ROYAL SOCIETY OF CHEMISTRY

DISCOVERY

Science Horizons

Leading-edge science for sustainable prosperity over the next 10-15 years

Contents

1.

Foreword & executive summary

The chemical sciences are entering an unprecedented era of discovery and achievement. Taking advantage of the new science and technologies of recent years, we have encountered amazing opportunities to further our understanding of the world, and to design and create solutions to a wide range of challenges.

To better define and evidence this we commissioned Science Horizons, which articulates the priorities, opportunities and challenges for chemical sciences research in the next 5-10 years. Through interviews, workshops and a survey, we gained the views of more than 750 people actively doing research in universities and research institutes around the world. These findings are framed by themes identified through desk research, data science analysis of publishing trends and scoping interviews that identified the wider policy and industry context.

For some questions, the hundreds of leading scientists produced an astounding range of answers: the fields of study that chemical science will enhance; the applications of chemical science that will benefit society; and the unexplored frontiers of science that we will chart with exciting new techniques in the near future.

On other questions, those hundreds of scientists spoke with one voice. Chemistry is essential to global prosperity. Applied research must be balanced with curiosity-based research, with the right environment and mechanisms to support both. Collaboration across disciplines and countries is vital to advancing the chemical sciences – it is notable that 90% and 85% of researchers surveyed had collaborated in the last five years with people outside their field and country respectively. Our community enjoys both a remarkable diversity of aspirations and a unified vision of the role of the chemical sciences in global prosperity.

This combination of creativity and drive is a hallmark of the chemical scientist, and is something we should encourage whole-heartedly among our peers and with the wider world. We are creators and innovators, with unquenchable curiosity in the world around us, and a keen sense of responsibility to consider the impact of our discoveries.

We have the ideas and capabilities to lead scientific advancement. As chemical scientists we must also have the confidence to step up, bring people together, and draw on the full extent of our diverse research community to discover new scientific knowledge and deliver amazing outcomes for society.

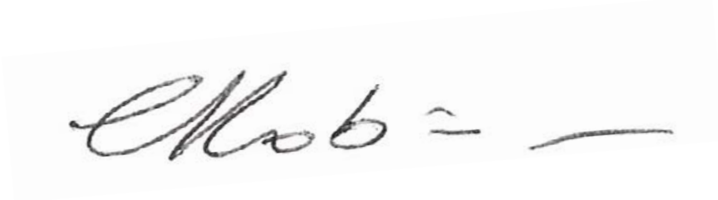
In our research for Science Horizons we found that finding paths to sustainable prosperity is the priority for governments funding R&D globally. The context of financial, societal and environmental upheaval in the last decade has focused global efforts to deliver tangible results that directly improve our lives.

The chemical sciences' role at the heart of this is clear, and the three areas we identified – delivering solutions, answering leading-edge questions and developing frontier techniques – complement and closely depend on each other. Our interviews brought to light an incredible range of advances across all these areas, which are summarised and explored in this report.

To take full advantage of the opportunities the chemical sciences offer, we need the right environment for them to thrive. We found that enabling curiosity, encouraging collaboration and developing leadership are all crucial to deliver advances in science, and Science Horizons expands on how global scientists feel these areas need support and development.

This report shows that hundreds of scientists worldwide are enormously positive and excited about what science will achieve in the near future – a view that every scientist I know would echo – and that the chemical sciences will play a vital and central role in leading these developments.

It is just the start, however. The thoughts and feelings shared in this report – the confidence and positivity – need to be repeated and multiplied, across the globe. Chemical scientists must be bold in communicating their ideas, bringing together diverse teams, and taking advantage of this amazing era for science.



Professor Dame Carol Robinson DBE HonFRSC FRS
President, Royal Society of Chemistry

In the context of a rapidly evolving global research environment, we commissioned our Science Horizons project to articulate the priorities, opportunities and challenges for chemical sciences research in the next 5-10 years.

The results in this report focus on what we heard through interviews, workshops and a survey in which we sought views from over 750 people actively doing research in universities and research institutes around the world. These findings are framed within themes identified through desk research, data science analysis of publishing trends and scoping interviews which set out the wider policy and industry context. Our methodology is in Appendix A.

Finding paths to sustainable prosperity is the priority for governments funding research and development (R&D) globally

Alongside the financial crisis, the past decade has been characterised by major geopolitical and societal changes that have set new expectations for scientific R&D. Demographic changes, escalating environmental challenges and growing fears about energy security have highlighted the urgent need for new paths to attaining sustainable prosperity, and R&D has been identified globally as a key enabler to achieve this goal.

The search for sustainable growth through responding to global challenges and driving industrial innovation has become the overarching theme shaping the outlook for R&D globally.

Advances in three interdependent dimensions of scientific research will be important to meeting this global R&D agenda:

i. **Solutions to global & industrial challenges**
Researchers expect significant advances in the chemical sciences to underpin new technological solutions to major societal challenges from environment and energy to human health and agriculture. Researchers are also deeply embedded in enhancing the efficiency, safety and profitability of industry, in sectors from electronics to pharmaceuticals to energy.

ii. **Leading-edge questions**
Researchers are tackling an incredibly broad range of questions relating to the structure, properties and interactions of matter across multiple length scales and levels of complexity – from atoms, molecules and materials to organisms and ecosystems. Starting with atomic and molecular insights, chemical scientists are designing, making and modifying new molecules and materials with applications from new medicines to batteries and solar cells.

iii. **Frontier techniques**
Advances across a staggering range of techniques are enabling researchers to reveal the structure and properties of matter at unprecedented resolution in space and time. Scientists and engineers are pushing the frontiers of: measurement & imaging; sensors & screening and modelling & simulations. Data and digital technologies are central to these areas as researchers gather and analyse data from increasingly complex studies, going on to use data and digital technologies in new ways to make predictions and discoveries, and to deliver new insights and products.

Curiosity, collaboration and leadership will be crucial to enable these advances

There are three key enablers where action is required to ensure that science contributes to its fullest potential to achieving the global sustainability and prosperity agenda:

i. **Curiosity**
Researchers consistently highlighted curiosity-driven research as a critical enabler for advancement of scientific knowledge and its application, particularly long-term and transformational advances. Lack of long term funding for this type of research (also called discovery, fundamental or basic research) was a universal concern. This emphasis on the crucial role of curiosity-driven research was coupled with a strong sense of duty that scientists consider the applications of their research.

ii. **Collaboration & interdisciplinarity**
Over 90% of the researchers surveyed had collaborated with people outside of their field and 85% have been involved in an international collaboration within the past five years. Collaboration between sub-fields of the chemical sciences, across science and engineering, between people in different countries and with industry were all highlighted as important. In an increasingly interdisciplinary landscape one size does not fit all as researchers instead develop strategies that best fit the question or challenge they are tackling. Scenarios range from individuals who consider themselves to be interdisciplinary researchers to large teams which bring together groups of people with diverse core disciplinary expertise and/or interdisciplinary individuals.

iii. **Leadership**
There is an opportunity for researchers to take a bolder leadership role in shaping the global research agenda and in translating scientific discovery into societal impact. It is also important that at least some academic researchers have opportunities and support to develop as effective leaders of research teams, large collaborations or programmes (see Figure 1).

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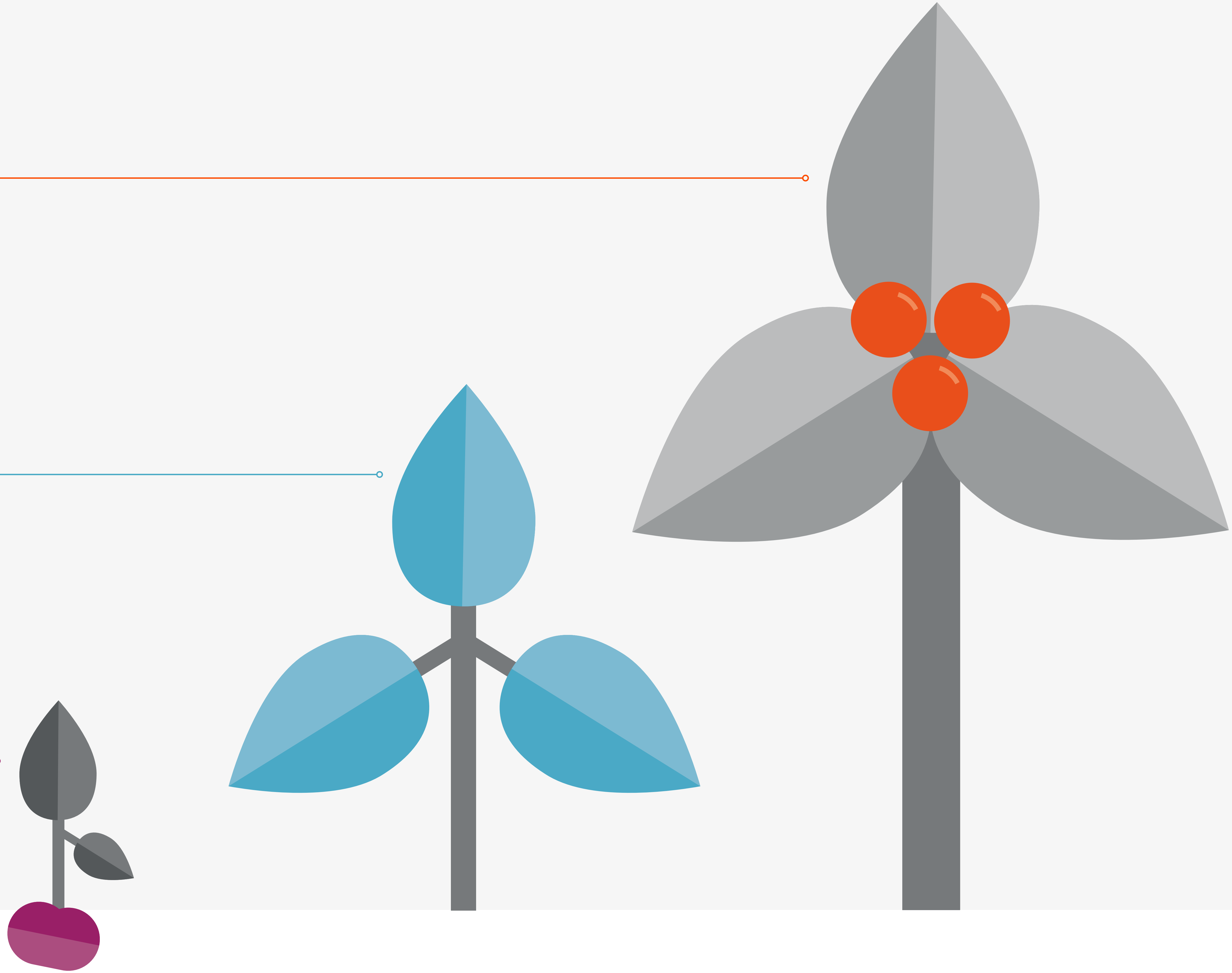
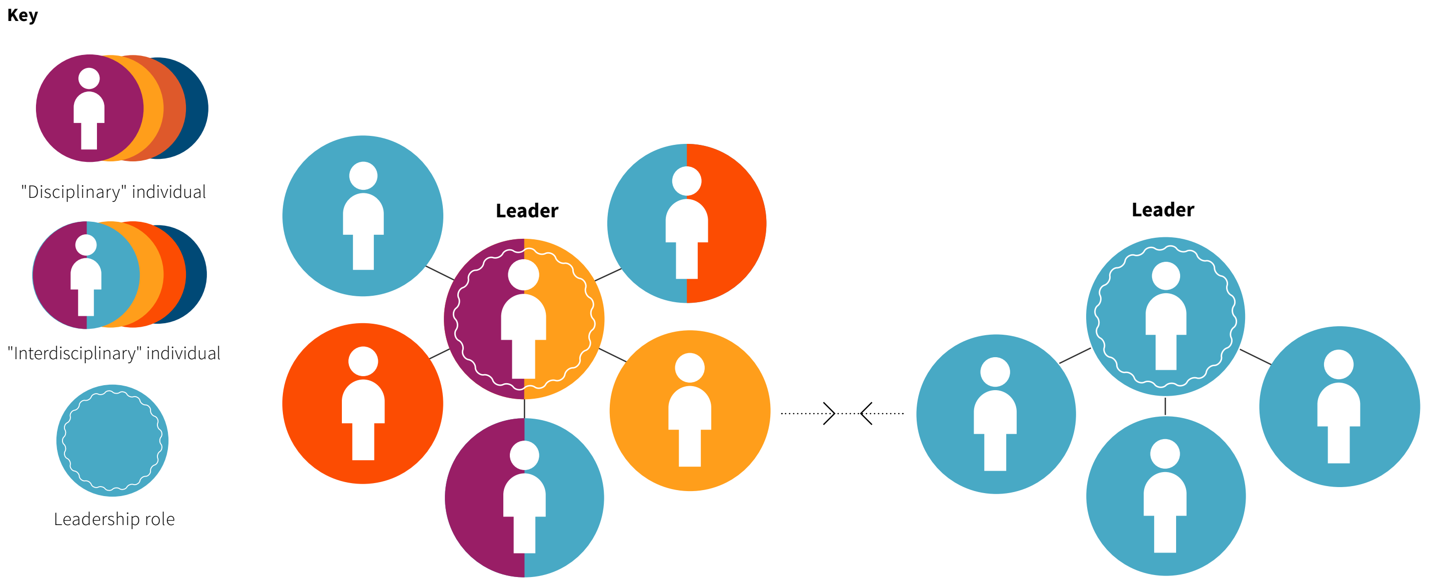
Curiosity, collaboration & leadership





Example of collaboration between two teams. Many combinations of "disciplinary" & "interdisciplinary" possible

Figure 1: Interdisciplinarity, collaborations and leadership

2.

Sustainability & prosperity

Total R&D investment remains strong

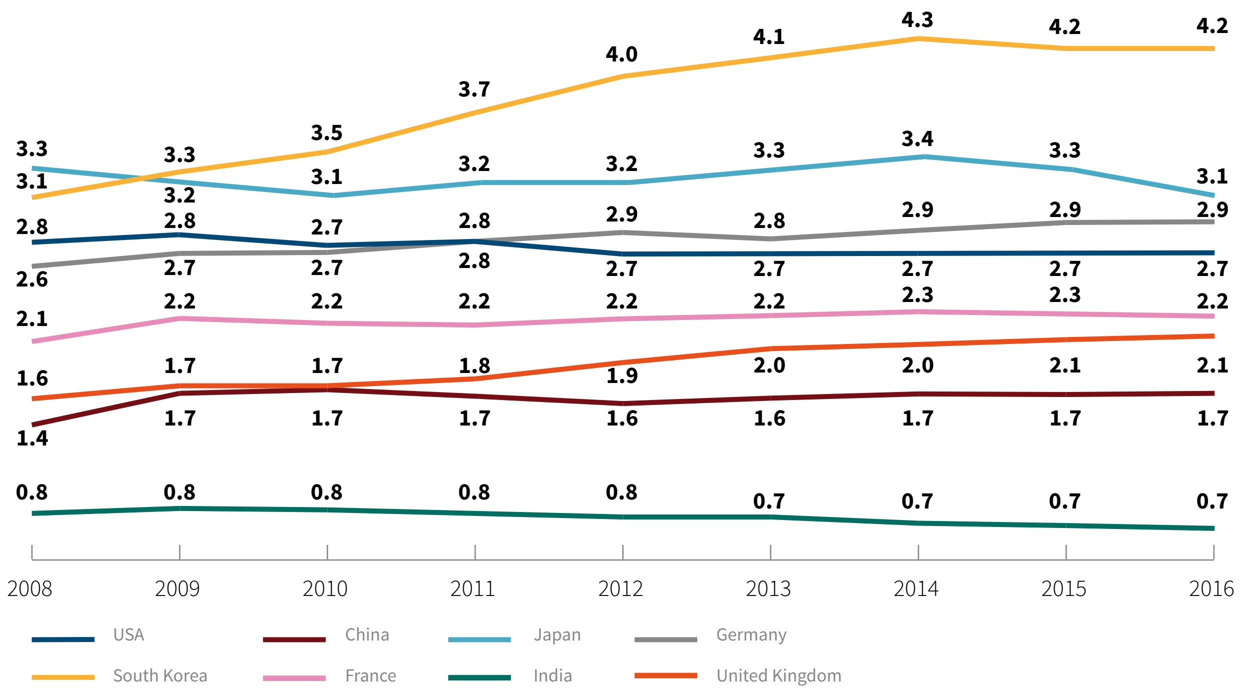
The financial crisis of 2008 set the global economy on a radically altered trajectory. Despite the ongoing impact of this crisis, R&D funding remains relatively strong reflecting ambitions to provide solutions to societal challenges and to stimulate economic growth through R&D. This trend is seen globally by all major economies with particularly strong growth in China and South Korea (see Table 1 and Figure 2).

Table 1: Estimated gross domestic spending on R&D (GERD) by selected countries 2008-16; billions of USD at constant 2010 prices

	2008	2009	2010	2011	2012	2013	2014	2015	2016	2008-16 CAGR*	Global Rank
USA	415	411	410	421	418	431	443	457	464	1.4%	1
China	149	188	213	243	281	316	345	375	410	13.5%	2
Japan	152	139	141	145	146	154	158	155	149	-0.2%	3
Germany	85	84	87	93	96	95	98	102	104	2.6%	4
South Korea	44	47	52	58	64	68	73	74	76	7.1%	5
India	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	6
France	49	51	51	52	53	54	55	56	56	1.7%	7
United Kingdom	38	37	38	38	37	39	41	42	43	1.6%	9

(R&D Magazine, 2018 OECD, 2018; Indian Department of Science and Technology, 2018; * CAGR: Compound Annual Growth Rate)

Figure 2: Estimated gross domestic spending on R&D PPP as a % GDP selected countries 2008-16



(OECD, 2018; Indian Department of Science and Technology, 2018)

Global challenges

The rapidly aging population, escalating environmental challenges and growing fears about energy have highlighted the urgent need for new paths to attaining sustainable prosperity (see Figure 3: example trends impacting R&D).

