Institution: University of Nottingham
Unit of Assessment: UoA8 – Chemistry
1. Unit context and structure, research and impact strategy

1.1: Unit Context/Overview

The vision of our School is focused on developing new science that underpins the delivery of atom-efficient, energy-resilient chemistries that address some of society's most pressing challenges. We have built a strong research community that shares this common goal and our strategy is implemented through four Research Themes that cut across all facets of chemistry: biological, computational, theoretical, materials, instrumentation and analysis, synthesis and catalysis.

We have developed and led major initiatives, seeded in our REF2014 strategy, which now forge links that span our University faculties. Looking to the future, we have initiated new and original research programmes that will form areas of strength beyond the current assessment period.

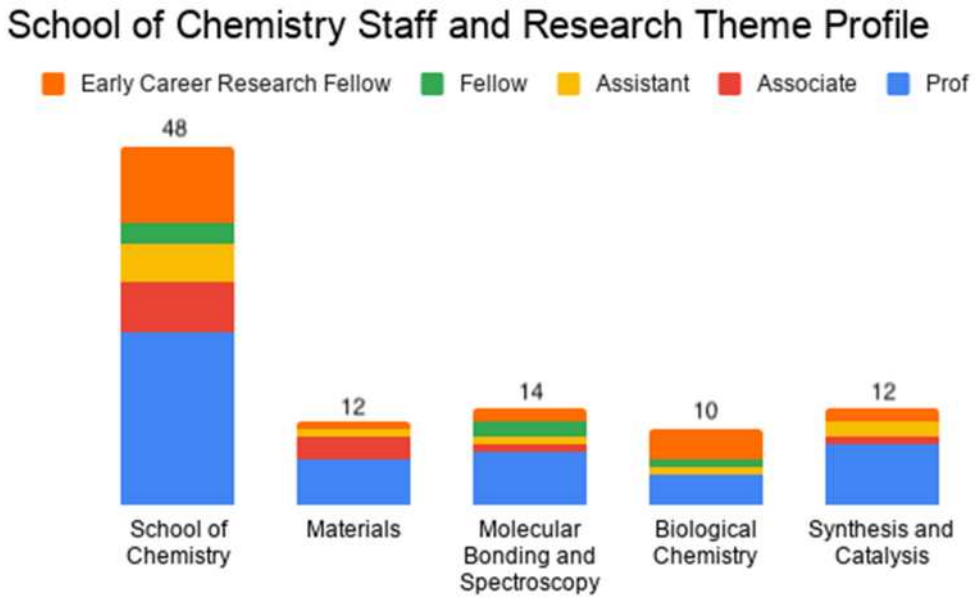
Over the REF2021 period we have delivered

- Major impact in sustainable chemistry with our Carbon Neutral Laboratory an exemplar for the future of sustainable laboratory-based research facilities.
- Our Centre for Sustainable Chemistry (CSC) that underpins the University's Green Chemicals Beacon of Excellence and has provided breakthroughs that will transform sustainable fine chemicals manufacture in the UK.
- Research funding of £44.13 million (including £747K R&D expenditure credit); a 36% increase compared to the previous REF2014.
- Investment in people including appointment of 17 new REF returned staff (13 of these are ECRs).
- Staff progression: 13 promotions (8 to Chair) recognising excellence in research.
- High-profile Honorary Professors, including Sir Fraser Stoddart (Nobel Laureate) and Paul Anastas, Academician Buxing Han (leading Green Chemist) and Natalia Tarasova (former President of IUPAC).
- A rich and vibrant research culture recognised by >50 national and international awards and fellowships including six RSC, Royal Society, two Royal Academy of Engineering, ACS, AAAS, Academia Europaea, UNIDO, Russia, China, USA and four Royal Society Wolfson Merit Awards.
- Publication of 1420 peer reviewed papers which have received >22,000 citations including influential outputs in *Adv. Mater., Chem. Sci., JACS, Nature and Science families, PRL*.
- Diversity Impact: Our annual "Women in Chemistry" conference, organised by School's PhD students on International Women's Day highlighted in 2020 by *Nature Chemistry* and the UoN Vice Chancellor's Medal.
- Global dissemination of our research with two Royal Society Summer Exhibitions and other live events with >40k attendees, and >130M views online with our Periodic Table of Videos.
- Filing of 14 key patents and 68 IP disclosures.
- Engagement with over 150 companies including strategic partnerships with GSK and Lubrizol.
- Graduation of 315 PhD students (6.7 per staff FTE).

1.2 Structure

The School of Chemistry supports a dynamic and vibrant research community and is returning 48 (46.7 FTEs) Category A researchers; 47 are fully based in the School. These include 23 Professors, 8 Associate Professors, 6 Assistant Professors, 3 Senior Research Fellows and 9 Early Career Research Fellows (ECRFs supported by a range of internal and external personal Fellowships).

Our research and impact strategy is supported and delivered by **four Research Themes**.



Names of ***staff returned in REF2021 are italicized***

Since 2017, our management has been led by the School Leadership Team (SLT) comprising Head of School (HoS) (*Howdle*) Deputy HoS for Research (*George*) and for Teaching (*McMaster*) and Directors of Operations (Chambers-Asman) and Business and Knowledge Exchange (Farren). The four **Theme leaders** of the four Research Themes and their *deputies* report into SLT. The Theme leaders also constitute the School's Research Committee (SRC), led by *Khlobystov*, reporting to the Faculty Research Board. Strategic decisions on teaching and research are discussed and enacted through this structure, which also ensures effective research line management (**Section** 2.1; **S**2.1).

- **Materials**: ***E. Besley***[P], *Amabilino*[A], *Kays*[P], *Champness*, *Howdle*, *Mokaya*, *Newton*[A], *Titman*, *Walsh*[P], *Johnson*[A,P], *Vandeginste*[A,P], *Pilgrim**
- **Molecular Bonding and Spectroscopy**: ***Licence***, *N.Besley*[P], *McMaster*[P], *Reid*, *Wheatley*, *George*, *Khlobystov*, *Teale*[P], *Wright, Argent*[A], *Rance*[P], *Cliffe**, *Alves Fernandes**, *Lanterna*[A]
- **Biological Chemistry:** ***Thomas***, *Oldham*[P], *Hirst*, *Mitchell*[A], *Soultanas*, *Williams*[P], *O'Neill**, *Ciano**, *Quaglia**, *Harvey**
- **Synthesis and Catalysis**: ***Lam***, *Hayes*, *Ball*[A], *Cuthbertson**, *Denton*[P], *Dowden*, *Moody*, *Poliakoff (FREng, FRS)*, *Stockman*[P], *Woodward*, *Silvi**, *O'Duill*[A]

[A]Staff appointed since REF2014; [P]staff promoted since REF2014, *ECRFs

A dedicated Equality, Diversity and Inclusion (EDI) Committee operates across all job families and our Athena Swan application and Action Plan adherence is driven by our Self-Assessment Team

led by *Hirst*. Our approach and the School structure ensure succession planning, a balanced working culture and addresses EDI for all staff and students (**S**2).

1.3 Research and Impact Strategy

Our strategic aims in REF2014 positioned Chemistry to lead in larger scale projects (nationally, internationally and industrially), to build upon existing strengths and to enhance impact. Central to this was a need to strategically appoint new staff to maintain our vitality and to allow flexibility to focus upon emerging research areas.

Specifically, our stated aims in **REF2014** were under the headings:

(i) Building research capacity.

(ii) Building collaborations and strengthening interdisciplinary interactions (reported in **S**4).

(iii) International partnerships (**S**4).

(iv) Sustainable Chemistry at Nottingham.

(v) Developing new instrumentation and theory.

1.3.1 Implementing Our Strategic Goals During the Assessment Period

(Below, "**IES-S**X" refers to relevant sections of the Institutional Environment Statement and "**ICS-1** to **ICS-4**" to our four Impact Case Studies).

The University's 'Research Vision' is to establish transdisciplinary Beacons of Excellence to direct >£200M investment towards targeted goals with societal impact building on research strengths across the University (**IES-S**2). Chemistry was instrumental in shaping the themes of the Beacons and contributes strongly to the research. *George* and *Licence* have major roles in **Green Chemicals** linking strongly to our Centre for Sustainable Chemistry. *Amabilino* and *Wheatley* have leadership positions in **Propulsion Futures** and *Harvey* is pivotal in **Precision Imaging.**

Our 117 REF outputs constitute a portfolio of cutting-edge internationally leading research which addresses major challenges in modern chemistry including developing energy and atom-efficient reactions, discovering materials with new functional properties and inventing new analytical and theoretical tools to study matter across the length scales.

Key breakthroughs supported by the actions and activities initiated through our REF2014 objectives include: innovative synthetic routes enabled by new metal catalysts (e.g. Au/Cu) and organocatalysts (e.g. phosphine oxides); materials with redox/photo-activity (e.g. mechanically interlocked and supramolecular); functional inorganic nanomaterials (e.g. metal oxides, sulfides) templated by self-assembled block-copolymers or nanotubes; time-resolved IR & XAFS spectroscopy characterising the bonding of transition metals (e.g. M-Xe or CH-M); diffraction and spectroscopic methods uncovering new f-block element bonding (e.g. U-As bond), and direct imaging of chemical reactions at the single-molecule level.

