemistry/biology interface by maintaining strong collaborations with life scientists;
- enhance work on nanomaterials and light-matter interactions by building new collaborations with the Department of Physics in photonics and nanomaterials (e.g. £1.7M near-field spectroscopy award with Tartakovskii, 2020-24; Leggett Programme Grant 2020-25) and by expanding the international reach of the Porter Lab.
- build on our strong portfolio of research on sustainability, by adding work on inorganic materials and solar energy capture;
- expand theory work on molecular modelling of biological and polymeric materials.

1.5. Open research

Consistent with best practice in the chemical sciences, metadata are typically published as extensive supporting information files accompanying every publication. Staff are encouraged to archive data using ORDA, the University's data repository. Structural data are submitted to crystallographic (e.g. Cambridge Structural Database) and NMR structural databases. To ensure maximum discoverability of our research, we aim to put all outputs in White Rose Research Online, our shared repository with Leeds and York (green route). This is our preferred route, ensuring equity in publishing opportunities regardless of available funding; we also publish outputs in fully OA journals or hybrid where required for funder compliance. In addition, staff increasingly submit papers to preprint services such as ChemRxiv, bioRxiv or arXiv.

We have contributed to driving forward the open research agenda. For example, *Jones* participated in an RSC initiative to define standards for metadata in synthetic chemistry. *Hill* has created an open repository for the basis sets he has developed, which are used in high-accuracy calculations on heavy elements in many types of quantum chemical calculations. This repository gets 2,000-4,000 hits per month.

Members of the department are also extending the open research ethos to experimental studies. For example, *Craggs* has developed an open-source single-molecule FRET (smFRET) resource that aims to democratise measurements, by providing designs, software and a list of all the components for a fully-functional, low-cost system. A key challenge in smFRET has been to establish data standards to enable the effective sharing of data between different laboratories. *Craggs* played a leading role in a consortium of 20 partners from Europe and North America that developed a unified, straightforward method to solve this problem (*Nature Methods*). The consortium proposed experimental and computational procedures for converting FRET efficiencies

into accurate distances and provided a quantitative assessment of the reproducibility of intensity-based smFRET measurements.

1.6 Research integrity

The University's Good Research and Innovation Practices (GRIP) policy governs research in the Department. All staff and all postgraduate research students (PGRs) receive mandatory training in research ethics and integrity. Maintaining strong integrity underpins our aim to conduct impactful research that is both transparent and reproducible.

Compliance is overseen by our Research Committee. All staff and PGRs are provided with training via away-days, staff meetings and targeted training for specific staff groups. As well as formal training, we aim to create an open and honest environment in which researchers feel confident to challenge inappropriate research approaches. Our Research Groups organise seminars that provide opportunities to debate and challenge research. Although most research in chemistry does not require prior ethical approval, the Department has an Ethics Lead (Burnham) who organises proposal reviews as required by trained ethics reviewers.

2. People

Our staffing and recruitment strategy aims to ensure that we have the breadth, depth and diversity of research excellence needed to achieve our research goals (**§1**).

2.1. Staffing strategy and staff development

Staff development strategy

An important goal in the current REF cycle was to develop a succession plan to maintain a well-balanced department with a sustainable future. To achieve this we appointed nine ECRs across all research groups. All have made excellent starts towards establishing their independent research programmes. Additionally, we appointed EPSRC Industry Fellow *Slark* to enhance our engagement with industry.

To enable these promising researchers to develop fully as research leaders, we implemented various measures, including a mentoring scheme and the creation of the role of Deputy Research Group Head to provide them with experience of leadership. To further balance our age profile, we will recruit mid-career staff across our research groups during the next five years to retain strong research leadership and bridge the gap between established senior staff and emerging ECR leaders.

All staff undertake an annual review with their line manager (research group head) in which they discuss their contribution over the preceding year and set agreed objectives for the following year, identifying training and development needs where applicable. The result is a portfolio of achievements that align with both Departmental and personal goals, enabling staff to maximise opportunities for promotion under the University's new Academic Career Pathways framework (see REF5a). In addition, staff have longer-term individual research planning meetings with their research group heads that enable them to discuss their three-year plans for funding, writing, and impact activities that can be signposted for relevant institutional and external support.

The Department supports ***study leave*** to allow staff relief from teaching and other responsibilities for one semester. For example, *Fowler* used study leave in 2019 to research 'Coulson's lost theorem' in The Bodleian Library. In 2019, the Faculty introduced an enhanced study leave programme, under which staff are eligible for study leave every seventh semester.

Support for ECRs

We strive to uphold the principles and implement the responsibilities of the 2019 *Researcher Development Concordat*.