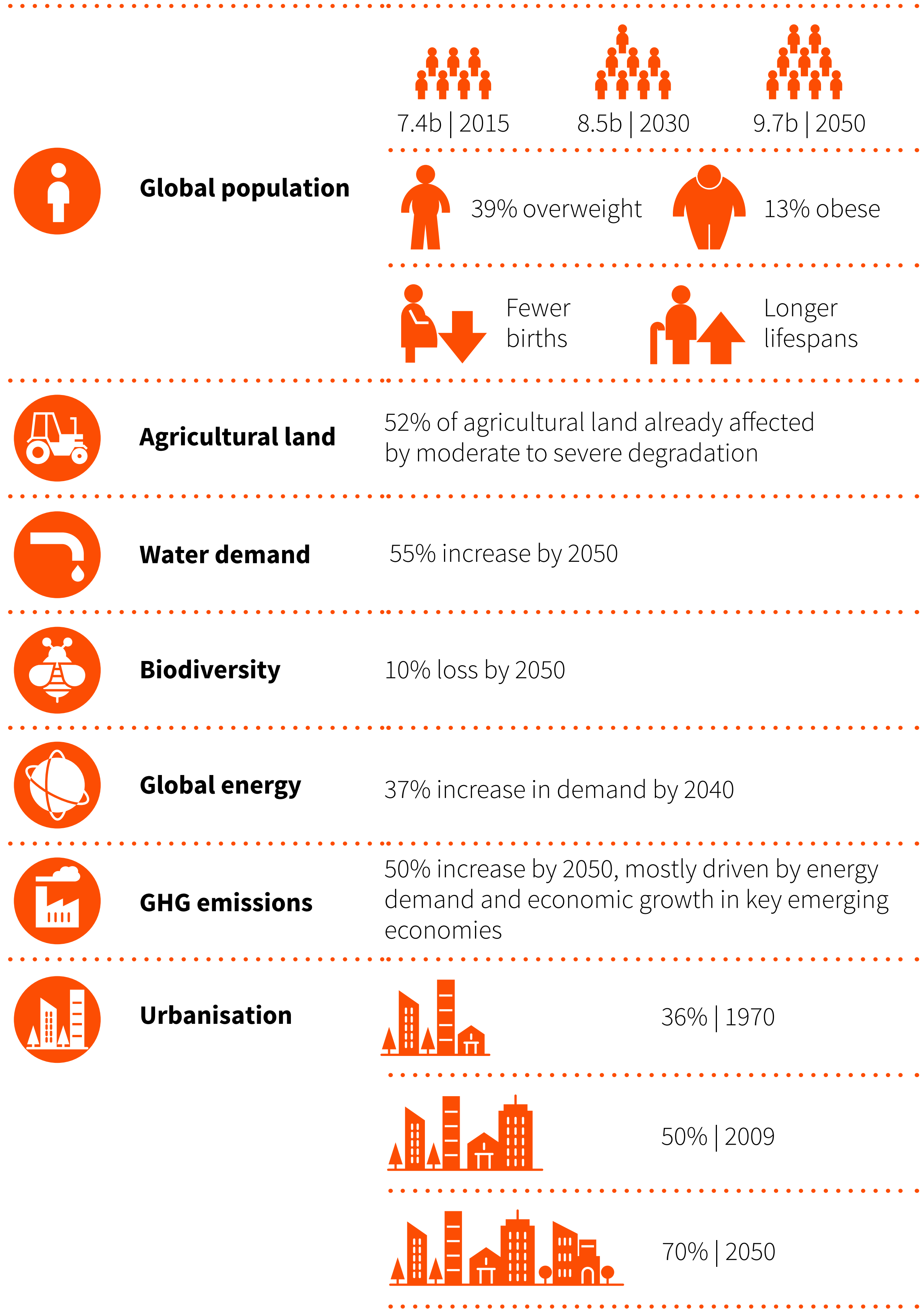


Figure 3: Example societal challenges impacting R&D (OECD, 2016)

This search for sustainable development has been the key focus of major international agendas such as the UN 2030 Sustainable Development Goals (SDGs), the World Economic Forum Systems Initiatives (WEF, 2018) and the World Business Council for Sustainable Development Work Programs (WBCSD, 2018) as well as international treaties such as the Paris Agreement on climate change in 2015.

As a result of these influences, governments globally have converged on a similar set of societal and environmental areas of focus for R&D funding with sustainability a key thread. The UN defines sustainable development as "development that meets the needs of the present without compromising the ability of future generations to meet their own needs" (UN, 1987) and its increasing importance as an output of R&D is highlighted by the 13% CAGR of 'sustainability' as a keyword in global chemical science research publications from 2014-17.

The exact priorities and their labels vary between nations, but we have classified the key global challenges which are a focus for research in the chemical sciences into five broad inter-related and overlapping areas shown in Figure 4 (see Appendix A).

Figure 4: Key global challenge areas

Energy
R&D focussed on secure, clean, efficient and affordable energy technologies

Environment
R&D focussed on climate action, resource efficiency, air quality and life on earth

Urban living
R&D focussed on sustainable cities, communities, transport and infrastructure

Human health
R&D focussed on advancing good health and well-being

Food & water
R&D focussed on food security, sustainable agriculture and water sanitation

Industrial innovation

In addition to encouraging a focus on societal challenges, governments globally are also pushing initiatives to accelerate innovation and to improve links between academic research and industry in order to drive economic development. This investment has broadly been focussed on four areas:

Figure 5: Key investment areas for driving economic growth

Technologies
Investment in key techniques identified as important for economic growth eg AI, nanotechnology

Industry
Investment in specific industries that are important for economic growth eg aerospace, electronics, computing

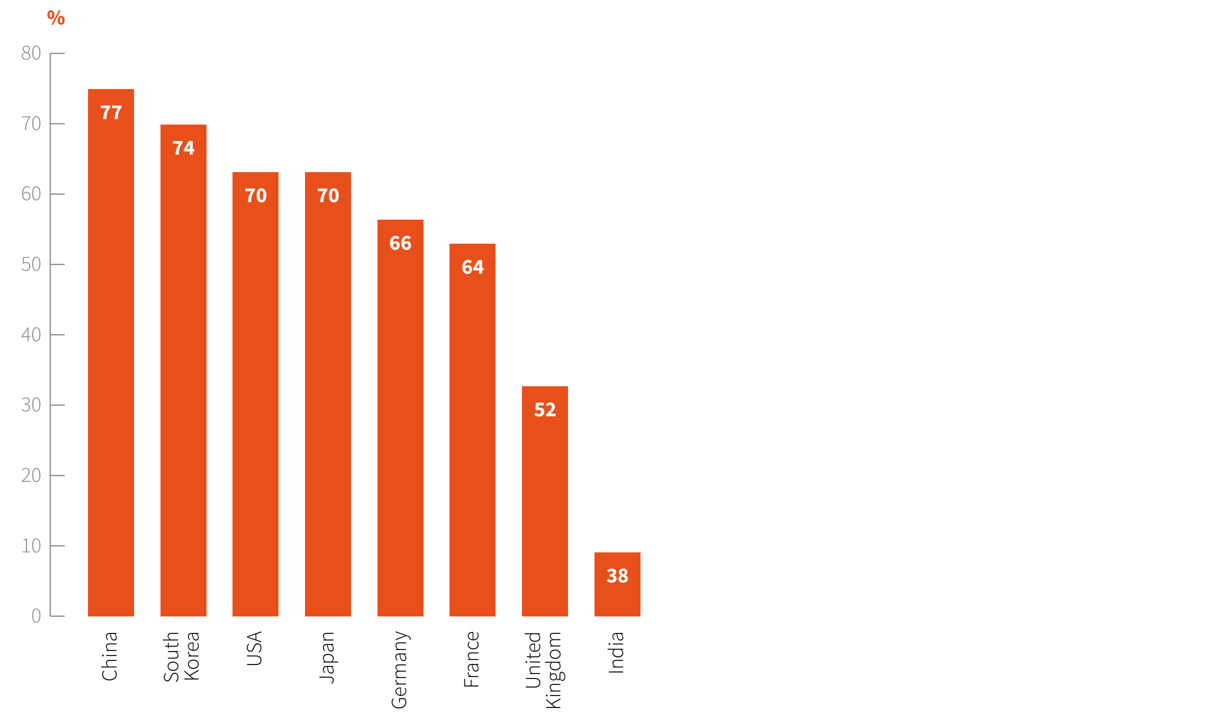
Innovation
Investment in programs to encourage innovation eg SMEs, links between academia & industry

Infrastructure
Investment in underlying infrastructure to enable sustainable economic growth eg cyber security, transport

A key goal of the European Horizon 2020 framework was for industry to contribute two thirds of Gross Domestic Expenditure on R&D (GERD). Performance has improved since 2010: for example, Horizon 2020 funded projects are 40% more likely to be granted patents (European Commission, 2017). Industrial innovation is also key to the major Asian R&D economies, for example both the Indian and South Korean government fund strong tax support for business R&D (UNESCO, 2016).

In line with the EU, UK Research & Innovation has a major focus on innovation in strategic announcements to date, with an ambition for the "UK to become the most innovative country in the world" (UKRI, 2018). In 2017, the Department for Business, Energy and Industrial Strategy launched the UK Industrial Strategy (GOV.UK, 2018) focused on boosting productivity by backing businesses to create jobs and increase earning power, and has set out "mission-based grand challenges" to "tackle specific challenges or opportunities for the UK" (UKRI, 2018). There have also been major environmental initiatives such as the Bioeconomy Strategy, UK Plastics Pact and Clean Growth Strategy that focus on delivering sustainable economic impact.

Figure 6: Estimated contribution of industry to R&D investment, latest available year

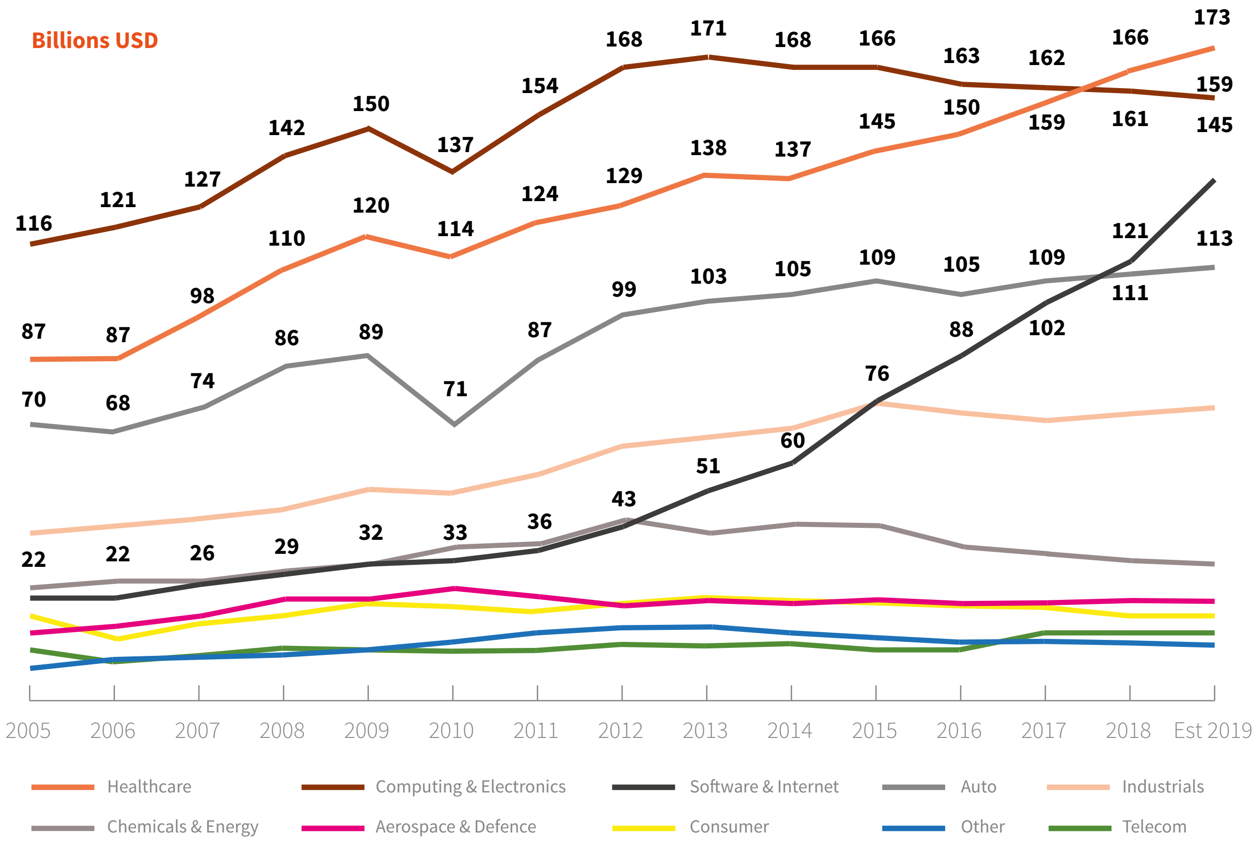


Sources: OECD, R&D Magazine, AAAS, Credit Suisse, UK Science & innovation Network, German Federal Ministry of Research & Education, Eurostat, ONS, Indian Department for Science & Technology

As a major source of R&D funding, businesses have a major influence on the direction of R&D. Globally, the top 3 industries in terms of R&D spending are Healthcare, Computing & Electronics and Software & Internet (see Figure 7), although there is significant variation between countries.

Going forwards, the speciality chemicals market is expected to show strong growth and is forecast to be worth $233bn globally by 2025 (Allied Market Research, 2018) with sectors such as construction, agrochemicals, wearable electronics and automotive driving this growth (Grand View Research, 2017).

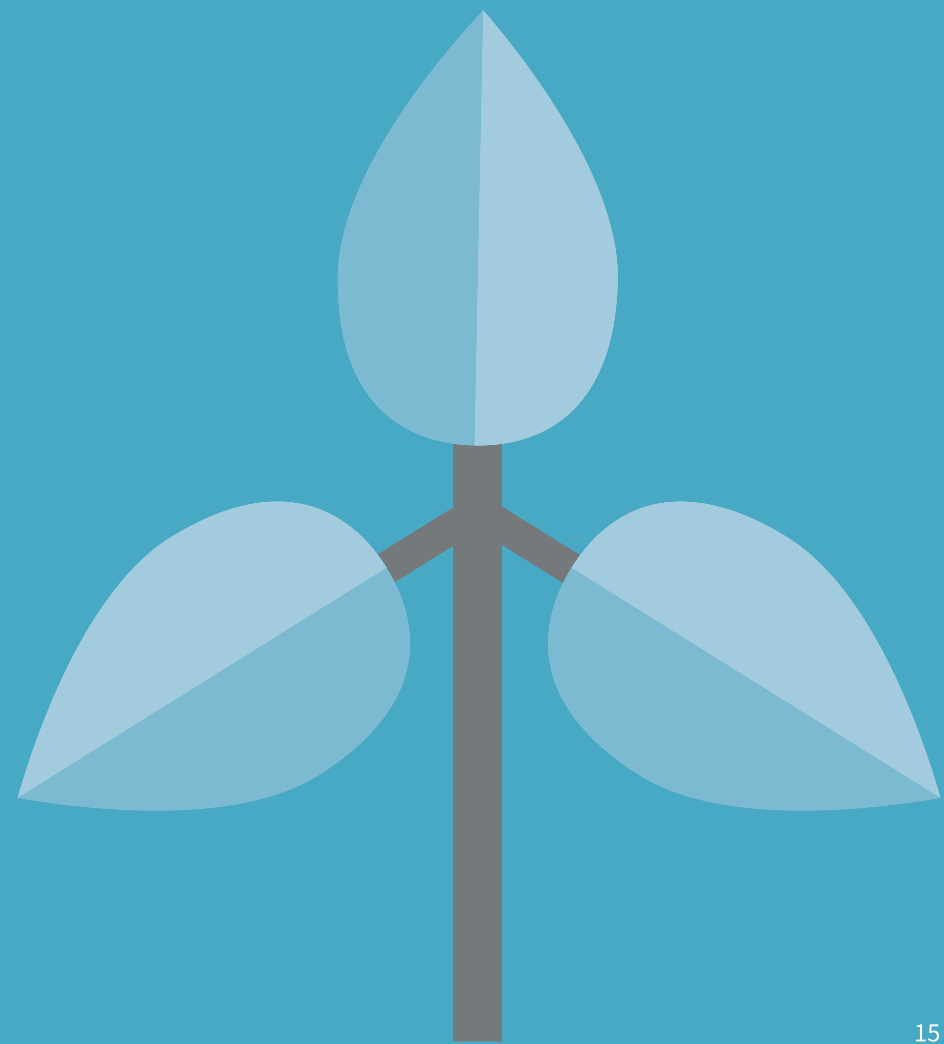
Figure 7: PWC Global Innovation 100 Survey: R&D spending by industry sector (estimates in billions of USD)



(PWC, 2017)

3.

Advances in science discovery & application



Through our interviews, workshops and survey, we heard that the scope of chemical sciences research today is vast. It encompasses deep questions about the structure and properties of matter from sub-nano to macrosopic scales right through to work with immediate application in fields such as human health and energy. Researchers are working across all of the global challenge areas and are deeply embedded in delivering industrial applications, with high expectations for what they can achieve over the medium term.

This breadth was confirmed in our data science analysis which showed that the top 20 fastest-growing topics in scholarly journals classified as chemistry included topics relevant to all of the major global challenge areas, some with strong industrial implications.