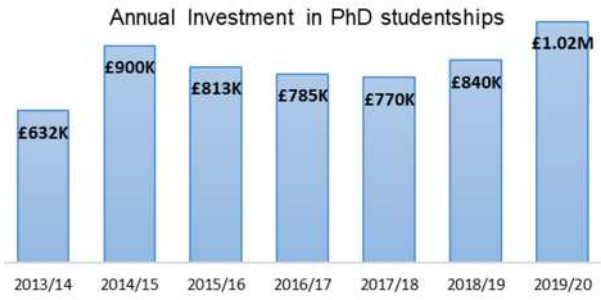
Building Research Capacity: We have ensured sustainability and vitality through the strategic appointment of new staff and continued allocation of resource for PhD support to drive new research ideas.

Staffing Strategy: We have appointed 17 new staff (~33% of our return), 12 as independent Fellows to ensure succession planning and to create our future research leaders. Nottingham

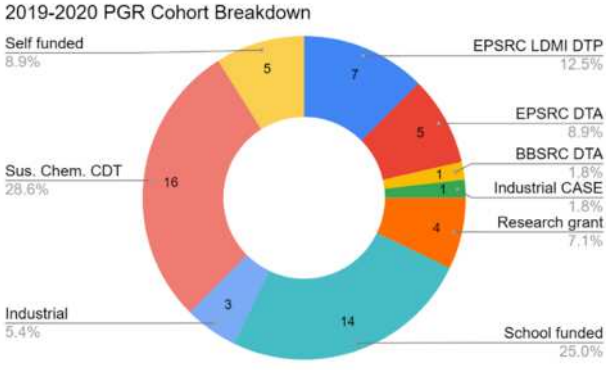
Research Fellowships (NRFs) are competitive 3-year posts (ca. 90 applicants to chemistry annually; **IES**-**S**3.2) with £75K research funds, a School funded PhD studentship and excellent mentorship and links to the wider University via our Research Themes. The first cohort, *Newton*, *Mitchell and Johnson* have moved to permanent academic posts. We have specifically aligned some NRFs with the Beacons: Propulsion Futures (*Alves Fernandes* and *Johnson*), Precision Imaging (*Harvey*) and Green Chemicals (*Silvi* and *Pilgrim*) whilst others are developing strongly at the heart of the discipline (Synthesis - *Cuthbertson)* and in multidisciplinary areas (e.g. synthetic biology - *O'Neill). Ciano* and *Quaglia* were appointed to Anne McLaren Fellowships targeted at women, and *Cliffe* to a Hobday Fellowship (**S**3.1.1), with identical levels of support and mentoring to the NRFs. Fellows are encouraged to apply for external fellowships and funding with 8 currently under assessment; significant successes so far include Royal Society URF (*Cuthbertson*), EPSRC-UKRI Innovation Fellowship (*Johnson*), and EPSRC New Investigator Award (*Silvi*).

The success of staff in delivering high impact publications and achieving international visibility has resulted in 8 Chair promotions since 2014 in Biological Chemistry (*Oldham,* Paradisi), Materials (*E. Besley, Kays*), Synthesis and Catalysis (*Stockman, Denton*) and Molecular Bonding and Spectroscopy (*McMaster, N. Besley*) as well as new appointments. *Lam* (GSK Professor of Sustainable Chemistry) leads our strategy around synthesis with expertise in organic synthesis and catalysis (ERC funding £1.35M, Starter Grant) and has a track record of securing significant funding from the EPSRC and UK Pharma. *Amabilino* (GSK/EPSRC co-funded Chair appointed 2015; £1.13M) is spearheading frontier research activity around energy materials. Dupont, appointed to a chair (2015), returned to Brazil for family reasons after three years. However, *Alves Fernandes*, a talented PDRA from his team has become an ECRF leading independent research focused on a novel "synthetic physics" approach to fabrication of highly active, naked nanocatalysts, linked to the UK Catalysis Hub and contributing to an EPSRC Programme Grant as a CI. Two assistant professors (*Lanterna, O'Duill*) were appointed in 2020 with three further posts advertised in December 2020.

To maximise research, we carefully balance teaching loads for research-active staff with support from a strong contingent of 11 teaching-focussed academics. This has enabled research to flourish whilst still recruiting ~240 undergraduates annually for the past 5 years, the largest chemistry cohort in the UK.



PhD Students are the next generation of chemistry researchers (**S**2.3). We have committed an average >£700K p.a. of School resources which, together with UKRI/Charities/Industry funding, supports ~45 PhD students p.a. (~1 per staff FTE). Since 2014, we have graduated 315 PhD students (6.7 per staff FTE). They are the lifeblood of our research base and 40% of our REF outputs include PhD students as co-authors.



Additionally, the School has led several CDTs/DTPs and EU consortia that contribute strongly to the vitality, diversity and number of our PhD students. Those centres supported by EPSRC are the Chemistry-centred CDT in Sustainable Chemistry (directors *Moody* & *Licence*, £5.30M), renewed as "Atoms to Products" (directors *Licence* & *Lam*, £6.24M); together with CDT in Sustainable Hydrogen (deputy director *E. Besley*, £6.55M); DTP in Low Dimensional Materials and Interfaces (*Champness*); DTP in Molecular Imaging and Analysis (*Khlobystov*). Other support includes Wellcome Trust DTP in Antimicrobials and Antimicrobial Resistance (AAMR) (*Soultanas*); BBSRC DTP (*Thomas*); and EU training networks "REFINE" and "SINCHEM" (*Howdle*) and Marie Skłodowska-Curie "ASPIRE" (*Reid*).

Sustainable Chemistry at Nottingham:
The **Centre for Sustainable Chemistry (CSC)** is a £30M project, led by *Licence,* supported by the flagship Research Partnership Investment Funding scheme (UKRPIF) (£10.3M) initiated by GSK (£12M) and supported by stakeholders including Rio Tinto, Invista, EoN, Lucite, AstraZeneca (AZ), Croda, Lubrizol, Syngenta, the Wolfson Foundation (£386K). A very high-profile success of the CSC, **The GSK Carbon Neutral Laboratory (CNL)** opened in 2016 led by *Licence.* This is a research community-scale experiment that is showing excellent results and defining how modern chemical research should be conducted and demonstrating the energy resilient laboratory systems needed to reduce the environmental impact of every single chemistry experiment that we complete.

The building has the highest possible recognition from both the Building Research Establishment and the US Green Building Council; collecting "BREEAM Outstanding" and "LEED Platinum" awards (only the second building of any kind in the UK to achieve these criteria); RIBA award "recognising design excellence" (2018); RIBA Sustainable Project of the Year (2018); the RICS Project of the Year (2017); and the international S-LAB "Best Physical Sciences Building" (2016); and also receiving favourable coverage in journals including *The Architects Journal, Chemistry World, Angew. Chemie, C&E News, Institute of Civil Engineers*.

Much more importantly, we have worked to reduce the energy/water consumption of the facility. The numbers speak for themselves; after only 18 months, electricity consumption was ~30% less and municipal water usage ~ 40% less than in an equivalent traditional chemistry building *without compromising research activities in any way*. The CNL includes the support and provision of a £4M suite of state of the art, energy resilient instruments; 3 high-field NMR spectrometers (including high-pressure and cryoprobe systems for multinuclear measurement) , a materials characterisation suite including time-resolved fluorimetry, solid state UV-Vis and thermal analysis. Our laboratories are equipped with industry standard reaction monitoring facilities including multiple in-situ HPLC and GC systems, in-line ReactIR/EasyMax (including process calorimetry) and mass spectrometry instrumentation that enables investigation of individual processes, from TLC plates through to complex biological mixtures.

The CNL has also stimulated innovative activity in energy materials and batteries (*Johnson/Newton/Walsh* **S**3.2.2) and in ground-breaking new sustainable organic synthesis and catalysis research which has grown out of our strategic partnership with GSK; e.g. high-profile joint publications (*Denton*) and also new licenced compounds (**S**4.3). The CSC was also pivotal in the initial winning (2014-2022) and renewal (2019–2027) of our EPSRC CDTs in Sustainable Chemistry.

Developing New Instrumentation and Theory:
We have matched significant inward investment in high field NMR, High Performance Computing and targeted refurbishment of labs (£5.7M). We have extended applications of Q-Chem, comprehensive *ab initio* quantum chemistry software for accurate predictions of molecular structures, properties, and spectra that enabled elucidation of the time-resolved X-ray spectroscopy of alkane and fluoroalkane complexes (*N.Besley*). We have discovered energy flow mechanisms in isolated molecules using in-house constructed instrumentation such as time-resolved photoelectron spectroscopy, two-dimensional laser-induced fluorescence (2D-LIF) and zero-kinetic-energy (ZEKE) spectroscopy methods (*Reid* and *Wright*); these complement solution-phase 2D-IR instrumentation (*George*).

A major academic and industrial partnership, “Photo-Electro”, a £6.48M EPSRC programme grant, between Nottingham (*George, Licence*, *Poliakoff* and UoN Engineers), Bristol and Southampton and 26 industries (including key multi-nationals, UK CROs and SMEs) exploits platforms for photo-, thermo- and electrochemistry to manufacture fine chemicals, agrochemicals and pharmaceuticals sustainably, yielding new reactors and approaches for continuous photo-, electro- and thermo-chemical reactions with successful prototype designs working up to a scale of 1 kg/day. Research in this area is also being applied to specific projects in a range of companies *via* Innovate UK, EPSRC IAA and direct industrial funding.