Postdoctoral researchers are supported by the extensive and outstanding (Times Higher Education Awards 2014) training and development programme, Think Ahead, which offers workshops, seminars, mentoring, networking opportunities, online resources, and job preparation sessions. Researchers benefit from a bespoke annual review tailored to their specific needs and receive peer support through the Chemistry Researchers Society (CRS, established in 2013, run by PDRAs and funded by the Department), which organises monthly coffee mornings and lunchtime or evening seminars and provides representation on departmental committees.

Transition to tenured posts. We recognise that precarity is a concern for our postdoctoral researchers, and aim to appoint them on open-ended contracts wherever possible. For example, *Mykhaylyk* (**Box 3**) was *promoted* to Senior Research Fellow following his successful EPSRC grant application for a world-class SAXS facility with *Armes*. We also support ECRs applying for independent research fellowships. The Departmental Executive, in consultation with the Research Committee, evaluates their fit to departmental research strategy and EDI considerations, based on CV, research plans and a departmental visit and seminar. Where reviews are positive, candidates receive support and advice from relevant senior staff in preparing their fellowship application.

Successful applicants are promised a permanent post, subject to satisfactory progress. For example, *Foster* was initially appointed as a Ramsay Memorial Fellow during the assessment period before transferring to a Vice-Chancellor's Fellowship via a highly competitive cross-institutional process. He took up a lectureship in 2019 and is making excellent progress towards completion of probation.

Box 3. Supporting researcher development: Sasha Mykhaylyk

2004 - 2011 Research Associate
2012 – 2016 Research Fellow (permanent)
2017 – 2020 Senior Research Fellow (equivalent to Senior Lecturer)

Sasha currently manages the £2M Soft Matter Analytical Lab (**§3.2**).

Academic staff appointed at lecturer level complete a three-year probationary period. In this supportive process, the probationer is assigned a mentor, who they meet monthly to review progress. Probationers have reduced teaching loads to enable them to establish independent research programmes. Each is provided with a start-up grant and a PhD studentship, and the CDT-PSC and the Grantham Centre have both supported additional studentships for ECR staff in the Department. Two years ago, we introduced an additional mentoring programme to support ECR staff after completion of probation. This will be extended to all staff from 2021.

2.2. Research students

PGRs are a vital part of a research-active chemistry department. Thus, we made support for PGRs a strategic priority for the current assessment period. Relative to the REF2014 period (average 103.8 FTE), our PGR annual enrolment for REF2021 (average 119.4 FTE) has increased by 15%.

Our PGRs are supported by a diversity of sources. In the assessment period, the CDT-PSC has had the single largest impact on student numbers (50, with 36 in Chemistry), although we have additionally benefitted from students funded by the Grantham Centre and by enhanced success in securing studentships funded by overseas organisations and governments. Studentships have also been funded by EPSRC, BBSRC, EU, industry, and overseas governments (including 155 students from 29 different countries in the REF period). The University's partnership with the A*STAR institutes in Singapore has created further additional studentships, and has facilitated international collaboration with these prestigious research institutes.

***Diversity among PGRs*:** In this assessment period we have implemented various methods to recruit a more diverse PGR cohort. We made a concerted effort to review and improve our recruitment materials and methods (e.g. using Textio to debias the wording of advertisements). Mandatory training is provided for all staff who chair interview panels, while all staff must complete unconscious bias training to ensure they are aware of the potential for bias and discrimination in selection processes. Illustrating the impact of these measures, the fraction of female PGR students has increased steadily from 33% in 2012/13 to 43% in 2018/19.

***Quality of training and supervision*:** Our goal is to provide students with a broad training in relevant transferable skills in addition to the in-depth training that they receive in their research specialism. New academic staff receive training in PGR supervision and support through mentoring. Students receive compulsory training covering e.g. health and safety, research ethics, information technology, and take a range of advanced courses tailored to meet their needs as determined through an annual training needs analysis undertaken with their supervisor. All PGRs are assigned an independent advisor, who checks their progress annually, provides pastoral support and discusses career progression with them.

During the assessment period, 57 PGR students have additionally benefited from the comprehensive advanced skills training provided by the CDT in Molecular-Scale Engineering, the CDT-PSC and the Grantham Centre.

A number of our students have won external prizes (e.g. Kirsty Smitten, Box 2). The Department celebrates the achievements of its PGR students through the award of our annual Turner Prizes: up to four prizes are awarded in recognition of students whose theses are judged to be outstanding by their examiners.

Box 4. Some of the attendees at our 2020 Global Women's Breakfast.