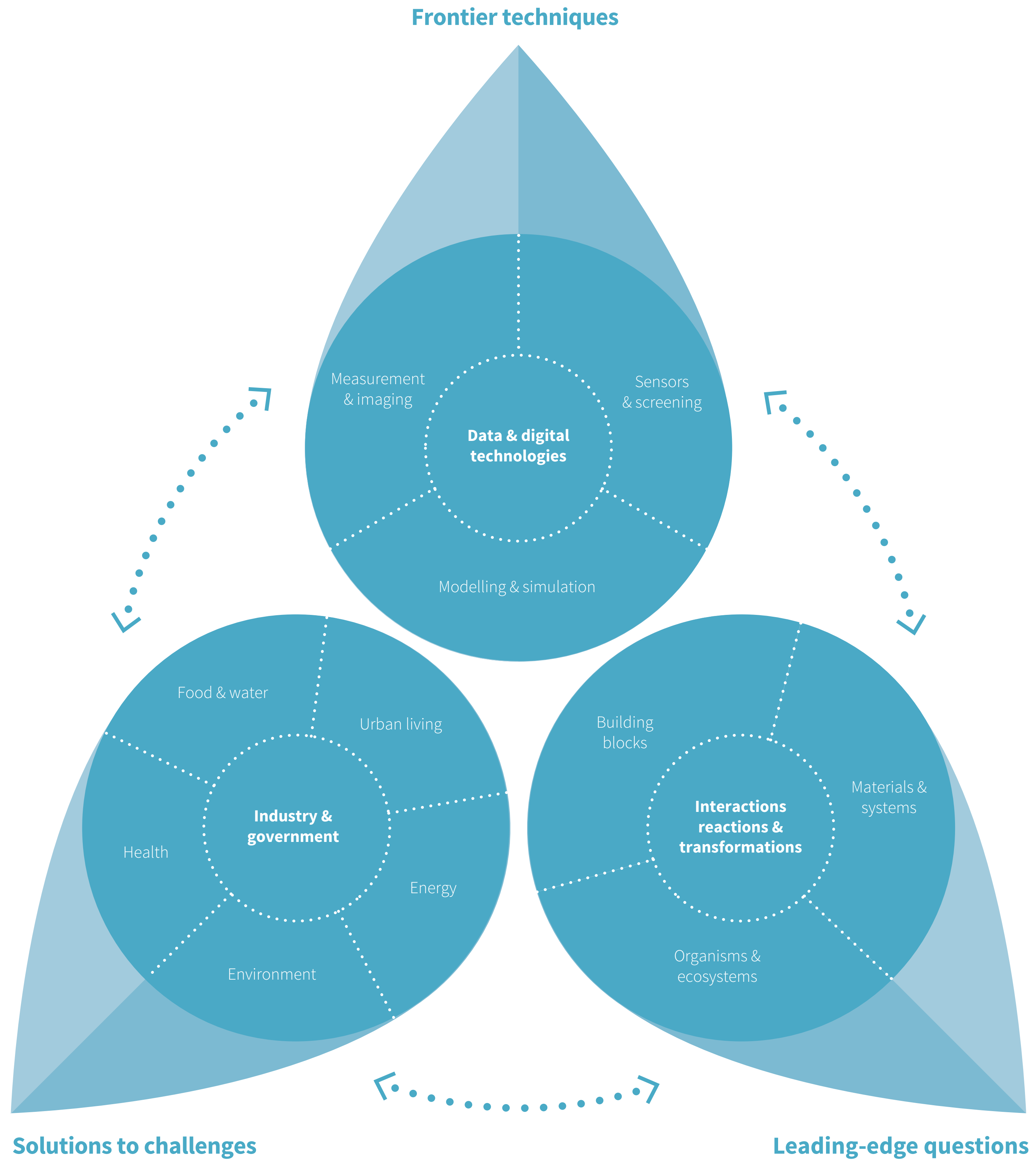
Combining analysis of publication trends with the expert views we heard through our researcher engagement programme, we grouped the mid-term advances we can expect from the chemical sciences into three broad areas:

- **Delivering solutions to global & industrial challenges:**
  Advances in understanding and application of the chemical sciences to major societal and industrial challenges
- **Exploring leading-edge questions:** Advances in understanding of the characteristics and interactions of systems from an atomic and molecular perspective along with designing, making and modifying molecules and materials.
- **Advancing frontier techniques:** Advances in a range of techniques that are critical for propelling the chemical and other sciences forward.

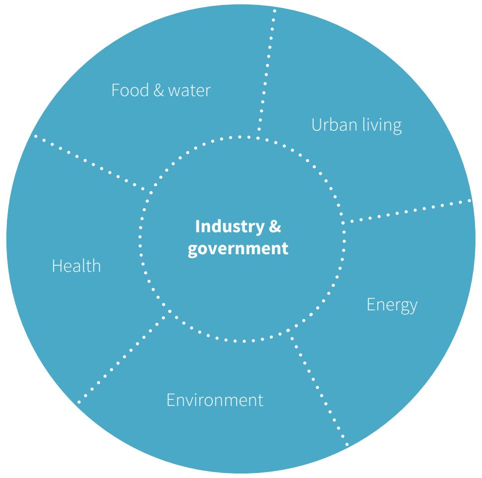
There is a high interdependency between these three areas. To make advances in frontier techniques researchers have to find answers to fundamental questions in theoretical, computational and analytical chemistry. These techniques in turn are critical in searching for answers to questions across and beyond the chemical sciences. Both frontier techniques and leading-edge questions are key to driving towards delivering solutions and as these applications emerge, they spur the development of new techniques and create new questions. The details of and interplay between these three areas is summarised in the following diagram.

In many cases an individual researcher or lab is making advances in all three areas. There is extensive collaboration within and across traditional disciplines like biology, chemistry, materials and physics as well as different engineering disciplines. Some researchers also described their journey moving between mathematics, laboratory experiments and digitally enabled prediction or analysis in seeking to answer a question or find a solution.

When we asked researchers about where the chemical sciences fit within this interdisciplinary science and engineering effort, a common theme was the combination of atomic and molecular insights, and the ability to design, make, isolate, characterise and/or modify molecules and materials.



3.1 Solutions to global & industry challenges



Researchers expect significant advances in the chemical sciences to underpin solutions to major societal challenges from environment and energy to human health and agriculture. In our survey, 99% of researchers stated that their work had potential application in at least one global challenge area with the average being 3.4 areas. Areas with the most potential for application are shown in Figure 8. A more detailed breakdown and list of specific examples of research advances are in Appendix B.

Figure 8: Potential application of research to global challenge area (% of respondents). Includes the top four application areas based on survey responses.

Potential application of research to global challenge area (% respondents)		Top 4 application areas
Environment	83%	• Substitution of toxic or hazardous materials • Environmental monitoring and/or remediation • Substitution of critical and scarce materials • Waste recycling
Human Health	75%	• Cancer • Measurement/sensing • Diagnostics • Antimicrobial resistance
Energy	68%	• Solar energy • Batteries • Carbon capture, storage and utilisation • Cleaner fuels and lubricants
Urban Living	57%	• Environmental monitoring and/or remediation • Waste recycling • Energy efficient buildings • Green transport
Food & Water	54%	• Drinking water quality and safety • Food safety • Water capture and recycling • Food production and security

Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Does your research have potential application in any of these <Urban living, Environment, Energy, Human Health, Food & water> areas? Please tick all that apply. N=549:554. Complete list of application areas given in Appendix B.

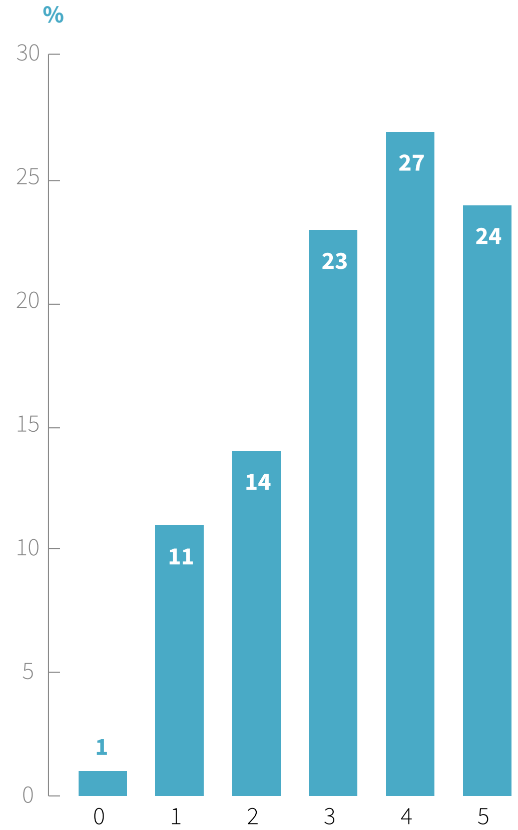


Figure 9: Number of potential research application areas selected by survey respondents

Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Does your research have potential application in any of these <Urban living, Environment, Energy, Human Health, Food & water> areas? Please tick all that apply. N=557.

Researchers consistently highlighted the importance of finding applications for their work and developing scientifically-based solutions to global and industrial challenges. For example, 23% of people who responded ticked three potential application areas. 82% of those surveyed agreed that considering the applications of research is in fact a 'duty' for scientists (see Figure 10).

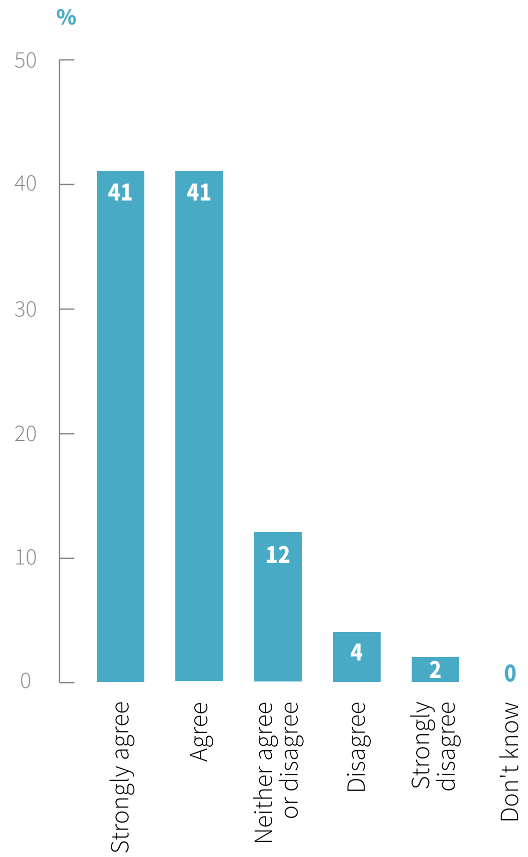


Figure 10: Attitudes to statement: "It is our duty as scientists to consider the potential applications of our research"

Source: RSC Science Horizons Researcher Survey, 2018. Survey question: To what extent do you agree / disagree with the following statement? "It is our duty as scientists to consider the potential applications of our research", N=531.

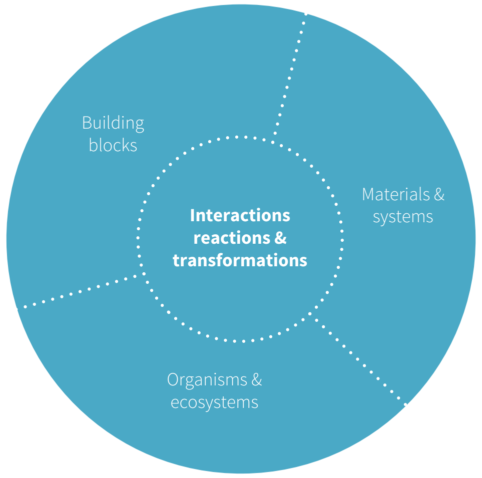
In order to translate research into application and mass adoption, it is critical for academic scientists to have close working relationships with industry partners. Academic chemical sciences researchers are deeply connected with current commercial areas of industry, ranging across everything from electronics to concrete and cement production. In addition, many researchers are engaged in advancing industrial processes, particularly in 'green industry' (eg alternative solvents or more efficient catalysts). Examples of the research chemical scientists are carrying out in partnership with industry are in Table 2.

Table 2: Examples of advances towards chemistry-based solutions to industrial challenges

Example topic	Specific research examples
Aerospace	Advances in corrosion-resistant steel coatings.
	Replacements for toxic metals (eg using aluminium, zinc or nickel as alternatives to cadmium).
Printing and lithography	Materials for extreme ultraviolet lithography.
	Environmentally-friendly materials for 3D printing.
Electronics and computing	Polymer materials for new display technologies (eg chiral helical polymers for 3D screen technologies, semiconducting polymers for flat and flexible displays).
	Molecules and materials that can be used as components of information storage (eg single molecule/crystal magnets and advanced polymers).
Food standards and safety	Robust measurement techniques and standards for verification of food contents (eg to detect plastic bulking agents in rice, verify claims about "free-from" or "gluten-free" foods).
Green industry	New supply chains based on converting industrial by-products (eg terpenes from paper industry) into useful functional molecules
	'Holistically green' alternatives to commonly used toxic chemicals and chemical processes (eg remove dimethylformamide (DMF), N-Methylpyrrolidone (NMP) and toluene from the production of commercial products including electric vehicle batteries, paints and apparel).
Industrial catalysis	Replacements for precious metals in catalysis (eg using earth-abundant metals such as iron, aluminium and zinc).
	More efficient catalysis at industrial scale (eg reduce use of volatile solvents, improve stability in air and at higher temperatures).
	Advances in enzyme-catalysed industrial processes (eg improving enzyme stabilisation, developing enzyme encapsulation materials, optimising flow chemistry).

Source: Science Horizons Survey, Interview and Workshop Programme Analysis, 2018

3.2 Leading-edge questions



Through interviews and workshops we heard that academic chemical sciences researchers are actively seeking answers to an incredibly broad range of questions, encompassing everything from the properties of main group elements to understanding the origins of life. The examples we classified in the leading-edge questions category are primarily driven by advancing fundamental understanding rather than seeking immediate practical applications.
In many cases answering these questions will contribute to advancing science and engineering knowledge more broadly and will enable new solutions to global and industrial challenges in both the short and long term.

We grouped the leading-edge questions being tackled by researchers into four broad themes:

- Building blocks: understanding the properties of the building blocks of systems, living or otherwise
- Materials & systems: understanding the fundamental properties of materials, systems and processes
- Organisms & ecosystems: understanding the properties of living systems and ecosystems
- Reactions, interactions & transformations: understanding chemical reactions and interactions within and between the three areas above, along with designing, making and modifying molecules and materials.

Classifying research topics into these categories is not an 'exact science' as some topics span multiple themes.

Learning from nature but not limited only to molecules and materials that exist in nature, we heard that researchers are using their knowledge, insights and skills to make new molecules and materials, using novel transformations to control important or useful properties, for example ultimately as new medicines or materials for energy. Researchers use frontier techniques to inform what they make, and to probe how molecules and materials behave or respond in different environments, for example depending on temperature, pressure, salinity or light.

It was striking that researchers are studying, creating or controlling matter across a huge range of scales - from hydrogen to DNA to plastics to our atmosphere. In some cases scientists are able to design new molecules or materials with desired properties on a computer or "in silico" before making them in a laboratory. For complex molecules like proteins or DNA researchers are making huge strides in elucidating structures, properties and interactions, and using approaches such as directed evolution to modify these.

As part of this interdisciplinary effort chemical scientists bring an atomic and molecular lens to the systems being studied and approaches used: for example, considering the different kinds of covalent and non-covalent interactions in non-living and living systems; thinking about how and why atoms, ions or molecules arrange in three dimensional configurations as they do; how and why charge is distributed locally and globally within systems; and how these aspects relate to molecular and material properties and interactions at different scales.

Table 3 gives some specific examples of research advances and there is a longer list in Appendix C.

> "Fundamental understanding at the molecular level and translation to controllable function at the macro level is where we have seen dramatic advances in the past decade which will only continue to propogate further over the next 5-10 years."
>
> **Professor Oren A. Scherman**
> University of Cambridge

> "Chemistry provides a molecular level of detail, for example identifying the pathways for many biological processes and disease mechanisms informs the design of interventions at the molecular level."
>
> **Professor Shu-Li You**
> Shanghai Institute of Organic Chemistry

Table 3: Example leading-edge questions (complete list in Appendix C)

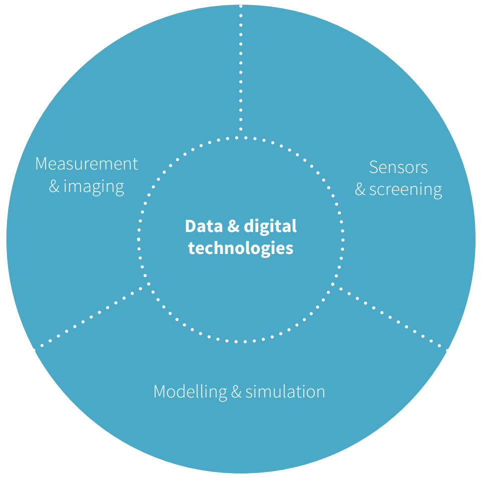
Theme	Example topic	Specific research examples
Building blocks	Single molecule chemistry	Advances in analytical, computational and synthetic chemistry are coming together to enable the study and manipulation of single molecules which presents exciting opportunities to control and design properties from the single molecule building block level. For example within analytical chemistry, developments in micro/nano-fluidic technologies and in spectrometry are enabling advances in this field.
	Protein dynamics & structure	Advancing our understanding of the fundamentals of the dynamics of protein structures using bioinformatics approaches to study the existing high resolution structural data and make predictions about new structures. We are now in a position to look at paradigm shifting questions in protein chemistry – not thinking only about the relationship between structure and function but rather thinking of proteins as an ensemble of soft states; different structural states facilitate different functions and roles in a protein.
	Main group chemistry	Systematic analysis of compounds of main group elements to develop fundamental understanding of the properties of different elements, with the aim of developing compounds with novel applications, as well as gaining access to previously unavailable bonding modes or unexpected structural features.
	Quantum effects	Advancing our understanding of the magnetic spin in materials and how to control it. This will have important applications in electronics.
Reactions, interactions & transformations	Complex organic synthesis	Advancing our understanding of C-H bond functionalisation – this has been a major fundamental synthesis challenge for chemists for many years, due to the highly inert nature of the bond. Discovering new ways to activate C-H bonds will allow chemists to optimise a number of key industrial transformations for example in pharmaceutical research.
	Next generation catalysts	Advancing our fundamental understanding of catalytic science by obtaining a detailed understanding of reaction mechanisms, using advanced spectroscopic techniques, high throughput screening and computational modelling. Advancing our understanding of how catalysts function will help us discover new catalysts and combinations of catalysts that will improve the efficiency of reactions and lower our reliance on scarce or toxic elements.
	Protein interactions	Advancing our understanding of protein - protein interactions and how to intervene or inhibit them; how they fold, mis-fold and interact with other molecules in living organisms. Examples of where this is critical for advancements in human health include peptide aggregation leading to amyloid formation implicated in Alzheimer's and Parkinson's.
Materials & systems	Intelligent polymer chemistry	Advancing our understanding of how mechanical and ionic forces trigger chemical reactions, in order to develop advanced 'autonomous' materials. With this knowledge we can, for example, begin to design materials that respond to external stimuli to self-repair.
	Bio-inspired materials	Understanding how nature facilitates CO2 capture from first principles (eg the function of photosystem II in photosynthesis) to develop bio-inspired porous metal-organic frameworks with large surface areas to harvest light energy.
	Systems chemistry	Next generation systems chemistry – understanding more complex systems and reaction networks will require better models, measurement and data analysis. This can inform our fundamental understanding of living systems eg cells. One of the grand challenges in chemistry now is the construction of functional far-from-equilibrium systems.