More recently, a high-throughput magnetron sputtering system (unique in Europe) has begun operation in our School, enabling fabrication of sub-nm metal cluster for heterogeneous catalysis on a preparative scale and stimulated a second EPSRC programme grant “Metal Atoms on Surfaces and Interfaces” (MASI) (£6.67M, *Khlobystov, Licence, Alves Fernandes, E. Besley*). Our developments in novel mass-spectrometry and electron microscopy imaging and analysis have also generated significant new research capacity (**S**3).

1.3.2 Future Strategic Plans for Research

Sustainable Buildings: Reducing the Environmental Impact of Chemistry
In delivering the CNL, we have learned much about the infrastructural aspects of chemical research, whilst developing new ways of working that embrace multidisciplinarity and partnerships with industry and academia alike. Inspired by this approach, we have embarked on an ambitious programme of increasing the sustainability of our architecturally important Grade 2 listed 1962 Chemistry Building which currently consumes more energy and water than almost all buildings on Nottingham’s UK-based campuses.

We will now apply techniques from the CNL to support and develop analytical services with reduced energy footprints and recyclable cryogens. We are deploying sustainable refurbishment to deliver energy-resilient laboratories. We have begun this process by testing the efficiencies gained with rebalancing fume cupboards and installing vented cabinets in some of our existing labs and our refurbished teaching laboratories have already demonstrated the proof of concept on a larger scale. We will publicise our solutions to enable others to improve existing facilities and our Strategic Advisory Board (**S**1.5.1) stress that this information will be particularly timely for the

industrial sector. More broadly, we are demonstrating leadership to influence our University to adopt science-based targets that support the goals of the Paris climate agreement and contribute to the City of Nottingham's aspiration to become carbon neutral by 2028.

Research Vision: Maximising the Impact of Our Chemistry

We will focus on the delivery of high-impact scientific programmes that address key societal challenges spanning the fields of energy, materials, manufacturing, medicine, and healthcare, harnessing the research capabilities of our four Research Themes. We have secured the critical-mass funding to begin to tackle some of the big questions in key areas:

Computational Chemistry: We will develop next generation methods for simulation and interpretation of chemical processes in application areas previously inaccessible to computation. We will lead the development of new electronic structure methods with extended scope to treat molecules in extreme electromagnetic fields (*Teale*) and to simulate high energy multiphoton spectroscopic techniques (*N.Besley*). Our development of advanced theoretical methods and modelling tools will progress the areas of electrostatic self-assembly and radiation induced processes in nanomaterials (*E.Besley*) and address grand challenges in energy-related research that cannot be solved by experiment alone. These advances will be made available to the world-wide user base through leading software packages (QChem, Dalton, DL_Monte).

Artificial Intelligence and Data Driven Design: Our development and application of AI to key chemical challenges, including catalyst design, solvent optimisation and multiparameter screening, will rapidly accelerate the rate at which new molecules can be developed and produced (*Woodward*), whilst significantly reducing the impacts of failed syntheses and low activity. Our innovations will transform 'design-make-test-analyse' cycles and will be spearheaded by *Hirst* (RAEng Chair in Emerging Technologies 2020). Explainable and interactive AI models will capture nuanced high-level knowledge from chemists, paving the way to a new generation of hybrid AI-human chemical discovery.

Structure and Interfaces at the Sub-Nanoscale: Founded upon our innovations in the field of nanoscience, electron microscopy and ionic liquids, we have created a unique magnetron driven nanofabrication suite that enables the creation of exquisitely controlled metal clusters of 10-15 atoms at or near the surface of condensed phases that straddle the boundary between hetero- and homogeneous catalysis (*Alves Fernandes*). The "MASI" EPSRC Programme Grant will exploit these new catalysts in topical reactions including CO_2 activation, the synthesis of ammonia and creation of drop-in synthetic fuels. Key to this will be the interdisciplinary academic collaborations across the UK and engagement with industrial stakeholders.

Novel Methodology: Building upon our synthetic expertise in drug discovery and in-situ reaction kinetics measurements we are developing new experimental and theoretical methods to control the selectivity of reactions; and to translate to medicinal chemistry and materials (e.g. polymers, organic electronics). As an example, phosphorus reagents have been used for over half a century in chemical synthesis but are inherently wasteful in stoichiometric quantities. Recent fundamental research in collaboration with GSK has demonstrated catalytic use of phosphorus species to eliminate waste (*Denton*). The new catalysts mediate valuable transformations of feedstock chemicals and will be developed and exploited for scalable, sustainable syntheses of high value pharmaceuticals in batch and flow processes.

Atom Efficient Synthesis: Building on expertise in the fields of catalysis, AI and Process intensification we have secured a UKRI-EPSRC Prosperity Partnership with GSK and the

University of Strathclyde, GSK (£5.36M, *Licence*) for “end-to-end" processes that deliver novel pharmaceuticals via atom efficient and energy resilient routes. This partnership showcases excellence in catalysis, process design/monitoring and manufacturing while defining new production routes to molecules of significant value to GSK.

New Approaches to Continuous Manufacturing of Chemicals are needed to keep the UK at the forefront of pharmaceutical and fine chemical production at a time when advances in personal medicine are creating demand for a greater variety of chemicals but in smaller quantities. We will combine innovative organic chemistry, novel flow reactor engineering and AI to deliver processing agility for future chemical manufacture. Photo-Electro is the springboard, with the invention of new photochemical, electrochemical and thermal reactors which combine very high productivity with very small physical footprints (*George, Licence, Poliakoff*). We will integrate these reactors into multi-step chains with data-driven self-optimisation for accelerated delivery of new processes towards pharmaceuticals and fine chemicals in a cleaner, more sustainable way.

Bioprocessing and Feedstocks: combining expertise in synthetic chemistry with molecular and structural biology, bolstered by AI computational approaches including neural networks we will harness and disrupt a wide range of biological systems; from single peptides and proteins through to bacteria, plants and higher animals (*Thomas, Ciano, O’Neill*). We will build upon recent success working with the Bill & Melinda Gates Foundation linking process chemistry and synthetic biology for the manufacture of the antimalarial drug Artemisinin together with the strong synergy between the CSC and the BBSRC/EPSRC Synthetic Biology Research Centre (SBRC) (Co-I *Licence*). This activity is poised to generate new chemical routes and engineered metabolic pathways for the sustainable synthesis of platform chemicals; identify new natural products; and improve understanding of biosynthetic processes and enzyme mechanisms using chemical probes and structural biology. A significant outcome will be new biopolymer-based materials for next generation therapeutics and performance applications.

Advanced Materials: We will target new classes of molecular materials and nanomaterials with bespoke chemical, electrochemical, electronic, optical or thermal properties (*Amabilino*, *Cliffe*, *Pilgrim*). New polymeric materials from renewable feedstocks will contribute significantly to next generation 3D printing technologies (*Howdle* with Engineering). Also, building on recent success with colour and colour mixing in 3D printing we will open up new markets and applications. Our strong profile in next-generation batteries will lead to a step change in energy storage. *Johnson*, *Walsh* and *Newton* are part of the Faraday Institution’s LiSTAR Consortium for improving performance of Li-sulfur batteries.

Decarbonisation of Performance Materials: A second UKRI-EPSRC Prosperity Partnership, with Warwick University and strategic partners Lubrizol (£2.3M *Licence* 2021), will address the challenges of sustainable use of renewables as feedstocks in fine and performance chemicals with a focus on lubricants and performance-based additives. These find application in fields as diverse as polymers, personal care products and e-lubricants to support electrified transportation; the latter will be a significant growth area in the next decades and there is strong interest in renewable and potentially recyclable approaches.

Our future research strategy, shaped by the CSC vision, builds on our innovations in synthetic, analytical and computational chemistry to allow chemists to break chemical bonds in energy-efficient ways, to form molecules through atom-efficient processes, and to control and predict

reaction paths. All these will contribute richly to achieving the UN sustainable development goals.

1.4 Interdisciplinarity

We are at the heart of three of the University's Beacons of Excellence strengthening interdisciplinary activities with links across our University, academia more broadly and with industry. We have strongly supported the Biodiscovery Institute (BDI) (**S**4.1), the GeoEnergy Research Centre (GERC) (**S**4.1), and the Nanoscale & Microscale Research Centre (nmRC) (**S**3.2.4) providing state of the art laboratory space and equipment and this interdisciplinary environment led to 18/117 (15%) of our outputs being used in REF returns for 9 other UoAs at Nottingham. Furthermore, our REF outputs were enriched by collaborations with Chemical Engineering (21%), Biochemistry (17%), Physics (9%), Materials Science (8%) and Engineering (4%). Our major research initiatives (e.g. CDTs, DTPs, programme grants) are firmly based on interdisciplinary collaborations across Science, Engineering, Life and Social Sciences (**S**4.1).