2.3. Equality, diversity, and inclusion

Over this assessment period a central goal has been to create a more diverse department by providing more effective support for under-represented groups. Our EDI Director is a member of the Executive, thus putting EDI considerations at the heart of departmental decision-making and driving policies and activities to support engagement by diverse groups of staff and students (e.g. **Box 4**). The success of our strategy is exemplified by Athena SWAN Silver Awards in 2015 and 2020, which built on the Bronze Award in 2013. Sheffield's commitment to eliminating discrimination and promoting diversity includes strong and active support for our LGBTQ+ staff and students, as evidenced by our ranking of 23 in the Stonewall *Top 100 Employers* 2019 survey. The University has launched an action plan with the aim of effecting transformational change targeting under-representation, progression, and attainment of Black, Asian and minority ethnic (BAME) staff and students with the aim to create a University community that is diverse and inclusive.

***Flexible working*:** We encourage staff to organise their work flexibly to balance family and other commitments, minimise stress and increase their personal effectiveness. Our Flexible Working Strategy includes many measures designed to support staff with non-standard working patterns, e.g. the identification of 'core hours' within which all departmental meetings occur and scheduling of staff meetings to ensure that no part-time staff are regularly excluded because of their working pattern.

We recognise that staff need to balance a wide range of responsibilities, which may vary over time. Thus, we endeavour to accommodate changes in working pattern. During the assessment period, eight staff (both female and male) have adopted part-time working for various reasons. Two of them have subsequently returned to full-time working. Thus far, all requests for changes to working pattern within the Department have been granted (e.g. **Box 5**).

***Support for EDI in the promotion process*:** We have taken action to address the gender pay and promotion gap. The Department has an inclusive approach to academic staff promotion: *all* staff

are automatically considered for promotion annually, a policy that avoids disadvantaging anyone reticent about putting themselves forward for promotion (a group that is thought to include a disproportionately high fraction of female staff). The positive impact of this approach is evidenced by our high success rate of promotions, particularly for female applicants: of 15 academic staff promoted, 6 were female (40%) (one part-time), significantly more than the proportion of female teaching-specialist and T&R staff (20%). In addition, 50% of female T&R staff are now professors.

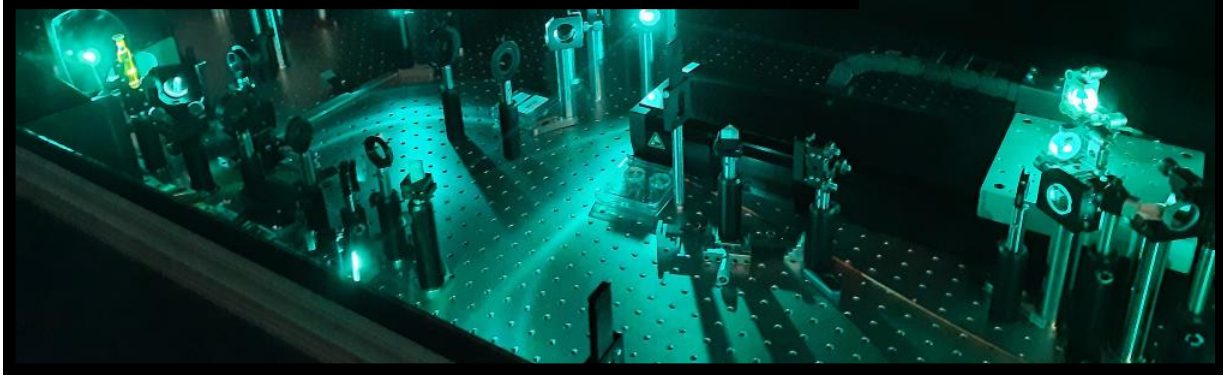
Box 5. Supporting flexible career pathways: Julia Weinstein

I joined the Chemistry Department as a Lecturer in 2005.

On return from maternity leave in 2007, I received support from WARP, which allowed me to retain a highly skilled postdoc in my group, easing the transition enormously.

I worked part-time for several years and was pomoted to Senior Lecturer in 2010, whilst I was still working part-time.

Subsequently, I returned to full-time working and was promoted to Reader in 2015 and Professor in 2016.



***Support for EDI in recruitment for leadership roles*:** Recognising that direct appointment to roles by the Head are susceptible to influence by unconscious bias, a new approach was introduced in 2018. Thus, for substantive roles within the Department, an invitation is issued for expressions of interest which are discussed by the Executive. Subsequently, eligible staff are interviewed. Posts are normally held for a three-year term.

***Support for parental leave*:** In addition to statutory support, female academics are strongly encouraged and supported to apply to the Women Academic Returners Programme (WARP). This scheme provides up to £10k funding for research staff costs, or to kick-start research on return to work by providing reduced teaching loads or funding conference attendance. Two Chemistry staff have used this scheme since 2014. Staff may also choose to work part-time after return from parental leave, with a guaranteed opportunity to return to full-time work in the future. One staff member changed to part-time and then back to full-time during the assessment period; her probation period was also extended to reflect the period of part-time working.