Table 3: Example leading-edge questions (complete list in Appendix C) (continued)

Theme	Example topic	Specific research examples
Organisms & ecosystems	Human physiology	Advancing our understanding of the human microbiome will help to inform such things as drug interactions; this will rely on development of new sensors that can be effective at point-of-use to accurately measure levels of specific microorganisms and molecular markers in the human microbiome.
	Chemistry of the ocean	Advancing our understanding of the chemistry of common pollutants and their interactions with biological systems in our rivers and oceans eg herbicides, pesticides and waste pharmaceuticals. These compounds are designed to interact with biological systems, but we don't really know how they interact with the biological systems in our rivers and oceans (eg with plankton).
	Chemistry of space	Understanding the molecules and chemistry of space using new instrumental techniques and light sources (eg broadband microwave spectroscopy, terahertz radiation sources) combined with astronomical observations to advance our understanding of the development of life.

Source: Science Horizons Survey, Interview and Workshop Programme Analysis, 2018

3.3 Frontier techniques



Measuring & imaging
Advanced analytical techniques for measuring increasingly complex systems in operando and to probe the real-time dynamics and interactions of molecules and materials.

Sensors & screening
Advanced sensor & screening technology that can detect, monitor and screen with high specificity under diverse conditions.

Modelling & simulation
Advances in theoretical and computational techniques for predicting the structure, function and properties of molecules, proteins, catalysts and materials.

In listening to researchers as they described their work three areas, within what we have called frontier techniques, stood out as being critical for the advancement of research over the next 5-10 years:

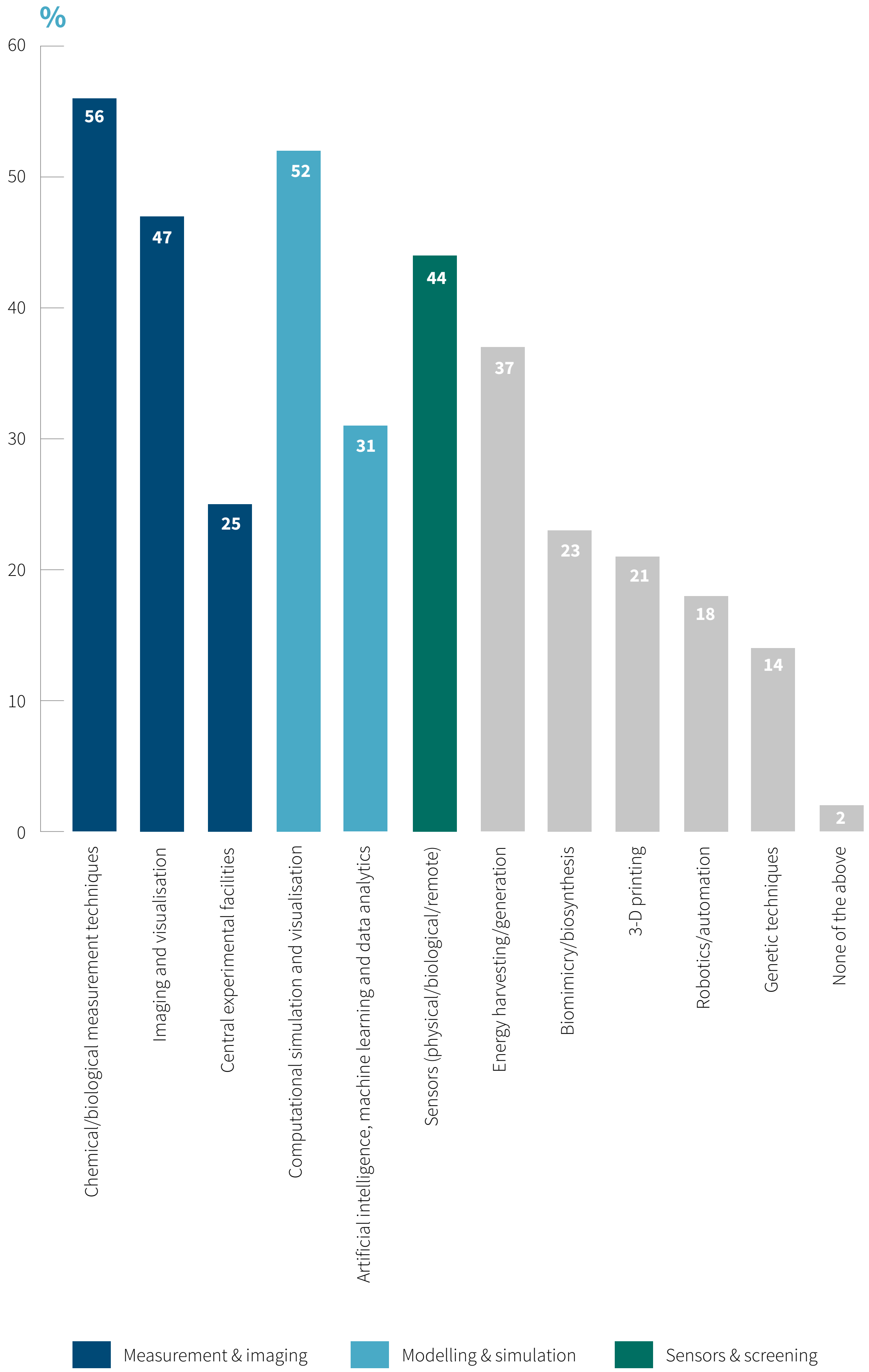
- Measurement & imaging
- Sensors & screening
- Modelling & simulations

Data & digital technologies sits at the centre of these three areas. Measurement & Imaging and Sensors & Screening, are critical for gathering data about observable structures and phenomena from across all fields of the chemical sciences.

Modelling & simulation is critical for the analysis and interpretation of data and for using data to make predictions and new discoveries.

Researchers expect major advances across all of the frontier techniques to enable data gathering from increasingly complex systems and samples and to get closer to 'real-time' observations, taking measurements at shorter and shorter intervals to provide increasingly detailed datasets. To support these advances, researchers expect further developments in the tools for data collection, alongside advances in miniaturisation, durability and portability.

Figure 11: Key technologies important for advancement of the chemical sciences



Source: RSC Science Horizons Survey Analysis, 2018. Survey question: Will advances in the following science and technology areas be important to development of your field of research? N = 555. Survey respondents were asked to select all that apply.

Measurement & imaging

We heard that advances in analytical measurement techniques are enabling researchers to study systems at greater resolution than ever before, from using single molecule spectroscopy to observe the properties of individual molecules to applying synchrotron X-ray and neutron sources to study catalysis at a molecular level as a reaction is taking place. Developments in ion mobility mass spectrometry provide researchers with greater information on the structure of biomolecules and by employing cryo-electron microscopy researchers can also study how they function.

Over 50% of researchers surveyed highlighted the importance of developments in analytical measurement and imaging techniques (see Figure 11). Advanced measurement techniques were also highlighted as a fast growing area in our analysis of publication trends and were consistently highlighted as critical in our researcher interviews.

In particular, researchers highlighted recent developments in ultra-fast and in operando measurement techniques, as well as advances in the complexity of species that can now be studied.

Researchers from across all fields of chemical sciences described the development of measurement & imaging as important for advancing their work, covering everything from understanding the behaviour of single molecules to studying the dynamics and interactions of complex systems. Specific examples included:

- Understanding charge distribution in individual molecules
- Investigating chemical reactions in ultra-dilute systems
- Exploring reactions at solid and solid/liquid interfaces
- Elucidating material properties
- Studying light-matter interactions at the femtosecond level in biological systems
- Studying proteins, lipids, peptides and metabolites in living cells
- Investigating protein–drug interactions

Continually improving resolution, miniaturisation and portability of measurement devices, eg high resolution spectroscopy, rapid mass spectrometry and bench-top NMR, were also identified as a critical priority in our survey.

“There are remarkable tools available that are changing the face of science such as those available at national facilities eg Diamond Light Source and the Canadian Light Source. Advances in measurement are critical – and we are getting better at using multiple measurement techniques to solve formidable problems by collating and merging different types of data.”

Professor Sarbajit Banerjee
Texas A&M University

“The ability to study systems both in situ and even more in operando will deliver valuable insights. For example, we can now study a catalytic system while it is operating, which is a huge benefit as it allows us to see how the catalyst changes in real time and to correlate structural changes with those in the product distribution. The next generation of light sources offer the exciting opportunity of following directly the mechanisms of reactions – probing systems under real operating conditions and monitoring how they develop over time.”

Professor Richard Catlow
University College London

“Using small molecules to probe biological mechanisms is very important. For example, we can identify bulk cellular lipids by mass spectrometry, and if they are tagged with small molecules we can learn more about their subcellular localisation and potential binding partners, which in turn will help us to understand the functions of these biomolecules.”

Professor Riki Eggert
King's College London

“Advanced measurement techniques allow you to look at complexity, reflecting not just isolated molecules, but how large numbers of these interact over different length and time scales. Being able to measure the intermediate processes between the molecular and macroscale states will deliver exciting new insights.”

Professor Richard Compton
University of Oxford

Sensors & screening

Developments in sensor & screening techniques were highlighted as important for the advancement of their research by over 40% of researchers surveyed (see Figure 11).

Advances in sensor & screening technology was highlighted as critical by researchers in a number of fields, particularly by researchers working in chemical biology and environmental areas. These fields in particular are looking to develop sensors that can detect, monitor and screen with high specificity in a vast array of diverse conditions eg outdoors, in hospitals. Advances in the underlying analytical chemistry will be critical to improving the sensitivity of the technology and developing tools that work effectively in real in-field conditions with high reliability. Developing sensors that can deal with multiple types of data in complex samples – for example, human secretions, soil etc – was highlighted as particularly important, as was miniaturisation of the technology.

Example applications highlighted by researchers include:

- Measuring atmospheric properties of complex urban environments for environmental monitoring
- Measurement of molecular markers (eg single molecules) in human breath, sweat, tears etc. for use in non-invasive diagnostics
- Tracking the bio-availability of specific substances (eg nutrients, contaminants), with applications in agriculture (eg fertiliser absorption), human health (eg toxin accumulation in food chain) and environmental remediation (eg more accurate measurement of soil contamination)
- Biosensors to detect pollutants in tissues/organs in a benign way and at small concentrations (eg detection of nano-metal oxides in the human brain, which may be implicated in neurodegenerative diseases)
- Measurement of airborne infectious disease markers
- Border security eg sensors for detecting drugs

“Developments in sensor technology for real-time analysis in the field will be important over the next 5-10 years. This will allow improved and faster monitoring of a number of key environmental markers including air quality, soil contaminants, pesticide levels and so on. Higher density sensor networks will enable more localised monitoring and interventions with applications in numerous areas such as agri-food, air quality, water and geo-energy. There is a need to improve the sensitivity of these sensors and to develop tools that work effectively in real in-field conditions that are highly reliable, connected, able to withstand temperature and humidity, as well as extreme environments. Advances in analytical techniques, materials, catalysis and engineering will be key enablers in developing sensors and to miniaturise these technologies making them portable – from something that works in laboratory conditions to being used on a farm or in a city.”

Professor Mercedes Maroto-Valer
Heriot-Watt University

“One of the biggest problems globally is a kind of infectious disease like the Zika virus - for the diagnosis of this infectious disease the most important issue is diagnosis being able to happen in the field. So we are trying to develop sensors for this with medical doctors.”

“Developments in portable optical systems are really important for the development of sensors. Also engineers are important for miniaturising the systems.”

Professor Jaebum Choo
Chung-Ang University

“Developing sensors, particularly nano-sensors, for in situ detection in real time requires research to improve the selectivity of sensors and a high level of accuracy at very low detection levels. This will be a collaborative effort involving researchers with expertise in microfluidics, chemistry, materials and environmental engineering. It is key to make the sensors robust enough for real world application.”

Professor Dionysios Dionysiou
University of Cincinnati

Modelling & simulations

Over 50% of researchers surveyed indicated that developments in modelling & simulation techniques are important for the advancement of their research fields. This was strongly reinforced in our researcher interviews. In combination with the data collected with advanced measurement and sensing tools, modelling & simulation techniques provide a powerful approach for advancing our understanding and our ability to make predictions.

In interviews and workshops researchers highlighted an incredible range of areas where modelling and simulation will be key to driving forward research. Examples illustrating the range from broad areas to specific research questions are:

- Molecular design and synthesis
- Materials discovery eg closed loop automated experimentation
- Optimising chemical reactions
- Improved experimental design
- Drug development and screening
- Discovery of new electrolytes for batteries
- Modelling interactions of complex pollutants with remediation technologies
- Improving design of probes for spectroscopy
- Making structural predications eg crystal structure of boron
- Understanding movement of cholesterol across lipid membranes

Advances in the underlying theory will be critical to developing models that can handle increasingly complex molecules and systems eg proteins, DNA–drug interactions or catalysis at material surfaces. New mathematical and computational approaches will be required to develop algorithms that can manage this increased complexity at a reasonable computational cost.

One of the key aims of modelling & simulation is to use atomistic calculations to predict and design molecules and materials with specific and desired chemical, electronic, and physical properties. With the potential for ‘in-silico experiments’ to eventually replace, or at least significantly enhance, some areas of experimental work, the area is also a key focus for industry (Deloitte, 2017).

“There is a frontier of big data for chemistry and other sciences – this is another potential transformative revolution coming down the pipeline. It is not a new concept, it is bringing to chemistry an enhanced culture of statistical literacy, which can better inform a lot of what we do and enable handling of more complex data sets. One thing that chemists do and that will not be replaced is make new things – organic or inorganic compounds – but it is now about to undergo a revolution with AI/ML. The science of synthesis that is at the heart of chemical sciences is about to change. In 10 years we will have a very different approach to synthesis. Not just a researcher in a lab coat. We won’t be supplanted by machines but half machine/half human science could be very real.”

Professor Sarbajit Banerjee
Texas A&M University

“Fundamentally modelling helps us to gain a better atomistic and quantitative understanding of molecular systems bridging multiple scales from electronic structure to a more macroscopic level. We are now studying bigger molecules than we ever dreamed we could understand, considering changes in molecular conformation alongside all types of intermolecular interactions, degrees of disorder etc. Advances in modelling itself and in the theoretical assumptions built into the models, for example going beyond assuming that building blocks are fairly spherical, will be crucial as we tackle more complex molecules and systems.”

Professor Sally Price
University College London

“Advances in theory, computation and experiment go hand in hand – improved theoretical understanding enables better computational modelling which can then be compared with experiment and in turn fed back into the theoretical models and experimental design. More collaboration is needed between theorists and experimentalists.”

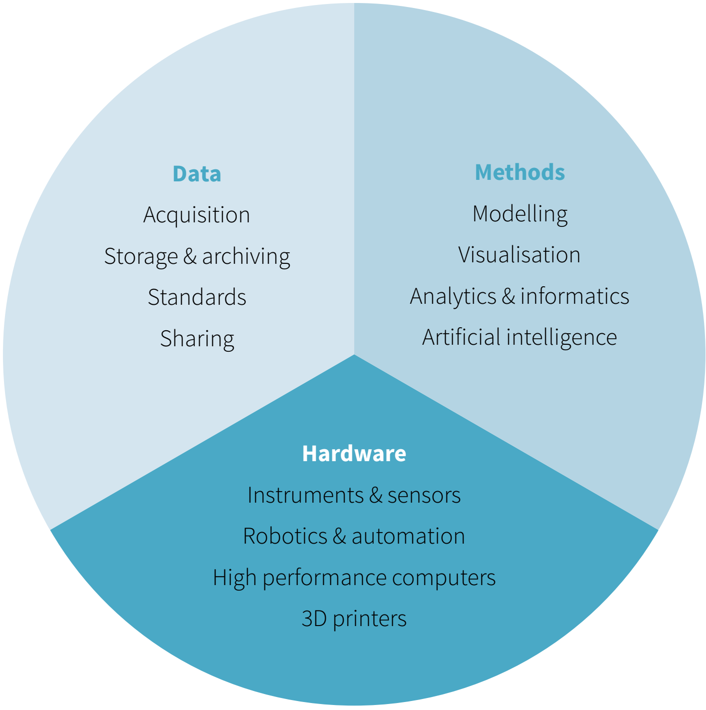
Professor Helen Fielding
University College London

Data & digital technologies

More broadly, through interviews and workshops we heard that researchers expect digital technologies to continue to transform and accelerate research, enabling faster understanding and prediction of more and more complex structures and properties.

Data and digital technologies are already integral to research, for example in computational modelling and in measurement techniques, and this will continue as increasing amounts of data are produced and as digital technologies such as machine learning and robotics are used in some domains.

Figure 12: Data and digital technologies in Science R&D



There are significant challenges in storing, standardising and sharing data in a useful way. It will also become ever more important that chemical sciences researchers have computational, mathematical and statistical skills so that they can meaningfully use digital tools and interpret results.

Artificial intelligence (AI) and, within it, machine learning (ML) were highlighted as important emerging fields in the context of application to scientific R&D. AI/ML in combination with big data has been referred to as the "fourth paradigm of science" (Agrawal, A & Choudhary, A, 2016) and researchers expect AI/ML to be deployed across a spectrum of studies – from inorganic molecules to proteins, and across both amorphous and crystalline materials – where it will enable faster and more reliable prediction of structures and properties (Isayev, O & Walsh, A, 2018). Our analysis of academic publishing trends also showed growth in publications related to AI/ML.