1.5 Increasing Capacity to Deliver Impact:

1.5.1 Impact Strategy 2014–2020

Our philosophy is that Research and Impact are mutually beneficial, and we have actively encouraged staff to build a mixed portfolio of curiosity driven and challenge led projects (**S**2.5.2). Impact from research is now included in our staff performance metrics and reward structure providing a strong incentive to engage.

We have expanded our engagement with industry through proactive use of our Strategic Advisory Board and the launch of a Sustainable Chemistry and Processing Industry Forum (**S**4.3). Valuable input from SAB has informed on the sustainable needs of the chemistry using industries, the effect of Brexit and to direct technical challenges for our research base.

We have successfully implemented new initiatives through our Business Partnership Unit (BPU) (**S**2.5.2) that have enabled staff to identify and achieve impact from their research, increasing the number of industrial collaborations undertaken, one example is our Prosperity Partnership with GSK.

1.5.2 Implementation of Impact Strategy and 2021 Case Studies

The success of our approach is reflected in all four of our selected impact case studies, which have been nurtured utilising the mechanisms that we have initiated and grown since REF2014 (**S**3.1.1) and they leverage research from across each of our four Research Themes.

- ***Increasing Public Understanding of Sustainable Chemistry*** (**ICS-1**) reports a sustained programme of public engagement, supported by our dedicated Outreach Officer, to communicate our world-leading research in Green and Sustainable Chemistry to a global audience of millions including schoolchildren, teachers, special interest groups, policy makers and the general public.
- ***New Antibacterial Agents for Farming (Akeso Biomedical Inc.)*** (**ICS-2**). Our entrepreneurial impact culture and access to BDI infrastructure empowered *Soultanas* to develop the commercial potential of Biological Chemistry through partnership and a start-up company.
- ***Protecting Critical Technology at Rolls Royce*** (**ICS-3**) *Licence* and *Champness* leveraged research expertise in nmRC to solve a challenge posed by Rolls Royce to our BPU. Collaborative development through a Nottingham researcher recruited into the company and effective and timely knowledge transfer ensured success.
- ***DABAL-Me$_3$: Novel Reagent for Industrial Synthetic Chemistry*** (**ICS-4**) This opportunity was identified through our BPU impact audit, leveraged Proof of Concept funding (IAA) to scale up and exemplify the technology and yielded a patent (*Woodward*). A licence with a major chemical reagent manufacturer resulted in worldwide sales and industrial application of this new and safer reagent.

1.5.3 Future Strategic Plans for Impact

Our regular impact audits identified >60 impact opportunities currently developing across the Research Themes. A member of BPU dedicated to each Theme supports their development by identifying funding opportunities and industry links establishing a healthy pipeline of impact activity at various stages of maturity (**S**2.5.2) and delivering impacts at local, regional, national and international scale. Currently projects with potential for significant future impact include:

- Improving the recycling of food packaging plastics (with a UK Industry consortium) using scCO_2 (*Howdle*).
- Collaboration with a pharmaceutical company applying NMR & computational modelling expertise to improve understanding of how molecules interact with biological receptors (*Williams*).
- Partnership with an international manufacturer developing an improved synthesis of a key intermediate for commercial painkillers (*Lam*).
- Partnerships with several companies to exploit continuous processing based on UoN reactor designs and approaches (*George, Poliakoff, Licence*).

We will continue to build upon our pipeline of impact opportunities from our Research Themes. With input from our SAB and other industrial stakeholders, we will ensure our research outputs are aligned to key societal and industry challenges with a focus on decarbonisation of the chemicals industry. Specifically, we will:

- Identify and nurture impact opportunities from cutting edge research teams working in areas of particular societal benefit such as next generation materials for batteries, AI enabled drug discovery, bio-based feedstocks for plastics, nanoscale catalysts reducing

precious metal use and photo/electrochemical processes for efficient chemical manufacture.

- Expand our engagement with local and regional companies to support the high growth cluster of chemistry using businesses in delivering post-Covid recovery and economic growth aiming to secure significant place-based Government funding.
- Build on our expertise in public engagement and our CSC to increase our interaction with policymakers to influence Government/Industrial strategy and promote development of green technologies in the chemicals sector.

1.6 Open Research and Research Integrity

We are committed to the University's approach (**IES**-**S**2.3) to open access publication, open research data and open science. All PhD theses are similarly deposited, with an embargo period for industrially sensitive research. We support a mixed Green and Gold open access model with agreements with major publishers to fully/partially waive article processing charges, and we use the UKRI/Charity Open Access Fund for research supported by UKRI / Wellcome Trust and others.

The UoN Code of Research Conduct and Research Ethics (**IES**-**S**2.4) provides a framework for governance, requiring adherence to the highest standards of performance and ethical conduct. Our Research Ethics Officer (Farren) advises colleagues and ensures our School procedures interface with institutional frameworks and policies providing secure data share facilities and policy compliant repositories for both data and published outputs.

Our School provides bespoke training in ethics, including IPR, publications, confidentiality, research transparency, and legal restrictions regarding data access. Our approach ensures an awareness of the wider consequences of new materials and technology platforms by building upon early start activities in the SBRC and EPSRC CDT in Sustainable Chemistry. Our research programme aims to develop Responsible Research and Innovation (RRI) skilled researchers and draws upon strategic collaboration with the UoN Institute for Science and Society. Our School provided a keynote lecture for the 2019 annual University-wide **Responsible Research Conference**, bringing together researchers from the humanities, social sciences, and STEM disciplines to exchange ideas and to seek synergy and communal benefit. Our chemistry graduates and ECRs take a working awareness of the principles and practice of RRI into their chosen careers, particularly in chemistry-using industries where the risk:benefit ratio is critical for large-scale, high-impact business decisions (**IES-S**2.3/2.4).

2. People

2.1 Staffing Strategy and Staff Dynamics

We are pro-active in supporting success and career development at all levels. A key aspect of creating the right research environment has been creating Research Themes with a clearly defined research-led management structure allied with a teaching-focused grouping. The Theme leaders and their deputies are responsible for mentoring and line management. This structure ensures that no individual manages more than 6 staff and there is excellent mentoring.

Our approach has allowed effective succession planning to ensure future vitality. Since REF2014, Stace (FRS), Powis, Jones, Blake and Searle retired. Others moved to Chairs: Schroder and Liddle (Manchester); Paradisi (Bern); Moses (Cold Spring Harbor); Loenarz (Freiburg); O'Reilly (Assoc. Prof UCD Dublin).

2.2 Career Development and Resources

Appraisal and Development Conversations (ADC) provide career mentoring and annual review. Our process sets benchmarks against key indicators, medium- and long-term goals, identifies career development opportunities and manages workload. All our ECRFs undertake teaching qualifications receiving training/advice on supervision, research group management and academic roles such as personal tutoring. We make good use of the University's mentoring and staff development programmes to develop leadership skills (**IES-S**3.1). We regularly refresh membership of our Committees and provide opportunities for all staff to engage with School governance. New staff have a reduced teaching load, and their independent research activity is supported with equipment, consumables and PhD studentships. As evidence of the success of this approach, all the ECRFs reported in REF2014 have now taken up academic posts; *Teale* (Nottingham, RS URF and ERC Consolidator); Gimenez-Lopez (Santiago), Robinson (Nottingham Trent), Gibson (Newcastle), Yang (Manchester).

We have established a mechanism for sabbatical leave in the School, open to all research-active colleagues. *Hirst* (2018), *Champness* and *Khlobystov* (2019-21), *Teale* (2017-18, Norwegian Academy of Science and Letters), *N. Besley* (2015, UC Berkeley) have developed new research ideas and established collaborations through sabbaticals.

The Covid-19 pandemic affected the School in multiple ways, including closure of laboratories and technical facilities from March-July 2020. Chemistry was the first building to reopen on campus and we led the way in preparing a Covid-safe research environment. Where possible we have reduced teaching and administrative loads to protect research time and we have identified individual staff or research projects that have been affected particularly badly and prioritised resource accordingly.

2.3 Our Postgraduate Community

Our PhD students (currently 231) are the largest UoN cohort of PGR researchers. We adhere to the UoN PGR governance (**IES**-**S**3.3), and locally we have enhanced the PGR experience through our PhD Forum who contribute by representation on the EDI Committee, Athena Swan SAT, Learning Community Forum and through direct access to the Postgraduate Studies Officer (*Dowden*). Recent interventions include "*Re:Action*" a peer supported network focussed on mental health and wellbeing. The School's Support and Wellbeing officer is always available, with on-line "drop-in" chats during Covid-19.

Training and support. In addition to UoN Researcher Academy's training and support (**IES**-**S**3.3), we offer a programme of colloquia, lectures on research skills, ethics and safety and relevant hands-on training for analytical and materials characterization. All PGR give short

lunchtime presentations to develop critical thinking and communication skills complemented by bespoke CDT and DTP activities. Participation at international conferences is supported with dedicated funding. Additionally, we deliver key transferable business skills modules in entrepreneurship, business awareness, research management and IPR (**S**2.5.2).

Progress and monitoring. Our training provision and rigorous safety induction meets external guidelines and is quality assured by a robust system of internal peer review. Training and research activities are monitored through electronically reported monthly meetings and Annual Review with written reports and a viva. The PhD process culminates in a final-year School-wide Research Symposium with prizes for the best presentations and 2nd year posters. During Covid-19 the event ran very successfully "on-line", a refreshing break from pandemic issues. We award annually the "*Sir Fraser and Norma Stoddart Prize*" (£2.5K and a plaque) in an open competition for all graduated PhDs to recognize outstanding citizenship and academic excellence.