***Supporting the wellbeing of staff and students*:** The Faculty recently established a network of trained wellbeing advocates that includes staff from every department, whose role is to assist anyone needing information or support to identify appropriate sources of specialist support within the University. Those in Chemistry are members of the EDI Committee, thus placing wellbeing at the heart of our thinking. Extensive work has been conducted to prevent bullying and harassment in the workplace. In 2019 the University rolled out the 'Report and Support' system for staff and students who have experienced bullying, harassment, verbal or physical abuse.

***EDI issues in the preparation of this REF submission*:** In accordance with the University code of practice, four principles were applied throughout all stages of our submission: *transparency*, *consistency*, *accountability* and *inclusivity*. All staff with a leading role in our REF submission have undertaken REF-specific EDI training, and 2/7 of these staff were female. Selection of outputs was guided by anonymous internal and external reviewers.

3. Income, infrastructure and facilities

3.1. Research income

We maintain a large, balanced portfolio of funding from many sources, including research councils, industry, government agencies and charities, which is essential for our long-term sustainability in an uncertain funding climate. Over the assessment period, our goals have been:

a) ***To prioritise interdisciplinary research*** by making targeted appointments to further strengthen our diverse activities at the chemistry-biology interface, and in light-matter interactions, nanomaterials, and sustainability.

b) **To increase income from industrial partners and from other sources outside the research councils,** primarily by developing new activities focused on sustainability.

c) **To update core equipment and to invest strategically in new capability** to drive forward our research strategy.

Our successes in **(a)** and **(b)** are illustrated below, while **(c)** is addressed in **§3.2**.

We have supported staff to win research funding through various measures, including compulsory peer review of research proposals organised by research group heads, who also provide advice on research strategy and the preparation of proposals, in addition to longer-term planning through research review meetings (**§2**). We have an internal database of successful applications and ongoing proposals to provide examples of best practice.

a) ***Interdisciplinary research and collaboration*** has been a central focus of many larger grants. Our staff have contributed as PI or Co-I to 26 active grants with award values of at least £1M during the assessment period. Highlights in EU funding include two £2.0M ERC *Advanced Investigator* grants for polymerisation-induced self-assembly (*Armes*) and synthetic biology (*Hunter*) respectively, three Marie Skłodowska-Curie ITN grants (€6M) in organic synthesis, and Horizon 2020 Future Emerging Technologies OPEN project "FLow Induced Phase Transitions (FLIPT)" for environmentally friendly plastics processing (€3.7M, €600k to Sheffield). *Leggett* has led two EPSRC programme grants on low-dimensional chemistry (£4.0M) and molecular photonic breadboards (£7.3M, ongoing). *Armes* and *Slark* hold EPSRC fellowships (each >£1.5M) and *Ryan* leads an interdisciplinary EPSRC programme on redefining single-use plastics (£1.01M). Eight other staff have been PI or Co-I in separate multi-investigator projects from EPSRC, MRC, EU and Wellcome Foundation. The research and impact contribution of selected major collaborations are described in **§4**.

   All nine ECR staff appointed to support our strategy have secured PDRA funding from EPSRC, BBSRC, NERC or the Leverhulme Trust, a direct result of the support and mentoring highlighted in **§2**. Highlights include construction and commercialisation of the

world's first low-cost (FRET) microscope for single-molecule detection (*Craggs*), novel computationally efficient high-accuracy models for intermolecular interaction and applications of AI in chemistry (*Hill*), novel dispersible porous polymers (*Dawson*), a high-profile in the emerging field of tunable 2D metal-organic nanosheets (*Foster*), development of spectroscopic tools for measuring phosphate depletion in soil (*Chauvet*, *Martsinovich*). Our grant spend per FTE has remained consistent despite several senior staff retiring or moving to other UK universities, providing good evidence of the success of our strategy to focus on the recruitment of talented ECRs.

b) ***Collaboration with industry has grown:*** *Portius* has received funding from QinetiQ, DSTL and The Home Office on energetic materials. *Ryan* is the lead Sheffield academic on a *Sustainable Coatings by Rational Design* (SusCoRD) AkzoNobel-EPSRC *Prosperity Partnership* grant (£1.53M to Sheffield over five years). This collaborative project involves the Universities of Liverpool and Manchester, Airbus, Crown Packaging and Tata Steel. To further strengthen industry-facing activities, *Slark* was appointed as a professorial fellow in 2018 to capitalise on his 20 years of experience working in industry. He works closely with the University's Advanced Manufacturing Research Centre (AMRC) on metal-composite adhesion and collaborates with *Ryan* and Rothman (Chemical and Biological Engineering) on single-use plastics in research funded by The Welding Institute.