There is also a healthy dose of scepticism about the level of 'hype' surrounding AI/ML and its potential impact on the chemical sciences, and a sense that the jury is out on where it will have its biggest impact. There is also a recognition that for ML significant progress needs to be made to develop high quality and appropriate datasets to train models.

"There is now an onus on researchers to be more statistics and data savvy so that we can more quickly and effectively get a deeper understanding of our own research – it is not good for research if data science is a 'black box' out of which an answer comes."

Professor Tom Welton
Imperial College London

"It is crucial that people developing computational tools and theoretical techniques closely collaborate so that they understand one another's language and can thus reach the desired goals more efficiently. This is particularly important in emerging fields."

Professor Fernando Martín
Autonomous University of Madrid

"AI/ML needs to be applied by the people who know what they are doing. It can be very good for interpolating between well-defined computational models and other comparably well-defined systems, and it will reduce the time and computational expense. However, people saying 'let's just apply AI/ML to your databases' is just pie in the sky as we don't necessarily have the data to train the models. The database may not hold all the critical information that determines the outcome, as this may not be known, or was not being recorded in the primary literature, let alone saved in the database. The data revolution brings huge challenges – the fields where we have enough data with enough controls related to it is currently quite limited. The quality of the data is really key as is having people with the right skills to use it."

Professor Sally Price
University College London

"Automation and ML is beginning to help atmospheric models as things are so complex that it would almost be impossible to manually operate the models and accurately interpret the huge amount of data that are generated. This is opening up the ability to deal with more complexity, interpret ever more detailed datasets and an increasing number of variables you can keep track of."

Professor Dwayne Heard
University of Leeds

"A trend of the last 5 years is the tremendous growth in data science. In particular, Machine Learning (ML) is a huge thing that cuts across many fields and sectors, including chemistry. People have started trying to use ML in materials science and drug design. However, there is a lot of information that scientists intuitively know, which is difficult to code into machines at the moment."

Professor Kieron Burke
University of California Irvine

"The computational side will become increasingly important for all researchers. We will need more and more maths and data skills to confidently use the tools needed for predictive modelling and analysis of complex data. Researchers without these skills will risk falling behind. Research is changing and we need to prepare students for this."

Professor Graeme Day
University of Southampton

"Better predictions of the structure and functional properties of new materials will allow us to design materials with specific desired properties that could have broad applications eg personalised medicine. These insights will enable chemists to make rationally-designed materials with specific properties, faster and more reproducibly."

Professor Molly Stevens
Imperial College London

"Computational tools are useful to rationalise experimental observations rather than as a replacement for experimental research. For many systems there is a large number of variables that need to be taken into account, which can limit the predictive power of the model."

Professor Catherine Cazin
Ghent University

"It seems very plausible that useful and important work will come out of the increased focus on AI and ML, but how deep the benefits will be, and realistic timescales for delivering them, really do vary by area."

Professor Fred Manby
University of Bristol

Other techniques

A number of additional techniques were highlighted by researchers, although with lower frequency in the survey (see Figure 11) and with less emphasis in the interviews and workshops. These are summarised in Table 4.

Table 4: Additional important frontier techniques

Technique	Summary
Advanced genetic techniques	Advanced genetic techniques for designing and constructing biological modules, systems and machines or re-designing existing biological systems for useful purposes ('synthetic biology'). For example, directed evolution techniques to enhance enzyme function such as artificial metallo-enzymes to enable Suzuki cross-coupling and modification of organisms (eg yeast, bacteria) to make useful substances
Robotics & automation	Advances in computer-aided experimental design (CAED) including automation and robotics, with particular application in synthetic chemistry eg formulation optimisation for consumer goods to drive performance improvement and cost-saving
High throughput screening techniques	Advances in biological screening techniques to allow high throughput screening for various biological properties and functions eg 'organ / enzyme on a chip' for experimental assays and fast diagnostics

Source: Science Horizons Survey, Interview and Workshop Programme Analysis, 2018

4. Curiosity, collaboration & leadership

Enablers for scientific discovery and application

Science and engineering research plays a pivotal role in driving forward the global R&D agenda, contributing to sustainability and prosperity. It is therefore important to ensure an environment that enables research to deliver to its full potential.

Through our conversations with researchers in interviews and workshops three key contextual areas emerged as critical in order that research contributes to its full potential to society today and in the future:

- Curiosity
- Collaboration
- Leadership

Table 5: Summary of enablers & challenges

Enabler	Why is this important?	What is holding us back?
Curiosity	Curiosity-driven research, also known as fundamental, discovery or basic research, was consistently highlighted as a critical enabler for long term and transformational advancement of knowledge and its applications.	Lack of funding for basic research Short-term thinking by policy makers and funding agencies Lack of funding for smaller groups and early career researchers
Collaboration	Over 80% of respondents in the researcher survey agreed that collaborations are critical for the advancement of the chemical sciences. This includes interdisciplinary, academia-industry and international collaboration.	Balancing depth of expertise with exposure to collaborative work during education and training Academic recognition and rewards culture that emphasises individual achievement too much Building, managing and leading interdisciplinary teams Ineffective mechanisms to work with industry
Leadership	Chemistry and other sciences have a critical role in driving the global research agenda but there is an opportunity to take a bolder leadership role across the spectrum from setting high level research agendas, to designing and carrying out research programmes, to translating researching into commercial and societal benefit.	Academic career paths do not always support or incentivise people in developing leadership skills Mechanisms to engage with the public and policymakers Not enough leadership in collaborative areas

4.1 Curiosity

Curiosity-driven research, also referred to as discovery, fundamental or basic research, was consistently highlighted as a critical enabler for the advancement and application of science. In interviews and workshops researchers spoke about how curiosity-driven research is where novel breakthroughs and transformative ideas come from. These open up new ways of thinking, new techniques and sometimes lead to entirely new directions of research spanning multiple disciplines.

These breakthroughs also pave the way for 'game-changing' disruptive technologies of the future. We heard numerous examples that illustrate the importance and long-term impact of curiosity-driven research, from the discovery of materials like Nylon and Kevlar to therapies like Penicillin and monoclonal antibodies to technologies like lithium ion batteries and LCD or OLED screens.

The importance of curiosity-driven research also came through strongly in our survey with 94% of respondents identifying funding for curiosity-driven research as important for the advancement of the chemical sciences (see Figure 14).

While 82% of those surveyed agreed that considering the applications of research is a 'duty' for scientists (see Figure 10), researchers based in every country represented in our interviews expressed a concern that the emphasis on societal challenges and economic growth has led to an imbalance in funding with insufficient investment in curiosity-driven research. Almost 70% of researchers surveyed agreed that funding agencies put too much emphasis on the potential applications of research (see Figure 13).

Most researchers expressed particular concern stemming from their perception of short-term thinking by governments and funding agencies:

“Scientists discover new beautiful things. It's important to do science to gain new knowledge and understanding, confident that this will lead to benefits to society. The discovery stage needs to be independent. There is a trend toward providing funding for task oriented research which is highly constrained. The power of curiosity-driven science is going into the unknown without bias.”

Professor Omar Yaghi
University of California, Berkeley

“Great discoveries often come from unexpected results rather than hypothesis-led research. It is therefore critical to take a long term view about research – it is like planting trees in a garden, the true impact of your work only becomes clear later.”

Professor Sir Christopher Dobson
University of Cambridge

“Curiosity driven science is very important – it means that in 50 years' time very superb things are realised. There are many examples of industrial applications from curiosity-driven science and it is beneficial to work in collaboration with researchers focused on this aspect.”

Professor Susumu Kitagawa
University of Kyoto

“As a complement to application-oriented research, we need to allow original serendipity driven research, as this will uncover real opportunities. It can be difficult to plan what the impact might be, and if we limit to defined outcomes we may miss opportunities and things not thought of before.”

Professor Stefanie Dehnen
University of Marburg

“Breakthroughs are by nature not predictable or linear. You can't programme them, but you can create environments that bring people together to exchange ideas and perspectives.”

Professor Bengt Norden
Chalmers University of Technology

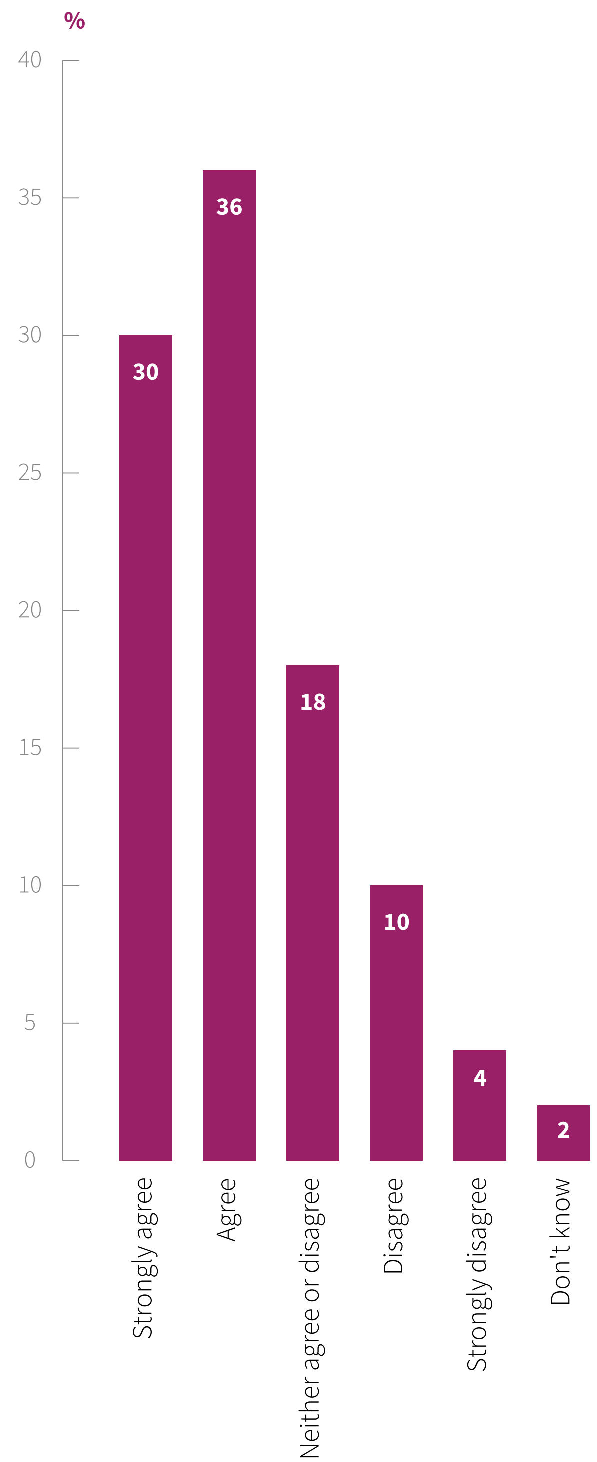


Figure 13: Attitudes to statement: "Funding bodies put too much emphasis on the potential applications of research"

Source: RSC Science Horizons Researcher Survey, 2018. Survey question: To what extent do you agree / disagree with the following statements? "Funding bodies put too much emphasis on the potential applications of research", N=530.

Scientists globally expressed concern about lack of funding for curiosity-driven discovery science. Researchers expressed views on how short-termism and over-concentration of investment in specific research areas or groups work against the long-term nature and impact of discovery science.

“Everything is on a three year cycle – if your research doesn’t produce anything in three years it is considered worthless. We need to look at mechanisms to deliver long term scientific impact.”

RSC Science Horizons Interview
Researcher based in North America

“Huge research centres have proliferated. They are a good idea to get people together to work towards a common mission. However, depending on how they are run and how funding agencies manage them, they can be restrictive on curiosity-based research. A good balance between medium sized centres and funding for individual PIs is important; a lot of smaller labs get less funding – smaller universities and smaller labs do not attract the funding. Big groups beget big funding.”

RSC Science Horizons Interview
Reesearcher based in North America

“There is a further push away from curiosity-based research to everything being linked to translation and applications. Even in the applied space it is all about short term optimisation, for example, how to scale this up in two years. This approach stifles research.”

RSC Science Horizons Interview
Researcher based in North America

“There is quite a lot of short-term thinking in how funding is being spent. Very short timescales in which very specific things need to be done – fine, but it has to be underpinned by funding for core curiosity based science.”

RSC Science Horizons Interview
Researcher based in the UK

“You need to be part of big teams to get good funding – it has gone too far in this direction so there is no funding for smaller endeavours and it gets in the way of creativity as you have to adjust your research interests to be part of a big team.”

RSC Science Horizons Interview
Researcher based in Europe (excl. UK)

“In many places, good research is only judged by its relevance for applications, or by the size of the corresponding community.”

RSC Science Horizons Interview
Researcher based in Europe (excl UK)

“The science effort is not well served by the amount of funding available for blue-skies research.”

RSC Science Horizons Interview
Researcher based in the UK

“The funding environment risks becoming a barrier to discovery. The balance of funding for basic versus applied research is a concern as well as the absolute amount of funding. Funders and agencies are focused on increasingly narrow areas, but without curiosity driven research we are unlikely to get any future breakthroughs.”

RSC Science Horizons Interview
Researcher, based in Europe (excl UK)

“The government is too short term and this runs the risk of no new discoveries.”

RSC Science Horizons Interview
Researcher based in Asia.

“There is a growing gap between the ‘haves’ and ‘have nots’ – smaller labs, particularly younger scientists, have to scrape around for their budget.”

RSC Science Horizons Interview
Researcher based in Asia

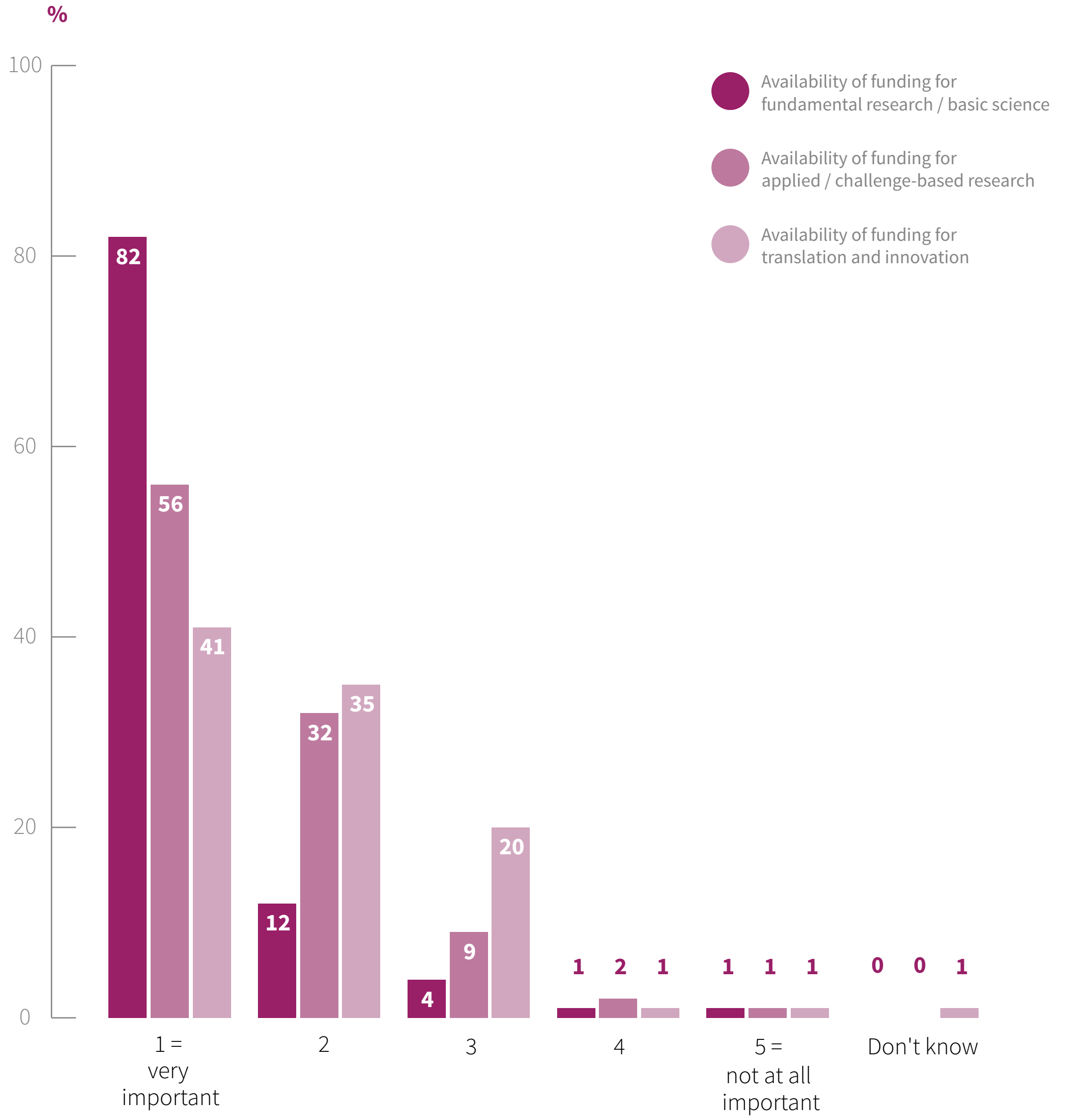
“The trend towards very application focussed funding creates too wide a gap between fundamental research and application. We must encourage approaches that focus on keeping agendas broad, to encourage curiosity while still providing a common direction.”

RSC Science Horizons Interview
Researcher based in Europe (excl UK)

A recent social science analysis of more than 65 million science and technology papers, patents and software products from 1954–2014 (Evans et al Nature, 2019) concludes that both small and large teams are essential to a flourishing ecology of science and technology.

The analysis found that smaller teams (which could include sub-teams within a larger team or centre) have tended to disrupt science and technology with new ideas and opportunities, whereas larger teams have tended to develop existing ones.

Figure 14: Researcher attitudes to the importance of different types of funding



Source: RSC Science Horizons Researcher Survey, 2018. Survey question: How important do you think the following areas will be to allowing the chemical sciences to contribute to their fullest potential over the next 5–10 years? Please score each area out of 5, where 1 = very important and 5 = not important at all, N=514.