2.4 Our Postdoctoral Community

Our PDRA Forum contributes to key School Committees e.g. EDI and Athena Swan and our PDRAs convene and chair our PGR presentations. PDRAs benefit from a bespoke appraisal process, with both supervisor-led project feedback, independent mentoring and entitlement of 5 days p.a. of external career development opportunities as well as support of proposal writing and fellowship applications and opportunities to develop business and entrepreneurial skills (**S**2.5.2). The annual RSC-sponsored Dan Eley Postdoctoral Symposium (est. 2013) provides a platform to publicise and promote PDRA research, this year running "on-line". We pro-actively support the career development of our ~70 PDRAs and we strongly embrace the principles of the Researchers Concordat (**IES**-**S**3.1). For example, more than 35 of our PDRAs have applied successfully for personal Fellowship and lectureship positions since REF2014, including *Alves Fernandes* (NRF Nottingham), and others now in posts in Manchester, Leeds, Oxford, Reading, Central Lancashire, Bangor, Dublin, Liverpool, Cardiff, GlynDwr, Chengdu, Shanghai, Addis Ababa and others. We hosted the prestigious RSC Joliot-Curie Early Career Researchers Conference 2019, aimed at promoting career development.

2.5 Support for Research Staff

2.5.1 Technical Support and Workshops

Much of our research relies upon dedicated support from highly skilled technicians spread across laboratories (5 staff) and workshops (9), providing technical support in electrical and mechanical engineering, IT and glassblowing. We have invested over £100K in four state-of-the-art computerised machine tools to enhance manufacturing capabilities. Expertise in the design and construction of bespoke instrumentation has underpinned UKRI and industry-funded collaborative projects. As part of our succession planning, we have embraced government apprenticeship schemes; two apprentices have seamlessly replaced retirees and two further apprentices were recruited in 2019. The School's Analytical Services team (7) underpin chemistry research and with a dedicated NMR Manager and a computational research fellow supporting training in molecular electronic structure calculations. We are proud that chemistry colleagues have been proactive in leading the UK's *Technician Commitment* (**IES**-**S**3.4). The contribution of our technicians to supporting research was highlighted by the 2016 RSC President's Award to Mr. Neil Barnes whose outreach activities were further recognized by the Russian Academy of Sciences in 2020.

2.5.2 Supporting Researchers to Deliver Impact

Fully integrated within our research structure, our Business Partnership Unit (BPU, is a team of knowledge exchange professionals and Business Science Fellows (BSF) that provides a focal

point for growing the School's business and impact related activities (**S**3.3.1 / 4.3). The BPU provides specialist advice, brokers new relationships with industry, facilitates technology disclosures in partnership with UoN Technology Transfer Office and secures investment for our portfolio of industry facing translational research and commercialisation.

Since 2013, we have trained 12 BSFs drawn from our PGR and PDRA talent pool. Each BSF receives mentoring from KE professionals, academics, entrepreneurs and industrialists. Our 30+ BSF alumni include two company CEOs and four patent agents who all give time to assist training our current BSFs and identifying commercial opportunities.

Our "From the Bench to the Bank" programme of interactive lectures is delivered by business figures and entrepreneurial scientists and enhances commercial awareness and business skills so that research impact is identified and realised. During the REF period our academic staff and 250 PDRA/PGRs have participated.

Impact Secondments have enabled our researchers to work in industry, and industry scientists to join us to facilitate knowledge exchange and research impact. For example, PDRAs working in collaboration with the National Nuclear Laboratory, Asynt, Spiber Technologies and Sustein were funded through EPSRC and BBSRC IAA schemes. Through our Chemistry Innovation Laboratory (**S**4.3) >20 recent graduates and PGR students were placed with 11 companies undertaking innovation projects; 3 were subsequently employed by those companies.

Funded by the RSC's placements scheme, a Croda employee utilised our state-of-the-art imaging techniques to support the commercial development of novel microparticles. We also seconded in two senior GSK staff, forming a research grouping addressing sustainability challenges with our staff and final year UG medicinal chemistry students. This yielded novel compounds licenced to GSK. An engineer from Lacerta Ltd. was seconded with *Howdle* to develop high pressure metrology and two scientists from Key Organics Ltd joined O'Reilly to transfer enzyme methodologies to the company.

2.6 Equality and Diversity

We enthusiastically embrace the University's guidance on EDI and REF (**IES**-**S**3.5). We strive for an inclusive and diverse working environment and culture that provides opportunities for all to realise their full potential. Our Athena Swan Silver Award (2016) recognized our recruitment of female students above HESA averages; excellent maternity and paternity support, appointment and promotion of female academics; and good mechanisms of communication, raising awareness and visibility of activities relating to inclusion and diversity. Our SAT team and EDI committee implement our Action Plan with robust governance through training, regular surveys, data analysis, embedding of pro-active policies in School processes and celebrating diversity and achievement. All staff and PGR undertake "equality and diversity" and "unconscious bias" training modules supplemented by expert-led workshops, most recently on communication, conflict, and respect. Line managers ensure uptake of training. The gender balance across our staff and PDRAs qualitatively resembles the pipeline statistics in the RSC's "Breaking the Barriers" 2019 report. Compared to 2016, our gender balance has improved (female PDRA: 30% → 33%; Assistant Prof: constant 38%; Associate Prof: 22% → 29%; Prof: 9% → 13%). Our 2020 Action Plan positively addresses these challenges. Our proportion of female PGRs (43%) is above the HESA average.

In recruitment, target thresholds for shortlists and composition of interview panels have been successfully implemented. All staff involved in recruitment must undertake specific EDI training. For our recent academic appointments, we worked with external experts to create an innovative

"Diversity by Design" approach with a complete overhaul of the advertisements and a process that anonymised applicant data to minimise traditional biases.

The UoN approach to create role models saw *Reid* appointed Faculty of Science Associate PVC for Teaching; *Mokaya* as PVC for Global Engagement has a very prominent role and is still the only black professor of Chemistry in the UK. *E. Besley,* one of our Research Theme leaders was nominated by the ERC to "AcademiaNet, an expert database for Outstanding Female Scientists and Scholars: Profiles of Leading Women Scientists". Both *Kays* and Paradisi were promoted to Chair and *Vandeginste* to Associate Professor, benefitting from mentorship by one of our female SAB members. The HoS promotes inclusivity by regular School-wide meetings (including PGRs and PDRAs) for open discussion of topical issues; these provide excellent support and reinforce our chemistry community. We also celebrate our achievements across the School with all staff and students contributing to our bi-weekly electronic newsletter (distributed to 2500 individuals). Chemistry has invited high profile external speakers and organised a Faculty wide Seminar to promote science by LGBTQ+ scientists. Our annual "Women in Chemistry" conference is organised by a group of PGRs who received the 2020 Vice Chancellor's Medal and was highlighted this year in *Nature Chemistry.*

A recent staff awayday focussed on a "Culture and Values" assessment, building on the University's Code of Practice for behaviour and the outcome was an independent Staff Focus Group that reports directly to School Leadership Team on respect, culture, values, health and well-being. In 2019, we welcomed our first cohort of 2+2 Chemistry undergraduates from Ningbo China, representing a positive cultural diversification of the School; cohorts 2 and 3 are already in place. Space in the School has been dedicated as a private, non-denominational prayer room; and there is a shared tea-room for all staff and PGRs.

Flexible working is vital. We have excellent uptake on maternity /paternity leave with a supportive return to work programme. We also facilitate career breaks to allow long-term absences to cover medical interventions and family based / caring requirements for all staff. We pioneered a new Faculty of Science "Return to Work Scheme" offering PDRAs whose fixed-term contracts end while they are on maternity leave the opportunity to return on a six-month contract; to minimise any impact that a gap in publications or employment may have on their career.