Knowledge transfer activities: Staff have carried out research projects co-funded by 46 companies spanning a range of commercial sectors including commodity chemicals (e.g. BASF), speciality chemicals (e.g. Lubrizol), custom synthesis (e.g. Peakdale Molecular), pharmaceuticals (e.g. Astra-Zeneca), agrochemicals (e.g. Syngenta), oil and gas (e.g. BP), defence technology (e.g. DSTL), coatings (e.g. AkzoNobel), cosmetics (e.g. L'Oreal), household & personal care products (e.g. Unilever, P&G), diagnostics (e.g. QuantuMDx) and materials (e.g. Scott Bader).

***New income streams*:** The Grantham Centre was established with a large philanthropic donation (£8.7M). It has funded a CDT focused on sustainability, which has involved seven staff and nine PGR in Chemistry, and has provided a nucleus for important new initiatives (**§4**).

The next five years: To complement our research strategy of important cross-cutting interdisciplinary research themes we will:

- Prioritise the development of proposals for large interdisciplinary collaborative projects.
- Build on our strong portfolio of research on sustainability, by adding work on inorganic materials and solar energy capture.
- Target enhanced funding for PGR training, through applications for CDT funding.
- Build on the established excellence of the Polymer Centre, by using our recent expansion of KE activities as a platform to construct a broader portfolio of industrial partnerships, and by taking advantage of opportunities offered by the sector-leading AMRC.

3.2. Organisational infrastructure supporting research and Impact

After REF2014, we identified the need to renew and expand our core instrumentation, and to develop strategic plans to ensure that all our research was supported by world-leading infrastructure. Therefore, we developed a strategy to secure funds to support these aims.

***Core facilities*:** include NMR (five spectrometers), X-ray crystallography (five diffractometers), the Faculty of Science Mass Spectrometry Centre (FoSMSC, five mass spectrometers for chemical and biological analysis), and an expanded computer cluster. These facilities are run by specialists, usually PhD scientists, who make significant contributions to our research output and provide vital training to our PGRs and PDRAs. The Department has many smaller items of equipment, which are available to all researchers and underpin our broad portfolio of research programmes, and shares access to imaging facilities housed elsewhere in the Faculty.

***Enhancing core instrumentation*:** We received £1.3M (EPSRC plus University funds) to support instruments underpinning a wide range of research in chemistry, including upgrades of NMR instruments; addition of single-crystal and powder X-ray diffraction instruments; addition/upgrades of three instruments in the FoSMSC; and upgrading and expansion of instrumentation for atomic force microscopy.

***Specialist facilities*:** The Polymer Centre provides state-of-the-art facilities for the comprehensive characterisation of polymeric materials, while the Centre for Chemical Biology provides extensive facilities for cell culture work, protein production and purification, biomolecular synthesis and biophysical characterisation. Our theoretical and computational capabilities have been enhanced by a new £63k computer cluster for artificial intelligence and molecular simulation, awarded to *Hill*.

Large investments in equipment to support research in chemistry

The Porter Lab*,* directed by Weinstein, opened in 2018. It hosts multiple ultra-fast (fs) electronic and vibrational techniques under one roof (transient absorption, infrared, 2DIR, fluorescence upconversion, diverse photoluminescence methods, at variable temperature and magnetic fields) that is unique within the UK. Ultra-fast spectroscopy was identified in REF2014 as a departmental strength and also offered the opportunity to develop interactions with other departments, e.g. Biological Sciences (photosynthesis), Medicine, Dentistry and Health (photodynamic therapy) and Physics (photonic materials and nanophotonics). The Porter Lab has been central to the successful pursuit of this strategy. It is managed by a dedicated facility scientist. Collaborations with 8 UK universities (to date), national facilities (RC@H,CLF, Diamond) and research groups in 6 countries spread across 4 continents have led to over 30 publications and have contributed to >£13M grant income.

The Soft Matter AnalyticaL Laboratory (SMALL) was established in 2016 by *Armes* and *Mykhaylyk* with the aid of a £874k EPSRC equipment grant and an £800k institutional investment to refurbish unused space. Its centrepiece is a world-leading laboratory SAXS instrument based on a liquid gallium MetalJet X-ray source which provides a viable alternative to synchrotron radiation for many studies (e.g. Armes, EPSRC Fellowship; Mykhaylyk *JACS* 2014, 2015, *Nat. Commun.* 2020). This facility serves research communities across the Northern Universities (N8) consortium.