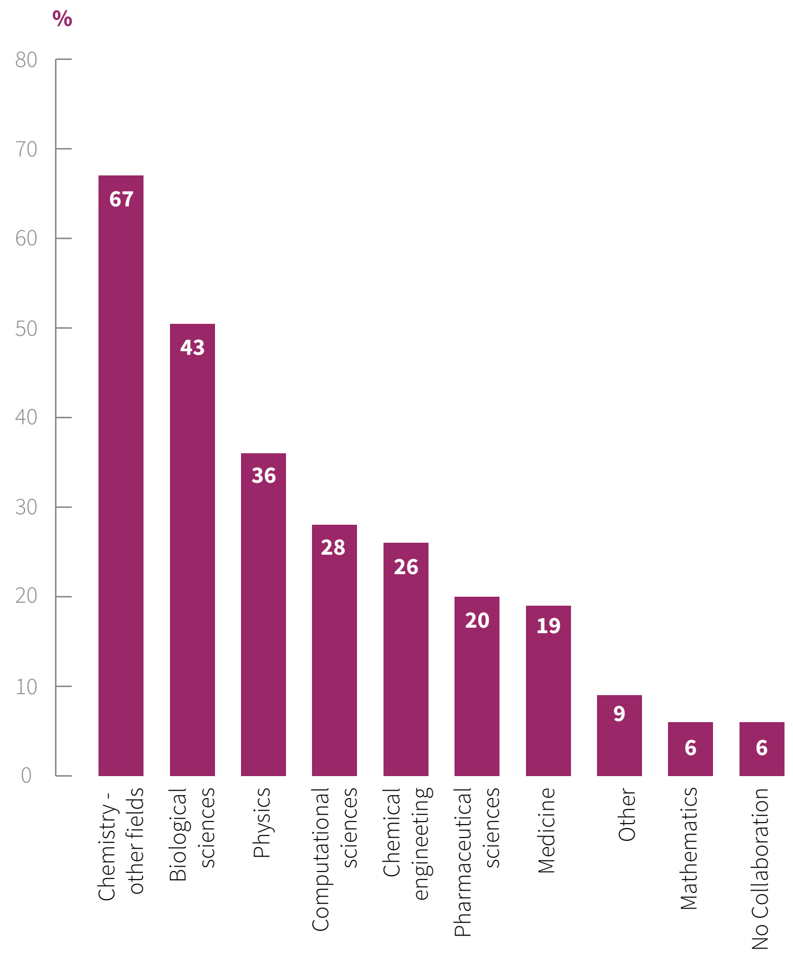
4.2 Collaboration

Collaboration was highlighted as an absolutely key enabler for advances in the chemical sciences, covering collaboration between and beyond scientific disciplines, with industry and internationally. Over 90% of the researchers we surveyed said that they had collaborated with people outside of their field in the past five years (see Figure 15). International collaborations also play an important role, with 85% of respondents having been involved in an international collaboration over the past five years. Over 80% of respondents agreed that collaborations are critical for the chemical sciences (see Figure 16).

“Really exciting science takes place where people cross disciplinary boundaries and work with industry. The way chemists along with other disciplines have used large facilities to really interrogate a problem has been revolutionary and will continue to be. It is essential to continually upgrade and invest in these facilities.”

Professor Graham Hutchings
Cardiff University

Figure 15: Collaboration with other fields of science



Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Have you collaborated with researchers / groups outside of your field of research within the past 5 years? Please tick all that apply, N=557. Note: ‘Chemistry – other fields’ counts as a field for this analysis.

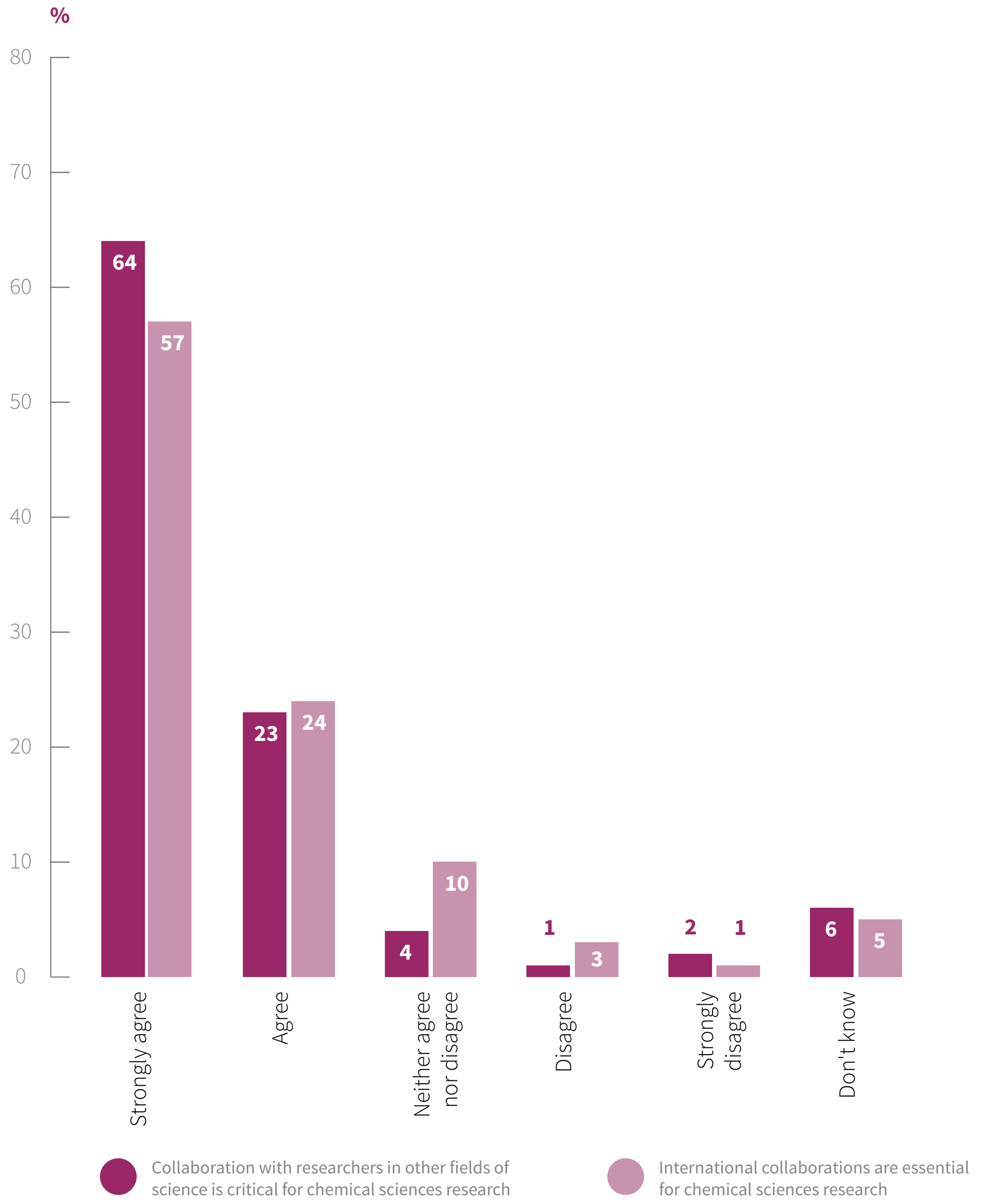
“It is of huge benefit to work with interdisciplinary groups and get new perspectives into the research, particularly if you include a researcher from a different sector such as industry.”

Professor Wolfgang Schmitt
Trinity College Dublin

“Bringing people together from different backgrounds lets you make progress really efficiently. Each discipline brings a unique insight to the problem, however it is increasingly hard to find the boundaries of what is chemistry, biology and physics.”

Dr Marina Kuimova
Imperial College London

Figure 16: Attitudes to collaboration



Source: RSC Science Horizons Researcher Survey, 2018. Survey question: To what extent do you agree / disagree with the following statements? Please tick all that apply, N=530. Note individual % are rounded to nearest whole number. important at all, N=514.

85% of researchers have collaborated with international partners in the past five years

90% of researchers have collaborated with researchers outside of their field in the past five years

2.7 is the average number of fields of science researchers have collaborated with in the past five years

Collaboration with other fields of science was seen as incredibly important:

The highly interdisciplinary nature of the chemical sciences themselves is further illustrated by how survey respondents classified their own research. When asked to classify research into twelve traditional subfields of chemistry, researchers picked on average 2.7 areas. Certain subfields are notably important for overlaps, for example materials chemistry has a particularly strong relationship with all other fields of chemistry. Fields of chemistry that co-occurred in respondents' description of their research > 50% of the time (see table X) are:

- Computational – Physical (64%)
- Environmental – Materials (54%)
- Green – Materials (64%)
- Inorganic – Materials (71%)
- Physical – Materials (61%)
- Synthetic – Materials (56%)
- Synthetic – Organic (68%)
- Theoretical – Computational (73%)
- Theoretical – Physical (73%)

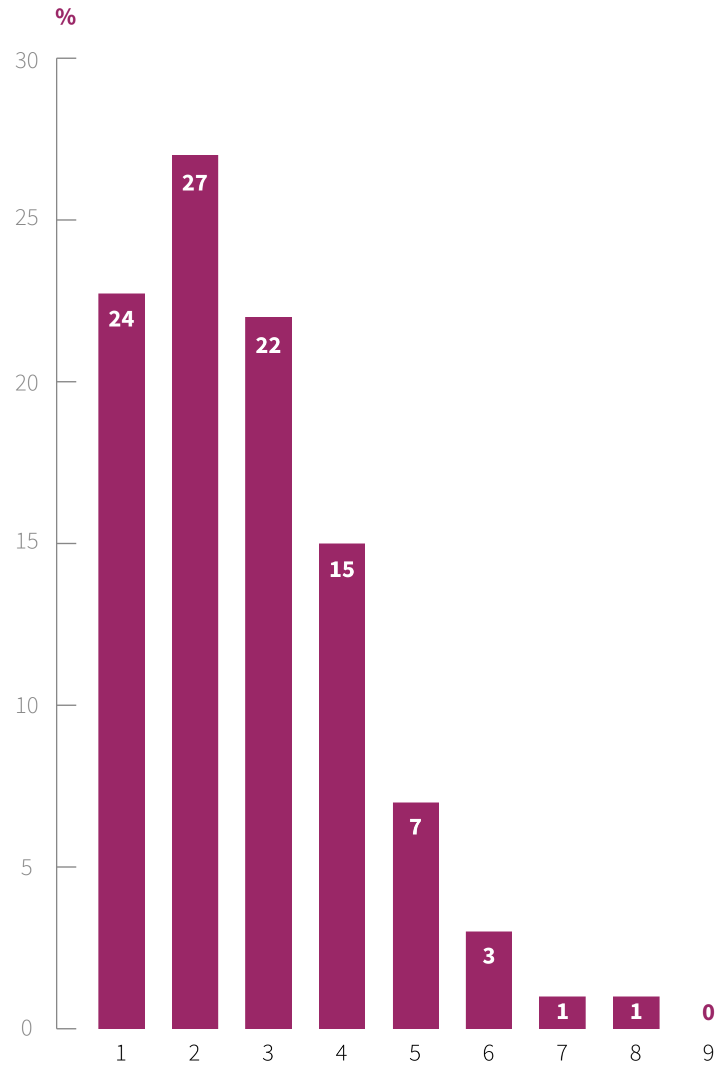
“As researchers we need to be open to new things, learning about different techniques and tools. We also need a range of mechanisms to bring researchers from different disciplines together via meetings and shared spaces.”

Professor Helen Fielding
University College London

“Many interesting fundamental questions are at the boundaries of chemistry and other disciplines. There is a lot of interesting chemistry to be done at the interfaces.”

Professor R. Scott Prosser
University of Toronto

Figure 17: Number of chemistry subfields into which respondents classified their work



Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Which of these areas does your research fit into? Please tick all that apply, N=557. For example, 27% of respondents ticked two different "chemistry sub-field" boxes.

Figure 18: Co-occurrence of chemical sciences sub-fields in researcher descriptions of their work

	Analytical chemistry	Chemical biology	Computational chemistry	Environmental chemistry	Green chemistry	Inorganic chemistry	Materials chemistry	Medicinal chemistry	Organic chemistry	Physical chemistry	Synthetic chemistry	Theoretical chemistry
Analytical chemistry	100%	23%	8%	34%	17%	20%	46%	9%	20%	40%	9%	6%
Chemical biology	31%	100%	17%	8%	12%	18%	32%	32%	30%	30%	22%	10%
Computational chemistry	13%	21%	100%	17%	17%	21%	45%	16%	21%	64%	19%	49%
Environmental chemistry	46%	7%	14%	100%	37%	26%	54%	4%	15%	43%	9%	7%
Green chemistry	20%	10%	12%	32%	100%	23%	64%	11%	38%	28%	26%	7%
Inorganic chemistry	20%	13%	12%	18%	19%	100%	71%	9%	19%	37%	27%	8%
Materials chemistry	21%	11%	12%	18%	25%	33%	100%	8%	21%	45%	18%	7%
Medicinal chemistry	18%	45%	18%	6%	18%	18%	33%	100%	56%	24%	36%	11%
Organic chemistry	19%	21%	12%	10%	30%	19%	44%	27%	100%	20%	47%	7%
Physical chemistry	25%	14%	23%	19%	15%	23%	61%	8%	13%	100%	7%	18%
Synthetic chemistry	13%	22%	15%	9%	30%	38%	56%	26%	68%	16%	100%	4%
Theoretical chemistry	16%	18%	73%	14%	16%	22%	39%	14%	20%	73%	8%	100%

Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Which of these areas does your research fit into? Please tick all that apply, N=557. NOTE: Table to be read horizontally eg 23% of people who classify their research as in 'analytical chemistry' also classified it as in the field of 'chemical biology'. See Appendix B for total number of researchers who selected each subfield.

In our survey researchers highlighted the importance of mechanisms for fostering collaboration (see Figure 19). We also heard about the challenges associated with developing effective collaborations.

From the point of view of education, it is a challenge to provide students with enough depth in the chemical sciences, while simultaneously preparing them for the collaborative, interdisciplinary world of academic research or other career paths, for example in industry.

Traditional university career paths do not typically prepare people to build collaborative, interdisciplinary teams and manage them as a research leader. Research leaders need to bring together a team with the right balance and breadth of skills. They must continually secure external funding and develop collaborations to support a long-term research programme. At the same time as team leaders they are responsible for developing and supporting the careers of people in their teams, as well as ensuring team performance and cultivating a positive, motivated culture with effective communication.

Researchers also flagged working closely with industry partners as particularly important in translating research findings towards application (see Figure 19). We heard that it can be challenging for potential academic and industry partners to find one another in the first place. Once they have found each other there can also be challenges in bridging differing expectations about timescales and levels of certainty required before starting projects.

For example, working with industry can require very tightly defined projects focussed on particular deliverables. This is a challenge if PhD students are involved because it is important for a student to have a broad scientific experience and to develop and pursue their own ideas.

We heard a sentiment that researchers need to be more flexible in the ways in which they respond to industry, but that this needs to be supported by university and funding structures. For example, academic structures need to have people with the flexibility to respond to new opportunities and not only organise in terms of typical 3-5 year PhD or 1-3 year post-doc cycles.

"It is important to enable networking between different disciplines – this is something that we should be trying to encourage – it brings very rich outcomes as you have people thinking very differently and being able to draw on the expertise from other disciplines of science. We also need to facilitate access for all to equipment from lab scale to large scale infrastructures, and to new instruments that are being developed."

Professor Catherine Cazin
Ghent University

"A really productive collaboration happens naturally; you can't engineer it. Ideally you want people who are happy at the interfaces and people who are happy at the core, so you need provision for independent funding of both areas of expertise, otherwise everything ends up too diffuse."

Professor Guy Lloyd-Jones FRS
University of Edinburgh

"The biggest challenge is getting all the disciplines to speak together and find a common language. When you have people with very different backgrounds all thinking about the same problem, it encourages and facilitates creativity. We require both interdisciplinary and also deep expertise in single areas. Quite different skillsets and ways of working."

Professor Floyd Romesberg
Scripps Research Institute

"Culturally, there has been a 'lone wolf' mentality in academia – scientists are aware that they are judged by their own ideas and results, and it can be hard to manage this in a collaboration context. Universities could do more to encourage collaboration, for example cross-disciplinary positions could be created and these positions would need to be properly supported."

Professor Tom Brown
University of Oxford

"We need to urgently start training the next generation of PhD students to have a culture of understanding across different disciplines and methods, in the way that is forward-looking, out-of-the-box and beyond the currently accepted concepts and established challenges - to enable them to drive science and innovation to the next level."

Professor Julia Weinstein
University of Sheffield

"I believe that the depth of understanding provided by traditional disciplines is needed to solve many of the big issues. Deep disciplinary knowledge has great value when working in multidisciplinary research teams who are tackling challenging questions."

Professor Vincent Rotello
University of Massachusetts Amherst

"Collaborating is not as simple as saying 'I need one chemist, one biologist etc.' To build useful interdisciplinary collaboration you really need to have a clear idea of the problem and topic you are exploring and an understanding of what skills you need to deliver the best outcomes."

Professor Gabriele Centi
University of Messina

“The word ‘interdisciplinary’ can send the notion that researchers should be very broadly trained and experienced. This is often misguidance, particularly for young scientists, who often get identified and initially hired on the basis of their expertise in a fairly specific subdiscipline – they then join a multidisciplinary team of researchers comprising experts in different, complementary fields. So collaboration is a more important aspect of education and training than interdisciplinarity. Young scientists need to be open-minded and appreciate the expertise of others – that is, it is good to be able to talk the talk with other fields, but you don’t need to have walked the walk to be an essential and productive team member.”

Professor Thomas Hoye
University of Minnesota, Twin Cities

“University structures are often built around individual achievement which can hinder collaborations. Universities have to value collaborations more, particularly for early career researchers who are trying to establish a distinctive profile through individual successes.”