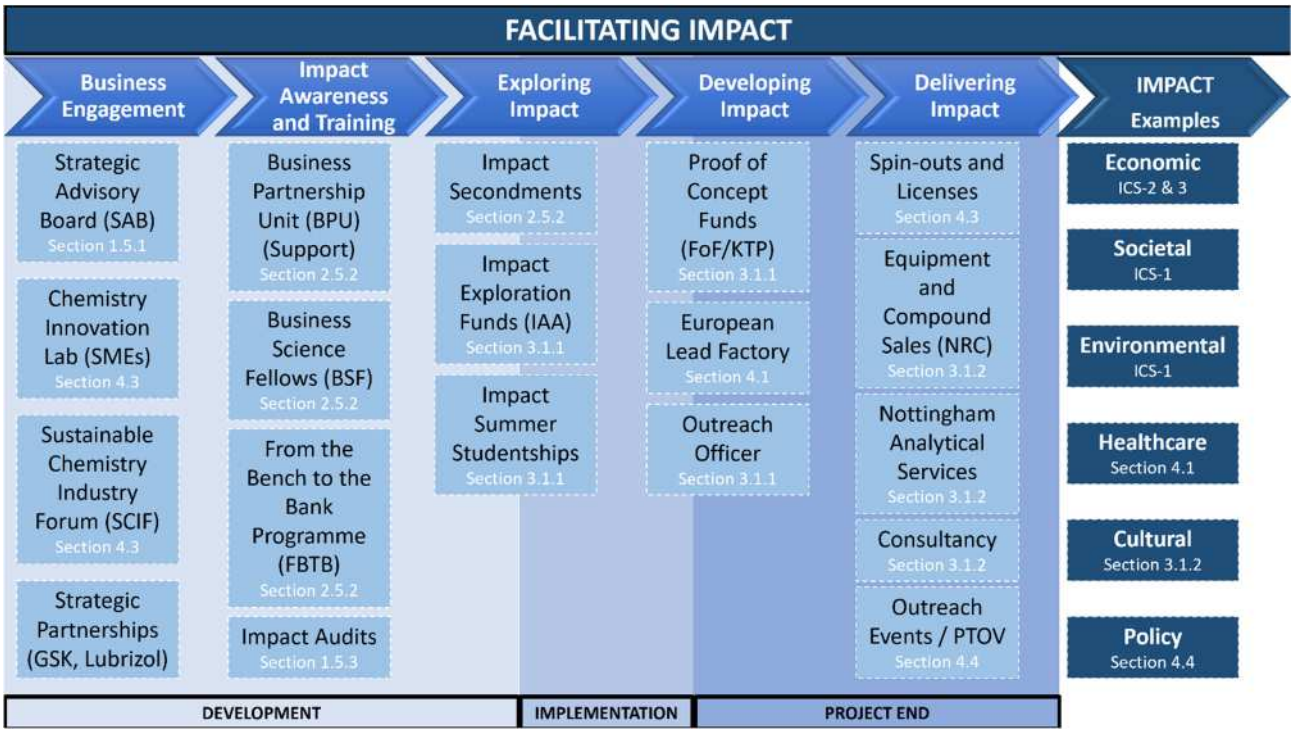
3. Income, infrastructure and facilities

3.1 Research funding portfolio

3.1.1 Research Lifecycle

Our portfolio of awards of £44.13 million (including £747K R&D expenditure credit) is a 36% increase upon REF2014 arising from Fellowships, single investigator and major UKRI awards (e.g. Programme, Platform, Prosperity Partnership and Strategic Equipment Grants). One REF2014 aim was to diversify our portfolio of funding; UKRI accounted for 72% of our research income (now 59%) with corresponding increase in EU awards (now 18%) industry (now 11%) charities (now 9%) and UK government bodies, local authorities, health authorities providing the remainder. We also received a legacy of £4M from alumnus Sir Gordon Hobday to support and stimulate research activities.

We drive the research lifecycle in a number of ways. At the *development phase*, we invest directly in fellowships, and we make appropriate investments in equipment to pump-prime new research directions and to leverage external funding. Staff can also bid for School-supported PhD studentships through a transparent and inclusive process. Additionally, Interdisciplinary Research Clusters (IRC) and Beacons of Excellence (**IES**-**S**2.1) provide further mechanisms for pump-priming new initiatives, e.g. three projects (*Newton*, *Alves Fernandes*, *Khlobystov*) were supported by the Advanced Molecular Materials IRC at £60K each. We support >30 undergraduate summer vacation projects to pump-prime research projects that could lead to impact and to provide valuable research experience; funding includes School resources, EPSRC IAA, UKRI, Charities, Alumni and industry.



During the *implementation phase*, opportunities are identified for enabling and accelerating impact, leveraging additional funding where required and disseminating research through policy and public engagement with our embedded Outreach Officer.

At *project end*, we enable impact, reporting and next steps. All phases are underpinned by stringent contractual, financial and procurement management to ensure value for money.

Our UKRI applications yielded £890K to support the delivery of Pathways to Impact during REF leveraging a further £1.8M from competitive internal and external schemes supporting 17 staff for 21 impact projects The outputs of these activities then led to an additional £2.6M to support commercial exploitation. Example projects include:

- Innovate UK funded Knowledge Transfer Partnership (KTP) with Cornelius Ltd scaling up and commercialising sustainable terpene-based monomers (*Howdle & Stockman* - £226K).
- BBSRC follow-on fund (FoF) underpinning synthetic spider silk technology (*Thomas,* Life Sciences) (£248K) leading to further funding; iCure grant and RSE Fellowship (*Thomas*).
- ERC proof-of-concept grants (€150k) developing carbon nanotubes for the detection/decontamination of hazardous compounds with DSTL (*Khlobystov*).

3.1.2 Income from Impact Related Activities

We have consulted for >20 companies providing expert opinion for example to help resolve patent litigation cases. Our ***Nottingham Analytical Services*** has delivered benefit and impact to ~100 businesses through access to our expertise and equipment and generated £840K income by solving process, product and regulatory challenges and supporting new product development. For example, work with Lanxess led to a new disinfectant product and with the Alfred Gillett Trust enabled the preservation of a heritage collection of shoes. Our partnership with BioCity Ltd. offers space and incubator support for start-ups and provides analytical services to tenants (e.g. Sygnature and Locate Bio).

Knowledge transfer from research projects generated income from sales of compounds and equipment. ***Nottingham Research Chemicals*** is our partnership with Key Organics Ltd taking new molecules from our research and making them available for sale worldwide with a product pipeline of 157 compounds from 11 research groups.

We have taken advantage of a range of collaborative research funding mechanisms leveraging industrial income from 39 Research Council Case and iCase awards in addition to fully funded research projects with a range of companies. For example, a GSK funded research fellow (£240K) helped secure the GSK Prosperity Partnership.

3.2 Infrastructure and Facilities

3.2.1 Laboratory Infrastructure

Since 2014, modernisation of research labs, instrument suites and office areas has been funded by UoN and competitively won infrastructure funds. Plans for a further £6M refurbishment of Synthetic Chemistry labs are well advanced.

3.2.2 Investments in Instrumentation

As well as the £4M investment in equipment at the CNL (**S**1.3.1), our strengths in multi-disciplinary NMR continued to grow with successful EPSRC Strategic Equipment Funding (£2.67M, 2014) to establish the UKs only High-field Dynamic Nuclear Polarization Magic Angle Spinning NMR Facility (*Titman* with Physics and Life Sciences) and £161K and £481K *Titman*) to maximise the sharing of the facility with the UK community. In addition, *Titman* is Deputy Director of the UK 850 MHz Solid-state NMR Facility with UKSBS funding (£2.67M 2015). Interdisciplinary CIF-funded research in high-field NMR spectroscopy has been upgraded through 'Very and Ultra-High Field NMR for the Physical and Life Sciences' (£966K *Williams*) with re-consoling and new probes making this one the few facilities for solids at 800 MHz and supporting the UK NMR Road Map for international competitiveness (*Williams*) through shared expertise and access to a national portfolio of collaborators.

Through the Beacons we have upgraded 'EPR facilities for the characterisation of Energy Materials' (£120K, *McMaster*), and launched a 'Battery Lab' initiative (£300K, *Johnson*) leveraging funding from the Faraday Institute (£0.9M, *Johnson*, *Walsh*, *Newton*, *Champness*) to allow for the development of lithium-sulfur batteries, nickel-rich cathodes/redox catalysts and new electrolytes. High Performance computing facilities (UoN £1.4M 2017) were further enhanced by the HPC Midlands Plus supercomputing hub (£3.2M 2016, £3M 2019 *Hirst*) to facilitate new interdisciplinary science and engagement with industry. Cutting-edge on-premise computational resources and a dedicated School computer cluster (ERC €2M 2018 *Teale*) allows effective method development and testing. A successful BBSRC 17ALERT bid (£423K 2018 *Soultanas*) for mid-range equipment delivered a multi-wavelength analytical ultracentrifuge to support investigation of biomolecular interactions.

3.2.3 Development of Instrumentation

Oldham is developing interfaces for liquid chromatography-native electrospray ionisation mass spectrometry allowing identification of active compounds from complex natural mixtures, e.g. microorganisms to overcome bottlenecks in drug discovery. A partnership with Waters Corp, interfaces in-line coupling of LC with native ESI-mass spectrometry to detect the binding of chromatographically separated natural products to selected protein targets; focussed on discovery of new immunosuppressants and antimicrobials.

Working with laboratory equipment manufacturer Asynt Ltd. we developed the "*PhotoVap*" high-throughput photoreactor (*George*/*Poliakoff*) and "*PressureSyn*" high-pressure reactor (*Howdle*) for national and international customers, which won the "Lions' Lair" competition for the best lab innovation. With our specialist workshop staff new vessels for scattering measurements under pressure were developed with ESRF facilitating in situ SAXS monitoring of structure evolution in nanostructured polymeric microparticles (*Howdle*). This has stimulated development an equivalent neutron scattering vessel with Oak Ridge National Lab (USA).