The Sheffield Surface Analysis Centre (SSAC), directed by *Leggett*, houses an extensive suite of equipment for X-ray photoelectron spectroscopy (XPS), secondary ion mass spectrometry and scanning probe microscopy (AFM and SNOM). It supports various research groups across the Faculties of Science and Engineering and provides contract services to large and small companies. SSAC was awarded £737k from an EPSRC capital equipment grant in 2015 to procure a new, state-of-the-art XPS instrument with the capability for non-destructive depth-profiling and enhanced imaging capability.

Impact: Our world-class facilities underpin a wide range of impact-generating activities, including collaborative research programmes with industry; provision of specialist technical support to industrial partners; consultancy; and the provision of contract research services including

sophisticated problem-solving for commercial customers. Farapack Polymers and Sheffield Synthesis Solutions are spin-out companies that were established to facilitate KE activities. They have each facilitated engagement with a wide range of companies in the pharmaceutical, polymer and speciality chemicals sectors. Several members of staff have acted (and continue to act) as expert witnesses in legal cases.

Cross-HEI sharing of research infrastructure: We provide essential services (surface science analysis, polymer analysis, SAXS/WAXS analysis, NMR and mass spectrometry) throughout the University and also for our industrial partners. The University is a member of the N8 Group of universities, and has agreed equipment-sharing arrangements with these partners.

Major facilities: *Ryan* is a member of STFC Council and was non-executive director of Diamond Light Source (DLS). *Brammer* (DLS, 2015-18) and *Clarke* (Institut Laue Langevin, 2014-16) chaired facility access panels, *Clarke* chairs the EPSRC e-infrastructure SAT, and *Brammer* was a member of 5-year review panel for DLS crystallography beamlines. A number of staff are substantial users of national and international facilities through competitive awards. (£5.15M in-kind income, REF4c), leading to major grants and high-impact papers. Examples include: Central Laser Facility (CLF) (*Weinstein,* £178k, *Science* + 2x *Nat. Chem.*); DLS (*Brammer,* £1.45M, *Nat. Chem.* leading to £1.3M EPSRC); multiple facilities (*Mykhaylyk,* £556k; *Parnell* £1.47M, *Ryan* £590k). Collaborative interactions with these facilities include four co-funded and co-supervised PhD students (*Weinstein, Brammer, Mykaylyk*) and involvement in major new equipment initiatives (STFC PORTO and UK XFEL, *Weinstein*)

The next five years: We plan to refurbish half of our research laboratories and to rationalise the estate to create a physical environment able to sustain us for the next two decades. To achieve this we will exploit and benefit from the recently announced £150M Science Estate Development Framework, a major new initiative that provides an exciting opportunity for significant investment in the Department.

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

4.1. Support for research collaboration

During the assessment period we prioritised collaborative research in the design of our new research group structure. Our aims were:

- to develop strong interdisciplinary research programmes (**§1)**;
- to maintain internationally excellent standards of research through collaboration with leaders in the field;
- to achieve impact by working with end-users in the co-creation of new knowledge and in knowledge exchange.

Since 2014, many staff have led substantial UK-based collaborative projects. Collaborative projects led by *Brammer* have attracted >£2M in EPSRC funding to study fundamentals of intermolecular interactions and dynamic behaviour in MOFs with collaborators in Chemistry, Chemical Engineering and Pharmacy at Cambridge, York, Bath and Strathclyde Universities. *Brammer* was a Co-I of the UK Catalysis Hub (EPSRC, £3M), which funded work with *Haynes* and collaborators from Liverpool, Oxford, and Imperial on organometallic catalysis in confined spaces

(MOFs). *Thomas* and *Weinstein* led a collaboration (EPSRC, £860k) with our Chemical and Biological Engineering department, Imperial College, U. Jena and the Central Laser Facility on the development of metal complexes as imaging probes, which led to the identification of new theranostic leads for photodynamic cancer treatment.

International collaboration: International best-with-best collaborative projects facilitate world-leading research. *Armes* published 50 papers in the assessment period involving overseas co-authors in academia and industry spread across 11 countries including Ober (Cornell), Klein (Weizman Institute), Wanless (U. Newcastle, Australia) and Tuinier (TU Eindhoven). *Armes* has had long-term collaborations with US scientists de Yoreo (PNNL) and Estroff (Cornell) on the efficient occlusion of nanoparticles within calcite crystals (*Nat. Commun*. and *JACS*, respectively). As part of a £663k EPSRC grant with Moore (Biology) on the long-term storage of pluripotent stem cells, *Armes* published joint papers with Whitesides (Harvard) and Wang (Louisville, Kentucky). *Clarke* collaborated with colleagues at U. Pennsylvania with funding from the NSF/EPSRC Materials World Network Program, leading to 14 jointly authored publications in the assessment period.