Professor Tony Cass
Imperial College London

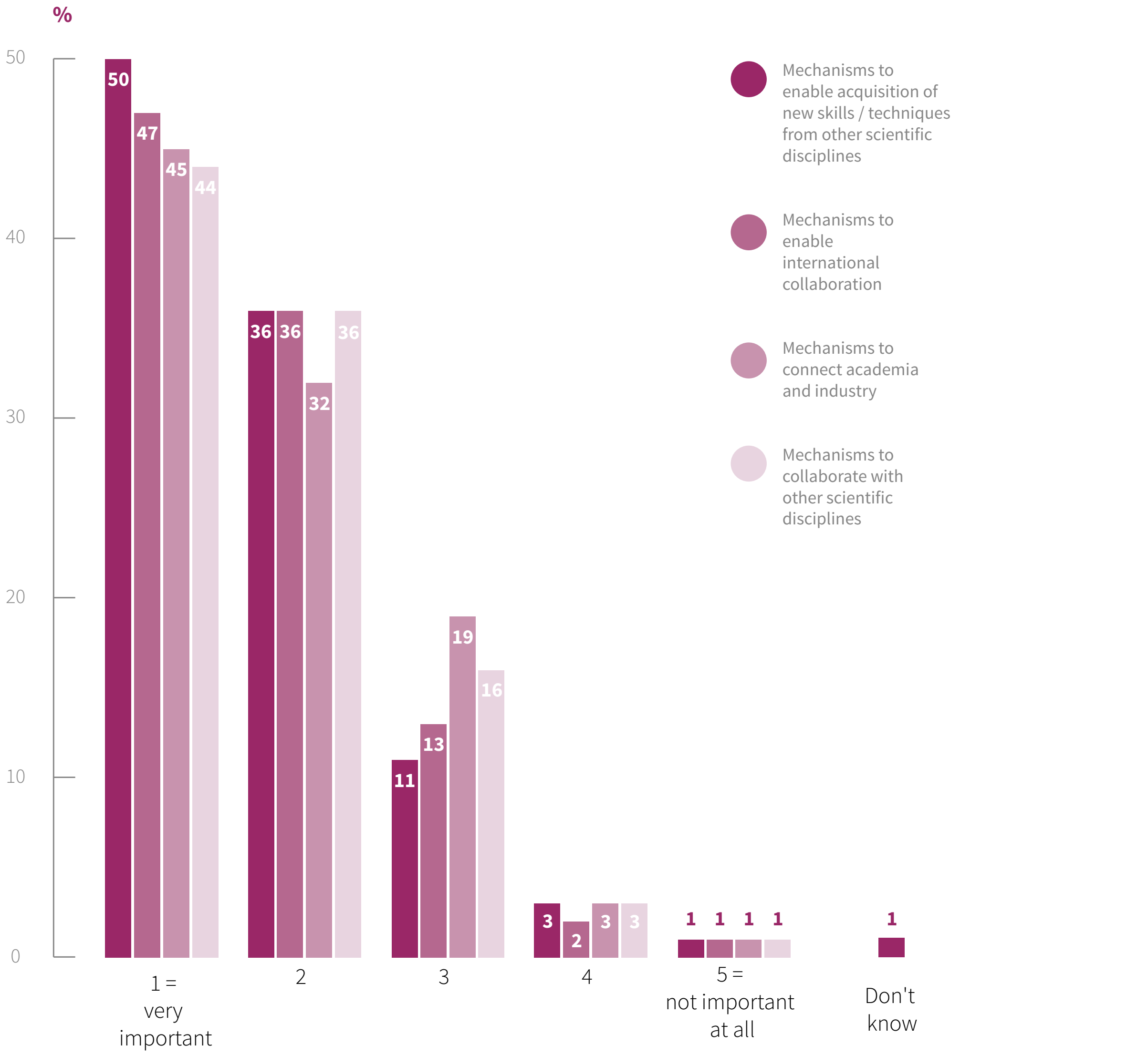
“Bringing the group together is a challenge – it is not easy to start. A lot of understanding and trust has to be built up.”

Professor Alexei Lapkin
University of Cambridge

“Discipline experts will always be needed and we should also educate people to have the skills to be able to communicate with other disciplines. For example to create new materials requires knowledge of the chemistry of the material but also some of the physics.”

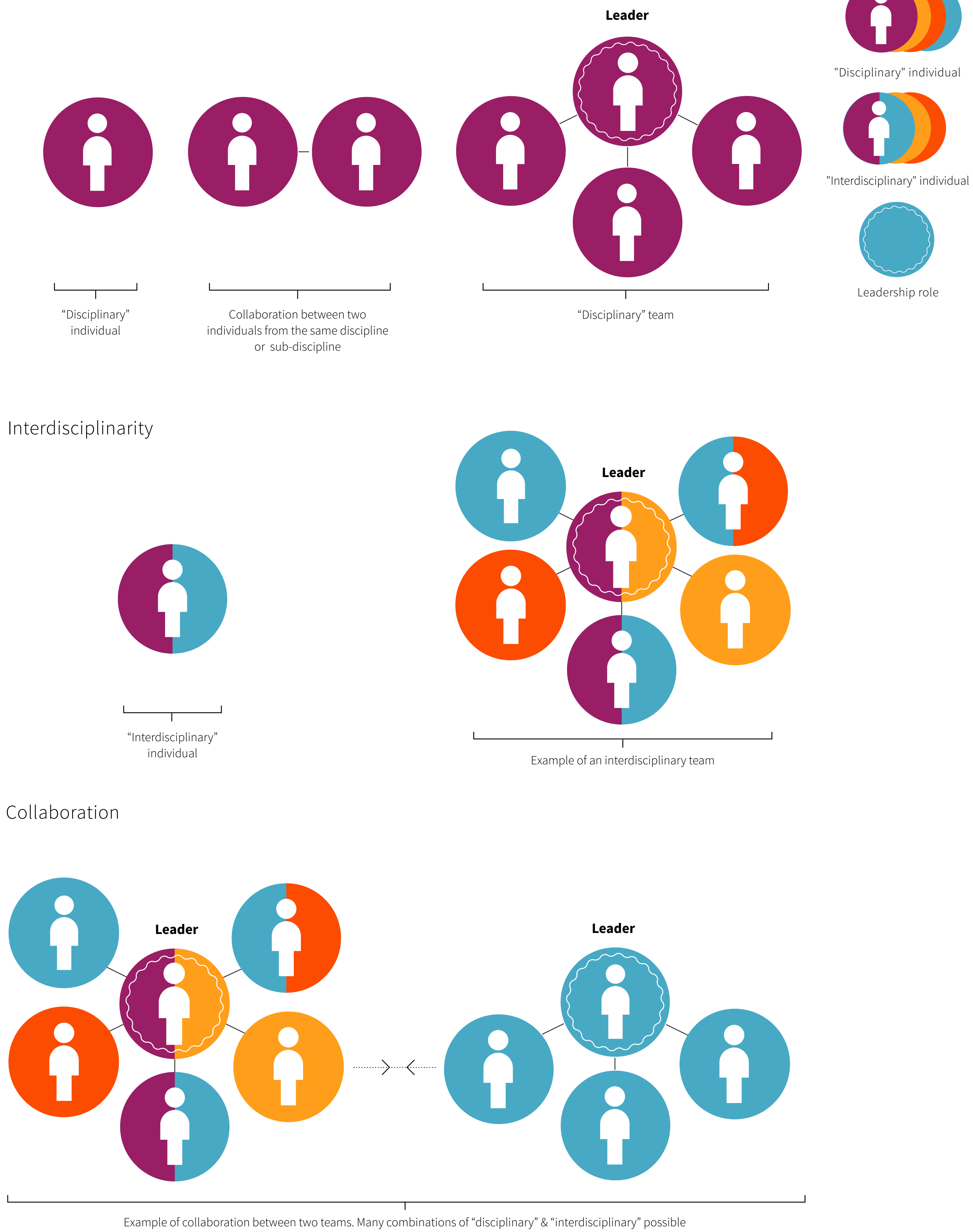
Professor Richard Winpenny
University of Manchester

Figure 19: Importance of collaboration mechanisms for science



Source: RSC Science Horizons Researcher Survey, 2018. Survey question: How important do you think the following areas will be to allowing the chemical sciences to contribute to their fullest potential over the next 5–10 years? Please score each area out of 5, where 1 = very important and 5 = not important at all, N=528:530.

Figure 26:
Individuals and teams



4.3 Leadership

The third key enabler we identified through analysis of researcher interviews and workshops is leadership. Chemistry and other sciences have a vital role to play in advancing knowledge, tackling global challenges and in innovation.

However, there was a sense amongst interviewees that the scientific community could do more to participate in shaping the research agenda and take a broader leadership role across fields in driving science forward collaboratively.

“It is important for scientists to bring their voice to shaping global issues such as climate and environmental issues. Chemists are working in an array of areas that will have applications in how we use, convert and store energy. Political backing is needed to translate this research into real change.”

Professor Silvia Bordiga
University of Turin

“Chemists are unique in that they understand science at the truly molecular level and it is important to maintain this identity, while still looking at the boundaries and where we can apply our knowledge and expertise across disciplines.”

Professor Tom Brown
University of Oxford

“It is important to have chemistry active and proactive, claiming our own space more. We shouldn’t be afraid to put our ideas and questions out there. We should be buoyant, confident and assert the unique value we bring.”

Professor Dame Carol Robinson
University of Oxford

“Curiosity is key, but it’s important that we take responsibility for ensuring potential applications of discoveries are pursued. That means being proactive, for example discussing results with colleagues in applied fields or from companies.”

Professor Andrea Schäfer
Karlsruhe Institute of Technology

“Chemistry will be part of nearly all the challenges we will face as a human race – energy, medicines, environment – what would these things look like without chemistry?”

Professor Paul Walton
University of York

“Chemists manipulate and control matter on the atomic and molecular level, for example reactions and dynamics. Working with other disciplines will enable us all to push the frontiers of fundamental understanding. Chemists have to step up and lead interdisciplinary groups and collaborations, bringing together the right teams, but doing so without losing the impact of sole principal investigator research.”

Professor Omar Yaghi
University of California, Berkeley

Figure 20 – Scientific leadership: From setting the research agenda to translating research to societal benefit

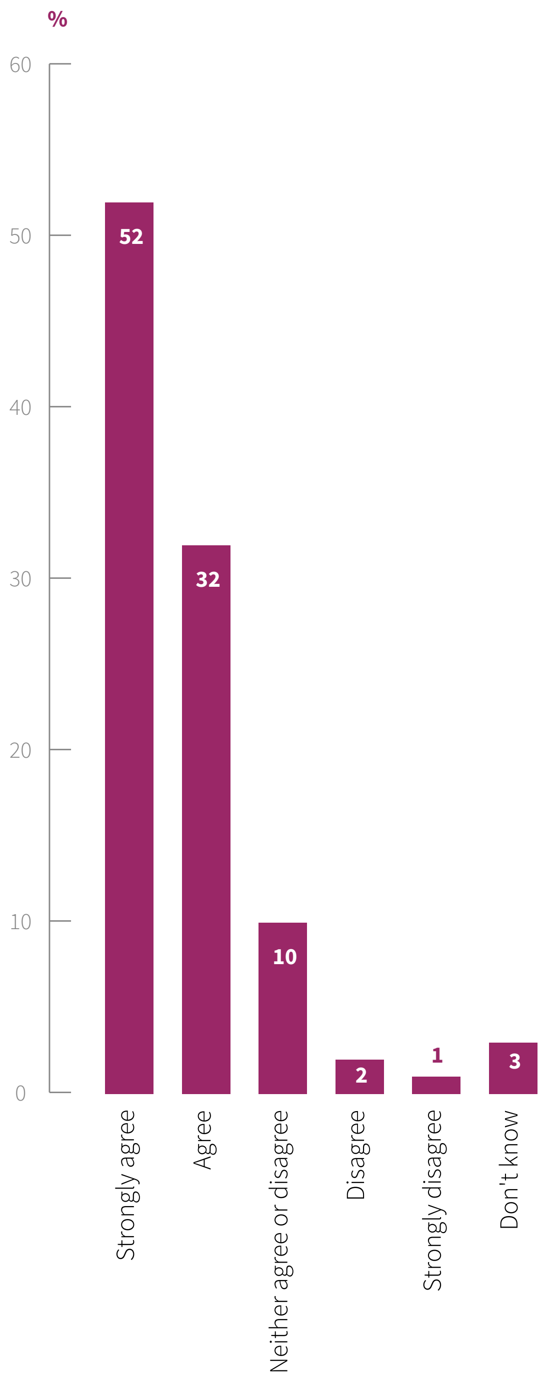
As well as taking a more prominent role inside the scientific and policy community, researchers also highlighted the importance of greater proactivity in engaging with the public.

Over 80% of researchers surveyed agreed that more needs to be done to engage the general public on the importance of the chemical sciences (see Figure 21).

> “There is opportunity for us to work with the media to highlight more the role of chemistry. Chemistry underpins our iPhones, the paints on our walls and the medicines we take – chemistry is everywhere.”
>
> **Professor Phil Baran**
> **Scripps Research Institute**

> “The real importance of chemistry in everyday life can sometimes be missed because chemistry is just about everywhere. We need to capture the public imagination about chemistry.”
>
> **Professor Greg Scholes**
> **Princeton University**

Figure 21: Attitudes to need for more to be done to engage the public on the importance of chemical sciences research



Source: RSC Science Horizons Researcher Survey, 2018. Survey question: To what extent do you agree / disagree with the following statements? More needs to be done to engage the general public on the importance of chemical sciences research. N=529.

5.

Conclusion

Chemical sciences research is key to achieving progress against the global agendas of sustainability and prosperity. This twin agenda is reflected in the move towards challenge-based research and the emphasis on R&D stimulating economic output.

In our Science Horizons project we engaged with chemical sciences researchers and found a positive, confident vision for research today and in the future. There is a sense of agency and energy among researchers – people are ambitious, breaking new research frontiers and actively engaged with other disciplines and sectors in translating their research for societal benefit.

Globally, researchers are developing cutting edge techniques and creating new knowledge and understanding about our world. Data and digital technologies are playing an ever-increasing role in scientific discovery, with the potential to accelerate and enable certain areas of science.
We found that researchers are deeply committed to delivering solutions to the urgent global challenges of our time across the spectrum from energy to environment to health.

Key themes that came through when considering how to ensure that academic research contributes to its full potential were balance and flexibility:

- Balance between funding for curiosity-driven and challenge-driven research
- Balance between funding for large research programmes and smaller groups.
- The need for highly skilled disciplinary experts and to harness interdisciplinary approaches to answering questions and delivering solutions.
- The importance of structures that support long term research endeavours and at the same time mechanisms to enable agile collaboration with industry.
- The importance of scientific research knowledge and competencies and the need for wider skills related to leadership, collaboration and engagement.
- The role of research culture in supporting individuals throughout their careers while fostering collaboration and translation.

The Science Horizons project provides a framework to inform strategy development across the Royal Society of Chemistry as we consider how to most impactfully support our community and work to advance the chemical sciences for the benefit of humanity. We will next host and share the outputs from a series of Strategic Advisory Fora in specific deep dive areas.

Appendix A

Research methodology

The project was informed by three categories of input

- Desk Research: Evidence based on existing reports, information in the public domain into global research and development (R&D) funding landscape and priorities.
- Data Sciences: Evidence based on analysis of publication trends and topics in the chemical sciences.
- Opinion: More than 880 current and future R&I leaders in academia from around the world participated in an online survey, and in interviews and workshops between August and October 2018.

In Spring 2019 we shared and tested initial themes and results with members of RSC Council, our Division Councils and Heads of Chemistry UK.

The results presented in this report are a synthesis and interpretation of evidence and views. They do not necessarily represent the view of any individual or group that participated in the project.

Desk research

We conducted an extensive programme of desk research into the global research and development (R&D) funding landscape, covering the USA, European Union, United Kingdom, India, Japan, China and South Korea. Areas of focus included government funding and priorities, trends in business / industry funding and key international development agendas.

Table A1: Major international development agendas

Organisation	UN	World Economic Forum (WEF)	World Business Council for Sustainable Development (WBCSD)
Programme	Sustainable Development Goals (SDGs)	System Initiatives	Work Programs
Background	On 1 January 2016, the 17 Sustainable Development Goals of the 2030 Agenda for Sustainable Development adopted by world leaders in September 2015 at an historic UN Summit – officially came into force. Over the next fifteen years, all countries will mobilise efforts to end all forms of poverty, fight inequalities and tackle climate change, while ensuring that no one is left behind.	The global, regional and industry challenges facing the world are the result of many "systems" – from global systems that influence the environment and natural resource security, to the economic systems that create inequality, to the regional systems that determine the fortunes of nations, to the industry systems that determine the effectiveness of supply and demand. To enable constituents to make sustained positive change, the WEF works with them to understand and influence the entirety of the system that affects the challenges and opportunities they are trying to address via systems initiatives.	As global business faces new and complex challenges and opportunities, the WBCSD's science-based approach and targeted business solutions aim to scale up business impact. They target the realisation of the Sustainable Development Goals (SDGs) through six work programs to achieve systems transformation.

Table A2: Major international development agendas continued

Organisation	UN	World Economic Forum (WEF)	World Business Council for Sustainable Development (WBCSD)
Themes	No Poverty	Consumption	Circular Economy
	Zero Hunger	Digital Economy & Society	Cities & Mobility
	Good Health & Well-being	Economic Progress	Climate & Energy
	Quality Education	Education, Gender & Work	Food, Land & Water
	Gender Equality	Energy	People
	Clean Water & Sanitation	Environment and Natural Resource Security	Redefining Value
	Affordable and Clean Energy	International Trade and Investment	
	Decent Work & Economic Growth	Food	
	Industry, Innovation & Infrastructure	Health & Healthcare	
	Reduced Inequalities		
	Sustainable Cites and Communities		
	Responsible Production & Consumption	Media, Entertainment and Information	
	Climate Action	International Trade & Investment	
	Life Below Water	Long-Term Investing, Infrastructure & Development	
	Life on Land	Mobility	
	Peace, Justice & Strong Institutions	Advanced Manufacturing and Production	
	Partnerships for the Goals		

Source: Agency websites

Mapping to RSC Science Horizons project categories

- Economic Growth
- Food & Water
- Human Health
- Energy
- Environment
- Urban Living

Note: Mapping is approximate and in some cases, themes could be mapped into more than one category.

Online survey

In October 2018, 557 chemical scientists responded to an invitation to participate in our online survey which comprised a series of closed and open-ended questions. The profile of survey respondents was as follows.