3.2.4 Development and Utilisation of Cross-Faculty Research Facilities

Partnership between Chemistry, Pharmacy, Physics and Engineering established the Nanoscale & Microscale Research Centre (nmRC 2016 director *Khlobystov*) in a newly refurbished building, providing 1,000 m^2 of high-quality research space and infrastructure for materials characterisation and consolidating 20 major instruments (£2.5M UoN investment and >£15M external, including £6.7M of EPSRC capital funding secured since 2014 (**IES-S**4.1). This new facility has leveraged multiple strategic initiatives to support local, regional and UK wide access. Additional grants stimulated new capabilities (**S**4.1), including a globally unique high resolution cryogenic analytical and transfer scanning electron microscopy (HR-CAT-SEM) (£1.56M *Khlobystov* 2019), a facility for 2D-semiconductor fabrication (£2.94M Co-I *Khlobystov* 2020), a 3D OrbiSIMS for label-free chemical imaging of materials, cells and tissues (£2.02M Co-I *Khlobystov* 2018), and a grant to pump-prime research stemming from this instrumentation (£250K *Khlobystov* 2018). In 2018-19, nmRC serviced over 500 researchers (including over 100 chemists), additionally the equipment and expertise actively shared with 17 universities in seven countries through 41 interdisciplinary research projects ("NanoPrime" *Khlobystov*). The Centre serves as a hub for the EPSRC DTP in Low-Dimensional Materials & Interfaces (LDMI) with 20 PhD projects over three cohorts (led by *Champness*), providing unique cross-disciplinary training environment where materials synthesis and characterisation are combined within each PhD project.

3.2.5 Utilisation of National and International Research Facilities

Our staff are major users of UK and international facilities, consistently securing competitive access and advising on development of synchrotron, laser and spectroscopic facilities. For example, a national resource 'Portable Femtosecond pump-probe' for dynamic structural science

(*George);* HPC access Archer 1.2 MAU (*Wheatley*), 9.0 MAU (*Hirst*) and significant access to national and international facilities including: 'Nottingham-Manchester Structural Chemistry BAG'; 'Catalysis Hub BAG' and single crystal diffraction at Diamond Light Source; Ultra Facility at Harwell; APS Synchrotron time-resolved XAFS; X-ray Scattering ESRF/DUBBLE; Neutron Scattering ORNL; light-source awards at Elettra (Sincrotone Trieste); DESY Petra III (Hamburg), Free Electron Lasers, Synchrotron Trieste FERMI and others that are summarised in the table below:

Facility	Value of Access £	Number of hours/shifts
ESRF (European Synchrotron)	1061500	193 shifts
MAX laboratory	230777	264 hours
EU laser lab	135000	21 shifts
Synchrotron Soleil (France)	1629787	4 weeks
ILL International Research Centre	373062	260 hours
High-field Solid State NMR*	28291	264 hours
CLF @ RAL*	741416	200 shifts
ISIS Neutron & Muon Source*	130530	1680 hours
EPSRC SuperSTEM*	35000	144 hours
Diamond Light Source*	1335000	120 hours
HPC Midland Plus*	80000	11000000 core hours
	£5,780,000	
Staff: *Alves Fernandes, Amabilino, Besley E,* Blake*,* Chamberlain*, Champness, Cliffe, Hirst, Howdle, Kays, Khlobystov, George, Powis, Reid, Titman* and *Wheatley*.		

*part of UKRI facilities

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

Our REF outputs include 57% with international and 20% with industrial/corporate co-authors illustrating a broad portfolio of collaborations across our Research Themes.

4.1 Cross-Disciplinary, Inter-Institutional and International Collaborations

In addition to nmRC (**S**3.2.4) the School contributes to collaborations with other disciplines via the *Biodiscovery Institute* (BDI, *Thomas* Deputy Director) which houses 700 researchers. *Soultanas*, *Thomas*, *Harvey*, *Quaglia* and *Oldham* all have researchers based in the BDI and contribute significantly to various research strands including Centre for Cancer Sciences and National Biofilms Innovation Centre and through supervision of PhD students in the Wellcome Trust AAMR DTP and EPSRC CDT in Advanced Therapeutics and Nanomedicine. Chemistry contributes strongly to the End to End Therapeutics IRC (*Thomas*) that brings a multidisciplinary strategy to better coordinate, focus and synergise drug discovery.

The *GeoEnergy Research Centre* (GERC) builds on collaboration with Engineering at Nottingham and Imperial, Manchester, Bristol and the British Geological Survey (BGS), strongly contributing to this *Vandeginste* initiated the *NERC-ESRC* Unconventional Hydrocarbons Programme Challenge 2 (£1.7M) and contributed to the EU consortium 'SECURE: subsurface evaluation of CCS and Unconventional Risks' (€787k to Nottingham) with participation from a raft of European Universities and the BGS.

Many other examples of successful collaborations have been stimulated through the Research Themes:

***Materials*:** collaborations with Physics on 2D supramolecular networks (£783K *Champness/George*) led to major strategic equipment awards (**S**3.2.4); *Newton* (Leverhulme Trust) and *Howdle* independently developed collaborations with Engineers on new materials for 3D printing (several publications and patents); *Vandeginste* linked to the Shell, Qatar Petroleum and the Qatar Science and Technology Park at Imperial College as Co-I in the £4.7M 'Qatar Carbonates and Carbon Storage Research Centre Project'; *Mokaya* led major initiatives in capacity building projects across Africa to improve research, teaching and technical capacity and to provide opportunities for researcher mobility and training; £1.2M Royal Society/DFID-funded research programme focussed on delivering research capacity in South Africa, Kenya and Cameroon targeted at replacements for fossil fuel e.g. porous solid stores of renewable energy and catalysts for sustainable production of renewable bio-fuels.

***Molecular Bonding and Spectroscopy*:** *Licence* established sustainable routes to platform chemicals funded by a major BBSRC grant (with Life Sciences) by integrating biology and chemistry (with SBRC), and *Alves Fernandes* on Green Ammonia synthesis and utilisation (with Engineering); *Khlobystov* developed new 2D materials based upon graphene and boron nitride (with Physics); *E. Besley* and *Khlobystov* led on electron microscopy research (with Ulm University) delivering 22 joint papers and leveraging over £4.2M of EPSRC, ERC and NERC funding for Nottingham in this area; *Khlobystov* expertise in nanoscale imaging underpinned the 2D-INK EU Horizon 2020 project aimed at printable electronics, and collaboration with marine biologists at Plymouth University on detection of nanomaterials in natural environment.

Synthesis and Catalysis: *Hayes* combined synthetic biology and synthetic chemistry to access high value anti-cancer natural products (with Life Sciences) forming spin-out company (RiboCell); *Dowden* on low-waste reactions; and *Stockman* on enzymatic approaches to antimicrobial which led to new antifungal approaches with Pharmacy; *Woodward* led a project

with Computer Science on Machine Learning for catalysis within the GSK Prosperity Partnership; *Moody* and *Stockman* expertise contributed strongly to the European Lead Factory project (*€196M; 1.2M to UoN*) - the biggest EU public-private venture aimed at accelerating the development of new medicines and involving a network of 50 partners, including 10 Universities, 7 major pharmaceutical companies (e.g. Johnson & Johnson, Sanofi and Bayer) and various SMEs; the initiative created new partnerships (e.g. with local SME Sygnature Discovery Ltd.) and yielded >100 publications and >200K novel compounds that were screened against 72 drug targets with >2400 'hit' compounds identified.

Biological Chemistry: Using high-field NMR capabilities and expertise Searle (with Biosciences £662K) produced new insights into 'Reducing Sodium in the UK Diet'; *Thomas* worked with the SBRC on optimising industrial gas fermentation for commercial low-carbon fuel and chemical production (BBSRC LOLA with LanzaTech NZ £2.396M); Paradisi participated in EU consortia EraCoBiotech (€1.13M) on heterogeneous biocatalysis for w-amino acids synthesis from renewable feedstocks and EraNet SUSFOOD2 (€1.29M) aimed at valorisation processes; *Oldham* collaborated on odorant binding proteins with UFAL, Brazil (£160K, Newton Fund - British Council/CAPES) and on in-line liquid chromatography-native mass spectrometry (FAPESP grant); *Hirst* worked on time-resolved circular dichroism for protein folding (£30K SOILEIL, France); *Thomas* exploited clickable recombinant spider silk through collaboration with Spiber Technologies AB, Sweden (BBSRC follow-on-funding).

4.2 Contribution to the Research Base

Our research contributions and their impact on the academic community, both in the UK and worldwide, has been recognised by a wide range of individual honours and leadership roles:

Outstanding Achievements, Awards and Prizes: Colleagues have been recognised and have played significant roles both nationally and internationally in setting the wider research agenda. For example: European Research Council (ERC) panel of 'Outstanding Female Scientists and Scholars' (*E. Besley*, 2014-present); Thomson Reuters Highly Cited Researcher (*Champness*, 2014, 2015, 2016); Fellow RAEng (*Poliakoff*, 2017); Fellow of the AAAS (*Poliakoff*, 2016); International Science and Technology Cooperation Award of the People's Republic of China (The Nation's highest honour for foreign scientists presented by President Xi in person to *Poliakoff* 2019); Special diploma of the Russian Academy of Sciences for "The Magic Table of Elements (Periodic Videos)" nominated by Academician Yu.Ts. Oganessian (*Poliakoff*, Barnes, 2020); Member of the Academia Europaea (*Champness* 2020).