D.Williams collaborated with Sturla (ETH Zurich) to characterise DNA alkylation damage. *Chen* collaborated with teams in The Netherlands, Spain, and Australia on broad-spectrum disease protection for enhanced plant growth in agriculture (*Nat. Chem. Biol.*). *Thomas* has two long-term collaborations with Das (CSMCRI, Bhavnagar and IISER Kolkata) and Felix (Aveiro) that have produced a series of publications including work on cell probes and therapeutic leads; with Williamson (MBB, Sheffield) he has collaborated with Keene (Adelaide) to determine the NMR structure of metal complexes threaded into duplex DNA.

Leggett's EPSRC low-dimensional chemistry programme grant yielded 60 publications, including joint papers with seven international authors, including Törmä (Aalto), Dutton (U. Pennsylvania), Schulten (Illinois) and Holten (Washington, St Louis). *Leggett*'s new programme grant on molecular photonic breadboards involves international collaborations with Spano (Temple, New York) and Ogilvie (Michigan).

PGR training building research critical mass: *Harrity* has led three Marie Skłodowska-Curie ITNs (total €6M) on synthetic chemistry of bioactive molecules, involving academic collaborations and exchange/training of PhD students across six European countries and companies in UK, Sweden, Netherlands, France, and Germany. We have led CDTs on polymers, soft matter and colloids and molecular-scale engineering (detail **§1.4**). Chemistry staff have been active in six other interdisciplinary CDTs either based or partially based in Sheffield. Moreover, 22 staff have supervised collaborative PhD projects with financial support from industry or national facilities such as Diamond Light Source (*Brammer*) and Rutherford Appleton Lab (*Weinstein*). Such studentships, which involve substantial (>6 months) placements at sponsor/collaborator sites, have been designed to significantly benefit the sponsor.

4.2. Engagement with key research users and beneficiaries

Over this assessment period our goal has been to expand our interactions with end-users in healthcare and to add new streams of activity aimed at generating humanitarian benefits and advances in sustainable manufacturing to our research portfolio.

Industrial engagement: Our staff have worked with 46 companies (**§3.1b**) leading to commercial impact and co-authorship of papers (e.g. *Mykhaylyk*, two papers on instrument development with co-authors at Anton Paar; *Coldham* and *Harrity* papers with co-authors at AstraZeneca). The Polymer Centre continues to play an important role in supporting and developing collaborations

with industrial partners. In addition, the Faculty has appointed two business development managers, who work closely with academic staff to develop relationships with prospective industrial partners. The CDT-PSC and the Faculty scheme to co-fund PhD studentships with external partners have further increased the number of academic-industrial collaborative projects. Finally, *Ryan* and *Craggs* have each acted as expert witnesses in separate patent litigation cases.

Departmental instrumentation underpins contract research with many companies, often brokered by our (wholly owned) spin-out company Farapack Polymers. For example, a wide range of companies and organisations, ranging from multinationals such as BP, L'Oreal and Unilever to local SMEs) have purchased analytical services from SSAC, and our SAXS and XPS instruments have also been used by companies and by academics working at Oxford, Leeds, Manchester, Huddersfield and Sheffield-Hallam Universities.

Healthcare challenges: With Skerry (Medical School), *Harrity* is a key member of an academic team that has developed a new first-in-class cancer therapeutic agent based on inhibition of the adrenomedullin-2 receptor. This team worked with a range of industrial scientists and consultants across the UK and China (e.g. Sandexis, Peakdale Molecular and Wuxi) to develop their academic ideas into a successful drug discovery programme. A Wellcome Trust Seeding Drug Discovery award (£2.95M; 2014-17) enabled them (i) to generate new, highly potent lead compounds and (ii) to demonstrate their efficacy both *in vitro* and *in vivo* (using simple models for pancreatic cancer). Follow-on Wellcome Trust funding (£2.0M, 2017-19) was secured for late-stage development of lead compounds for clinical development, leading to two patent applications and an associated publication in *ACS Pharmacology & Translational Science*. The team is currently spinning out a company *Modulus Oncology* to develop the IP on their proprietary compounds for clinical cancer therapies.

Humanitarian challenges: *Portius* received funding from QinetiQ, DSTL and the Home Office while Hippler received a two-year £186k grant from the 'Find a Better Way' charity for spectroscopic studies aimed at humanitarian demining of former war zones.

The Za'atari camp in Jordan is recognised by the UNHCR (the UN Refugee Agency) to be a safe haven for 80,000 refugees from the Syrian war. In the harsh, arid conditions in the camp it is difficult for refugees to grow their own food. With GCRF funding, *Ryan* has developed soil-free, hydroponic food production systems by repurposing discarded, unrecyclable polyurethane foam mattresses as growing media, thus enabling refugees to grow fresh produce, leading to better nutrition and improving mental health (**Box 6**). The Za'atari project is now self-sustaining, and *Ryan* is implementing similar schemes elsewhere in Jordan and Syria. With UNHCR's support, it is planned to take this humanitarian solution to refugees all over the world.

Environmental Challenges: *Ryan* is the lead Sheffield academic on a *Sustainable Coatings by Rational Design* (SusCoRD) AkzoNobel-EPSRC *Prosperity Partnership* grant (**§3.1(b)**). He leads a 'Circular Economy'' EPSRC grant (*Plastics: Redefining Single-Use*; £1.01 M) and presented findings from this programme at the House of Lords and to a Commons Parliamentary Inquiry (May 2019), and provided evidence to four policy consultations with HM Treasury and DEFRA. Our local MP, Paul Blomfield, highlighted this research project during a debate in parliament on unsustainable packaging and this project has also featured on the BBC's Inside Out programme and ITV's Calendar local/regional news programme.

4.3. Engagement with diverse communities

We have a vigorous and well-organised strategy to engage with diverse communities, especially in the Sheffield area. During the assessment period we have run sessions for local school students in our dedicated Kroto Schools Laboratory which have reached >7,000 school students from largely POLAR4 schools. CDT outreach activities, run by PGRs and sponsored by RSC and industrial partners, have reached >3,000 school students in the local area. Exploring STEM for Girls targets schools in the Sheffield region where there is a need for widening participation. Events have run annually since 2014. The most recent event in March 2020 welcomed 350 Y9-11 girls from 18 local schools. Our Taster Days, aimed at sixth formers considering pursuing a career in science, reach students from all over the country, with 27% coming from post-code areas with the lowest rates of engagement in higher education. Members of staff also go out into the community. For example, *Craggs* gave the annual RSC Christmas lecture for >200 Sheffield-area school children and *Ciani* presented at the Lowry Museum and at the LightNight Festival in Leeds. In addition, *Craggs* has been working with Channel Talent to deliver lectures to >100 schools around the country.

4.4. Contributions to the sustainability of the discipline and indicators of wider influence

Armes was elected FRS in 2014 and received a number of prizes over the assessment period. Highlights include the 2014 RSC Interdisciplinary Prize for his development of synthetic mimics for micrometeorites, in an international collaboration with space scientists, and the 2018 Royal Society Armourers and Braziers' Company Prize for his work on colloidal nanocomposite particles, which led to the development of successful commercial products by BASF, Cabot and DSM. He has been awarded the 2021 Sir Eric Rideal Lectureship, a lifetime achievement award in colloid science. His fruitful decade-long collaboration with Lubrizol was recognised by the Society for Chemical Industry with its 2020 SCI Innovation in Formulation award.

Staniland was awarded the 2016 RSC Harrison-Meldola Memorial prize for her exploitation of biomineralisation to produce magnetic nanoparticles via biomimetic syntheses; the Suffrage Science award, which recognises the achievements of women in science (2017); and the Wain Medal for research in biochemistry (2017). *Harrity* received the 2018 RSC Bader award in recognition of his outstanding contribution to synthetic organic chemistry. He also worked closely with Peakdale Molecular in 2014 and 2015 under the auspices of a Royal Society Industry Fellowship. *Weinstein* was awarded the 2017 RSC Chemical Dynamics Award for her seminal work in advancing the fundamental understanding of photoinduced charge transfer and the development of a new IR-laser induced control approach. *Ward* (now HoD, Warwick) received the 2016 RSC Supramolecular Chemistry prize for his leading contributions to the synthesis, characterisation, host-guest chemistry and functional properties of self-assembled coordination cages.

Brammer was elected President of the 700-member British Crystallographic Association (2015-18). *Leggett* led the EPSRC Grand Challenge Network on Understanding the Physics of Life “From Molecules to Systems” (2013-16), establishing a thriving community of 200 UK academics distributed across the physical and life sciences. Its “Roadmap for Biological Physics” was used by EPSRC and UKRI to guide the expansion of funding for this field. The network has been refunded twice and the network management group was awarded the 2020 IoP Rosalind Franklin Medal.

Staff have delivered plenary/keynote lectures on four continents (e.g. *Brammer* 10 lectures; *Armes* 5 lectures). During the assessment period, staff have been members of 18 journal editorial or advisory boards, including *Chemical Science* (*Weinste*in); *J. Mat. Chem. B* (*Staniland*); *ACS Nano* (*Leggett*); *Langmuir* (*Armes, Leggett*). Wider engagement with overseas institutions includes a visiting professorship at Cornell (Ryan); 5-year departmental review panels for Universities of Cape Town and Witwatersrand, SA (*Brammer*); German and Swedish Research Council panels (*Weinstein*); major facility access panels or science committee in France, Germany, USA (*Mykhaylyk*, *Ryan*, *Brammer*).