Overall, our staff have received >50 major internationally recognised honours, awards, and fellowships, including a Queen's Honour, KBE for Services to the Chemical Sciences (*Poliakoff*, 2015); Foreign Secretary and Vice-President of the Royal Society (*Poliakoff*, 2011-16). We have received significant national and international recognition: RSC Surfaces and Interfaces Award (*Champness*); United Nations Industrial Development Organisation (UNIDO) Bronze Award in Chemical Leasing (*George*, *Licence* & *Poliakoff*); Meggers Award, Society of Applied Spectroscopy, USA (*George*); ACS Grady Stack Award (*Poliakoff*) RSC Chemistry of the Transition Metals Award (*Kays*); RSC Corday-Morgan Medal (*Khlobystov,* Liddle); RSC Harrison-Meldola Prize (O'Reilly); RSC Lord Lewis Prize (*Poliakoff*); Royal Society Wolfson Merit Awards (*Champness*, *Mokaya*, *Khlobystov*, *E. Besley*); RSC Longstaff Prize (*Poliakoff*); IRDG Norman Sheppard Award (*George);* RS Michael Faraday Medal (*Poliakoff*); Honorary Professorship at Beijing University of Chemical Technology (*Poliakoff*); Thieme Chemistry Journals Award (*Ball*).

Prestigious funded Fellowships have been held by Nottingham colleagues: ERC Starter Grant (*Lam*) and four Consolidator Grants *(Khlobystov*, *Liddle*, *E. Besley*, *Teale*); EPSRC

Midcareer (Liddle) and two Established Career Fellowships (*Khlobystov*, *Champness*); Leverhulme Trust Research Fellowship (*N. Besley*); Royal Society University Research Fellowship (*Teale*, *Cuthbertson*); EPSRC-UKRI Innovation Fellowship (*Johnson*); EPSRC Fellowship (*Lam*); Royal Academy of Engineering (*Hirst*).

Invited Professorships and Fellowships: We have been recognised internationally with the award of distinguished fellowships and Honorary Chair appointments: Jilin University, China (*Hirst*); Polish Academy of Sciences, Krakow (*Mokaya*); University of Tsukuba, Japan (*Newton*); Zasshikai Lectureship, University of Tokyo (*Newton*); UC Davis USA (Paradisi); Ethiopian Academy of Sciences (*Poliakoff*); Moscow State University (*Poliakoff*); University of Oslo (*Teale*); Centre for Advanced Study, Norwegian Academy of Science and Letters, Norway (*Teale*); GDL Foundation, USA (*Vandeginste*); University of Toronto (*Ball*).

***Memberships of National and International Advisory Boards / Funding Panels*:** We have contributed to scientific governance, management, development and resource allocation of national and international facilities as members of >60 Science Advisory Councils, Funding, Fellowships and Awards panels across the UK, Ireland, Portugal, USA, Korea, Canada, Israel, Estonia, Qatar. We actively exploit new research opportunities and drive national research priorities by engagement with industry and UKRPIF, EPSRC Portfolio Shaping, and advisory boards: including EPSRC National Facilities Statement of Need Panels (*Howdle*), UK National Crystallographic Service Management & Advisory panel (*Champness*), STFC Facility Access Panel (*Cliffe*), Royal Society/British Academy Newton Fellowships Committee (*Poliakoff*), and BBSRC Committee C (*Thomas*). In addition, 12 colleagues have served on international advisory boards; Irish Research Council (*E Besley*), Royal Society DFID Africa Building Panel (*Mokaya*), Organisation for Prohibition of Chemical Weapons (Green Chemistry Working Group) (*Poliakoff*), European Academies Science Advisory Council (*Poliakoff*), IUPAC Group on Green Chemistry Metrics (*Licence*), RS Newton International Fellowships Committee (*Champness*) and many other organisations contributing to scientific governance of management, development and resource allocation of international funding agencies.

Other highlights include, ERC peer review panels, Royal Society University and International Fellowships Committees, Chairs of UK EPSRC panels; RSC Award Panels, Science Advisory Group on Grenfell & North Kensington, STFC Global Challenges Research Fund Panel, and Future Leaders (FLAIR) Fellowship panel, Commonwealth Scholarship Commission, ACS Catalysis Young Advisory Board, Vice-President European Academies Science Advisory Council, Institute of Basic Science, Korea, Royal Commission Exhibition of 1851 Committee, Royal Society University Research Fellowship panels, RSC Observer for 2014 International Review of Chemical Engineering, RSC Advisory Group for the International Year of the Periodic Table, Royal Society Premier Awards panel, Founding Members RSC Pan African Chemistry Network.

Journal editorships: Our staff have taken on editorship roles with 6 major international journals, and a further 10 staff are members on the editorial boards of 25 high profile journals. Highlights include: Associate Editor of Chemical Society Reviews (*Amabilino*, 2013-present); Editor-in-Chief RSC Theoretical & Computational Chemistry (*Hirst*, 2008-present); Editor, Journal of Theoretical and Computational Chemistry, and RSC Computational Nanosciences (*E. Besley*, 2016-2019); Executive Editor, Biocatalysis and Biotransformations (O'Reilly, 2017); Executive Editor (Ethics), ACS Sustainable Chemistry and Engineering (*Licence,* 2014-present); Section Editor, Genes: Molecular Genetics (*Soultanas*, 2017-present).

4.3 Contribution to the Economy

We have developed productive relationships with over 150 companies ranging from strategic partnerships with multinationals to local SMEs.

Our Chemistry Innovation Laboratory (ERDF £1.1M) has secured new partnerships with regional chemistry-using SMEs helping them innovate and grow through access to our facilities, expertise and placements. 45 SMEs engaged with the research activities of 25% of our academic staff, improving business performance (ca. £200K GVA per company) and creating 14 skilled jobs. An independent evaluation concluded that CIL "*has delivered a considerable level of economic impact measured by turnover/sales generation and associated GVA*" and "*The impact data indicate … a tangible effect on the economy. The extent of this impact was higher than we anticipated*". For example, a project with Upperton Ltd analysing spray dried polymers resulted in significant growth, new clients and increased staff from 4 to 22 and a move to new facilities. CIL also initiated "*MidsChem",* a regional network of chemistry using businesses delivering themed network events on regulation, IP management and building industry-University collaborations that were highlighted in CIKTN and East Midlands business support guides.

We launched the *Sustainable Chemistry Processing Industry Forum* where 45 senior industrialists, academics and government representatives meet biannually to share best practice, inform policy and identify challenges that have shaped the CSCs research programme. For example, participation in the forum has informed Croda's laboratory refurbishment plans. We have also engaged with the Chemistry Council, presenting our plans at stakeholder meetings and hosting meetings in the CNL.

***Technology Commercialisation*:** The School made 68 innovation disclosures yielding 14 patent filings. In addition to those described in impact case studies (**ICS**2-4) other outputs included:

- two company exits (Critical Pharmaceuticals and CellAura Technologies);
- growth of existing spin out company (Promethean Particles);
- formation of spin-out Ribocell in collaboration with Biosciences (*Hayes*);
- new company under development commercialising integrin technology (*Moody*);
- licensed lead compounds to GSK as potential treatment for respiratory diseases;
- assigned patent on novel molecules for fuel additives to Lubrizol (*Kays*);
- novel translation inhibitors licenced to Naturalea SA (*Hayes*).

4.4 Contribution to Society

All our staff and students participate in outreach targeting audiences from primary school to octogenarians in the University of the Third Age. Some events are held in the University, e.g. science fair for Year 5/6, "A Level spectroscopy" workshops, the FIRST LEGO League regional tournament and community open days. Other events are held in the city and regionally; Science in the Park, Pint of Science; Festival of Science, Curiosity etc. Our events also take place nationally with lectures for pupils from Edinburgh to London and worldwide in USA, Malaysia, China, Australia, and to schoolteachers in Russia, Ireland and Portugal. Our expertise in public engagement and schools outreach is sought by overseas groups: we led the 1st World conference on Science Literacy in Beijing (2018); the Indonesian government sent a delegation to learn from Nottingham, and we shared best practice with Ethiopian scientists to establish their first science centre (2015). The original idea of the International Year of the Periodic Table (2019, UNESCO) celebrating the 150th anniversary since Mendeleev's discovery the Periodic System, emerged from our School.

We have engaged with government Ministers at official events such as the Nottingham in Parliament Day 2016 and the All-Party Parliamentary Group of Malaria and Tropical Diseases in 2019, encouraging policy makers to adopt new ways of thinking about chemistry. We have twice exhibited our research at Royal Society Summer Exhibitions (2015 and 2019 with typically >10k visitors over a week), and our CDT students exhibited at the Cheltenham Festival. We have a strong presence on social media with multiple Twitter accounts (the School, the CDT, individual research projects and we take part in local and national TV and radio broadcasts in the UK and beyond (e.g. Russia, Estonia). Our chemistry channel on YouTube, Periodic Table of Videos (PTOV) has > 1.45M subscribers and >247M views and was described by the ACS as "*one of the most popular chemistry-related channels on YouTube*". We collect structured audience feedback at our outreach events, and this is almost uniformly positive. We have been particularly successful in communicating our research on Green Chemistry to a wide-ranging audience (**ICS-**1). Our science communication has been recognized by UK, Irish, Chinese, US and Russian awards and prizes. The total audience for our live events over the REF2021 period is *ca.* 40,000 and for our on-line engagement *ca.* 130 million.