Figure A1: Type of employment

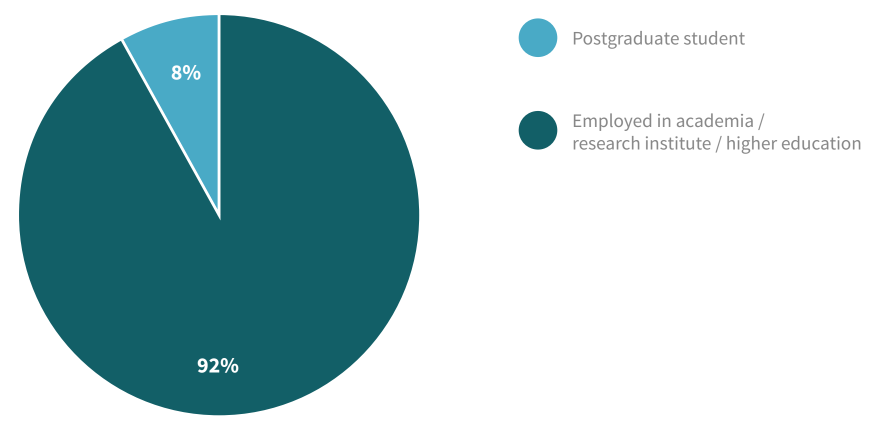


Figure A2: Level of education

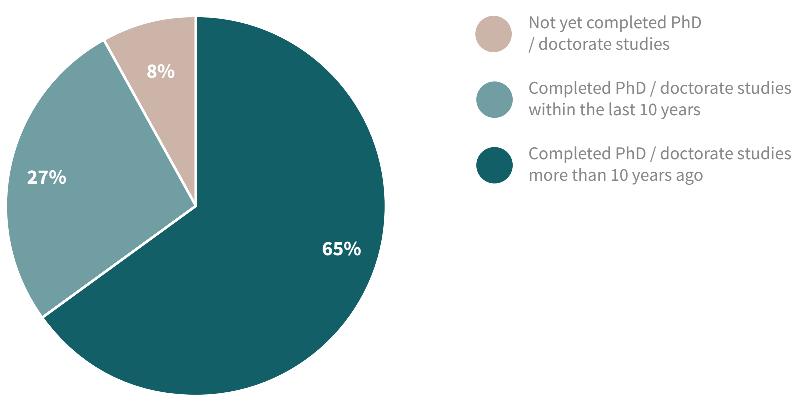


Figure A3: Current role

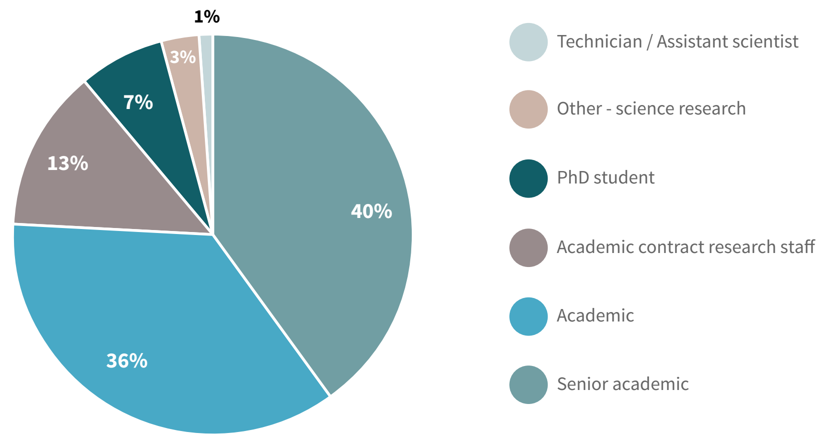


Figure A4: Region of the world

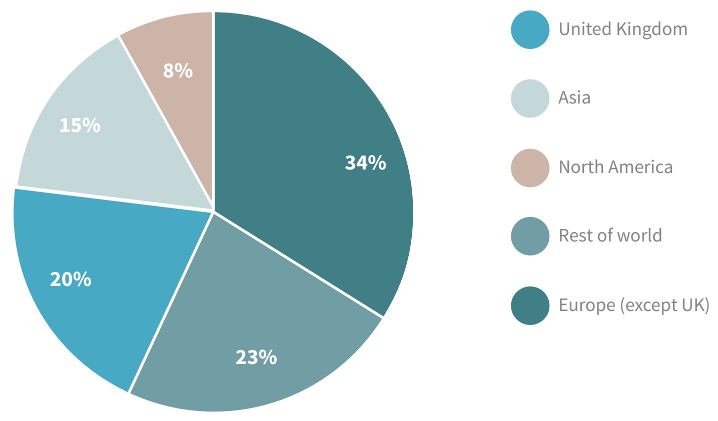


Table A3: Area(s) of research (noting that respondents could choose more than one area)

	Number of survey respondents
Materials chemistry	283
Physical chemistry	208
Organic chemistry	135
Inorganic chemistry	130
Analytical chemistry	127
Green chemistry	109
Environmental chemistry	94
Chemical biology	93
Synthetic chemistry	93
Computational chemistry	75
Medicinal chemistry	66
Theoretical chemistry	51
Other	52

Interviews

We interviewed 81 chemical sciences researchers in Autumn 2018. Each interview lasted 30-90 minutes and focused on the key scientific advances in the interviewees' research area, the enablers and blockers for these advances and the evolution of chemical sciences and its boundaries. The profile of interviewees was:

Figure A5: Interviewee regions

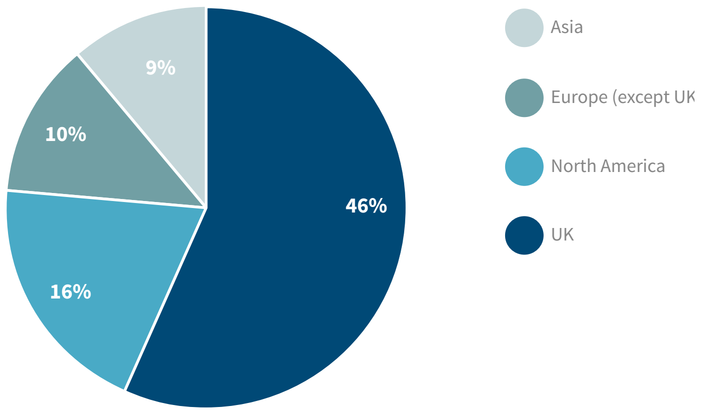
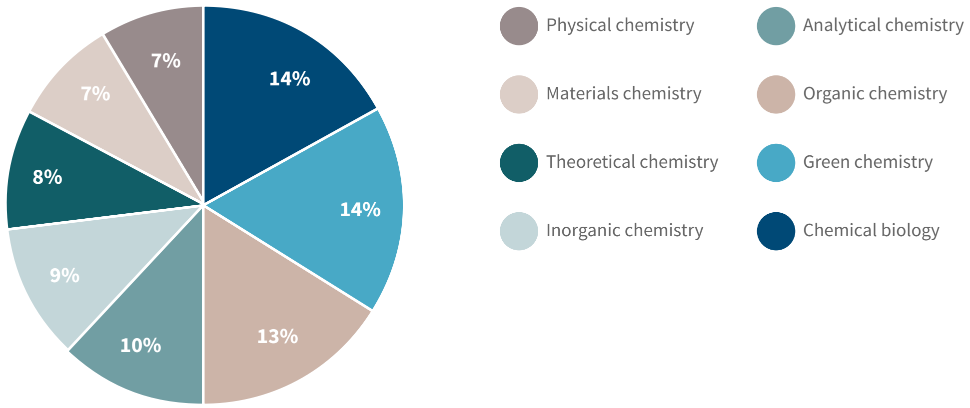


Figure A6: Interviewees' main research area (classified by interviewers)

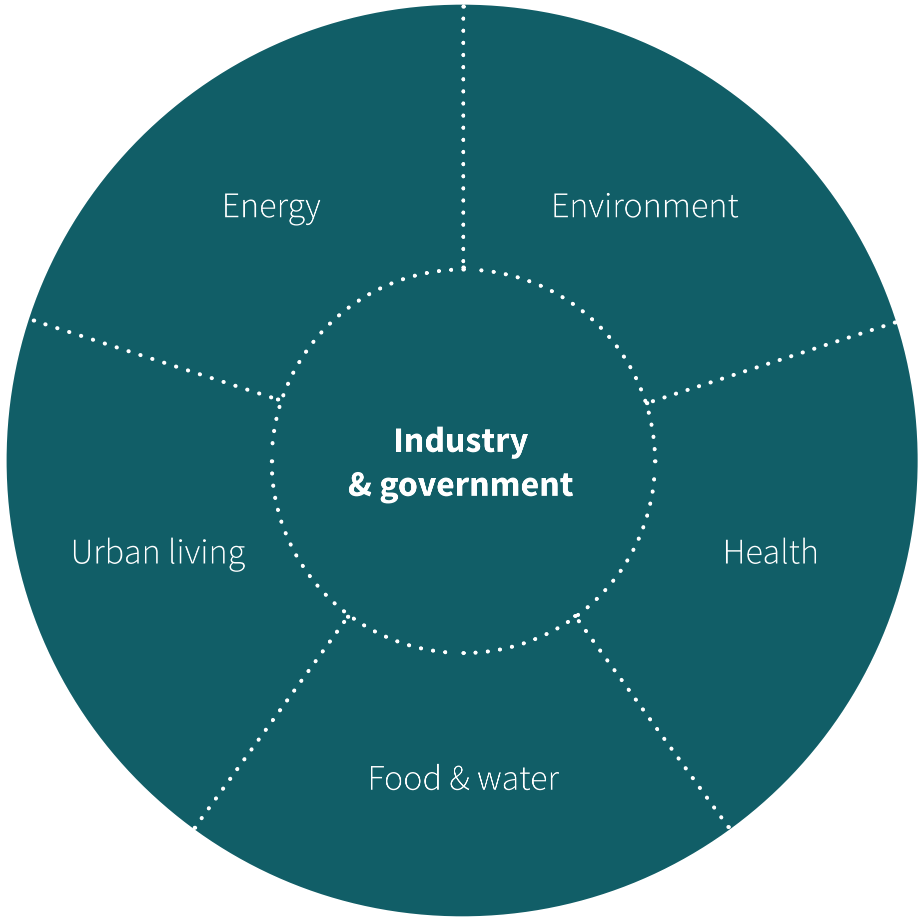


In October 2018 we ran workshops with seven of our Division Councils: Analytical Division, Chemistry Biology Interface Division, Dalton Division, Environment, Sustainability & Energy Division, Faraday Division, Materials Chemistry Division, and Organic Division. 92 researchers participated across the seven workshops. Workshops focused on the key scientific advances in each Division Council's field of the chemical sciences as well as enablers and blockers for these advances.

We conducted two workshops at the RSC Member Networks Conference in October 2018, comprising approximately 150 participants from RSC Interest Groups and Geographical Networks. The workshops consisted of an introductory presentation followed by discussions in roundtables where members gave their views on the advances in chemical sciences research that most excited them, their likely impacts and enablers and dependencies.

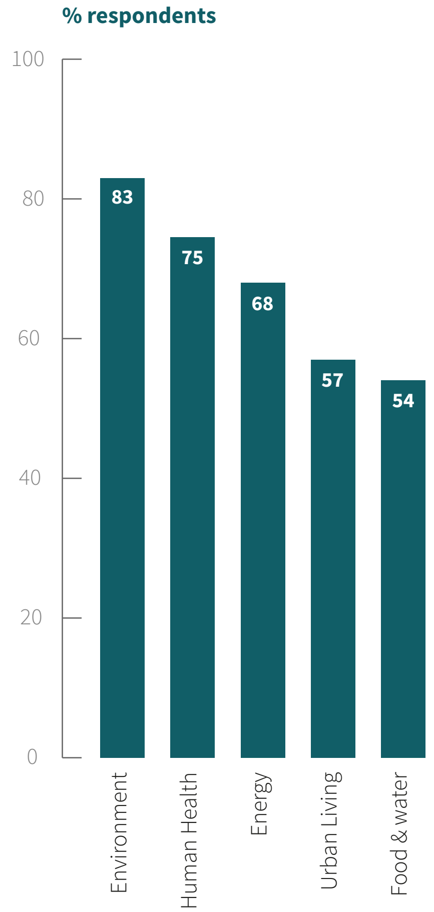
Appendix B

Solutions to global & industry challenges: specific research examples



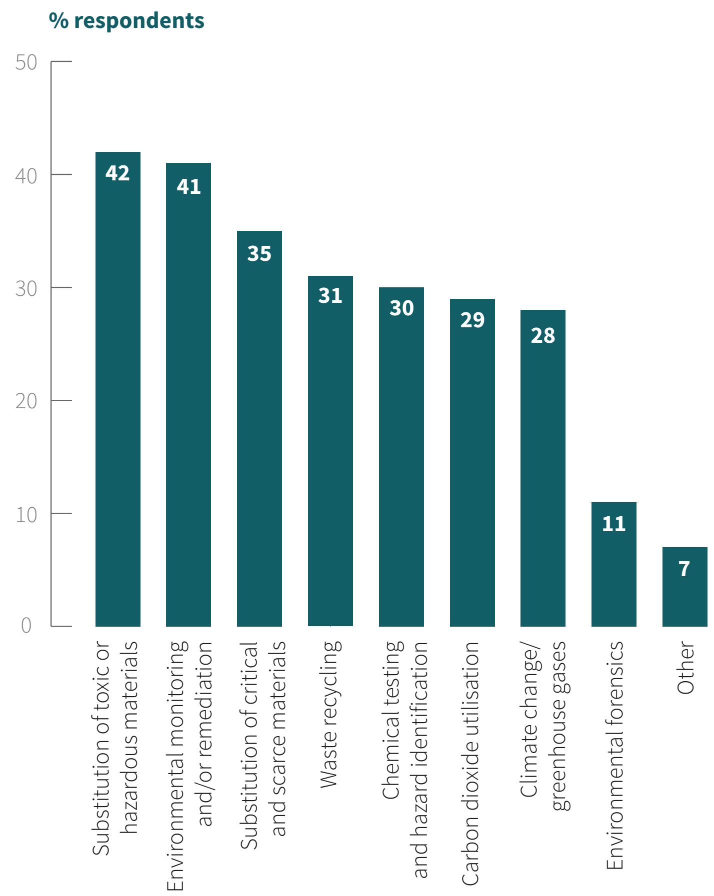
In our survey we asked people about potential applications of their research in global challenge areas. Within each global challenge area we then asked people to select more specific applications. In all cases people could select more than one option. A person doing research on a specific measurement technique, with potential applications as a tool for diagnosing multiple types of disease would likely select almost all of the options in the Human Health category. Similarly people working in certain areas of research in materials, catalysis or electrochemistry might select multiple options for applications of their research in Energy.

Figure B1: Areas of application for research



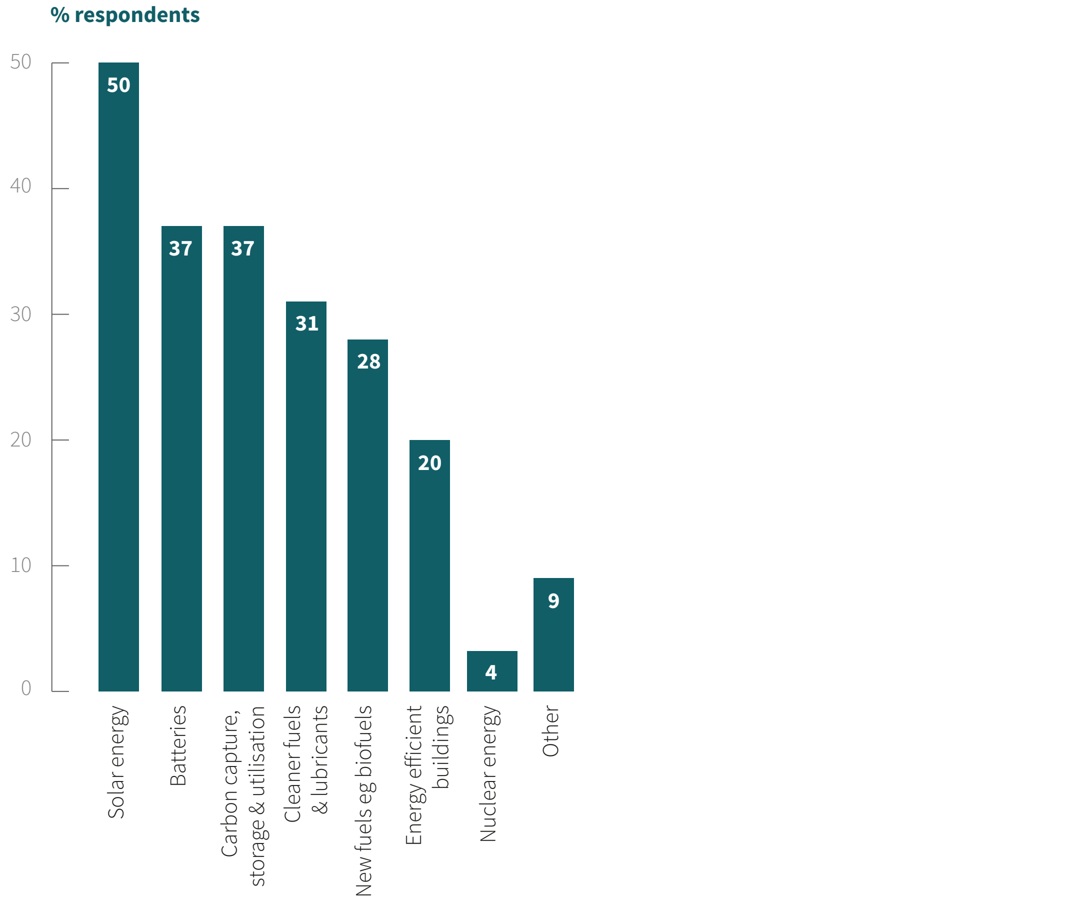
Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Does your research have potential application in any of these <X> areas [X= Environment, Human Health, Energy, Urban Living, Food & Water]? Please tick all that apply. N=549:554

Figure B2: Areas of application for environmental research



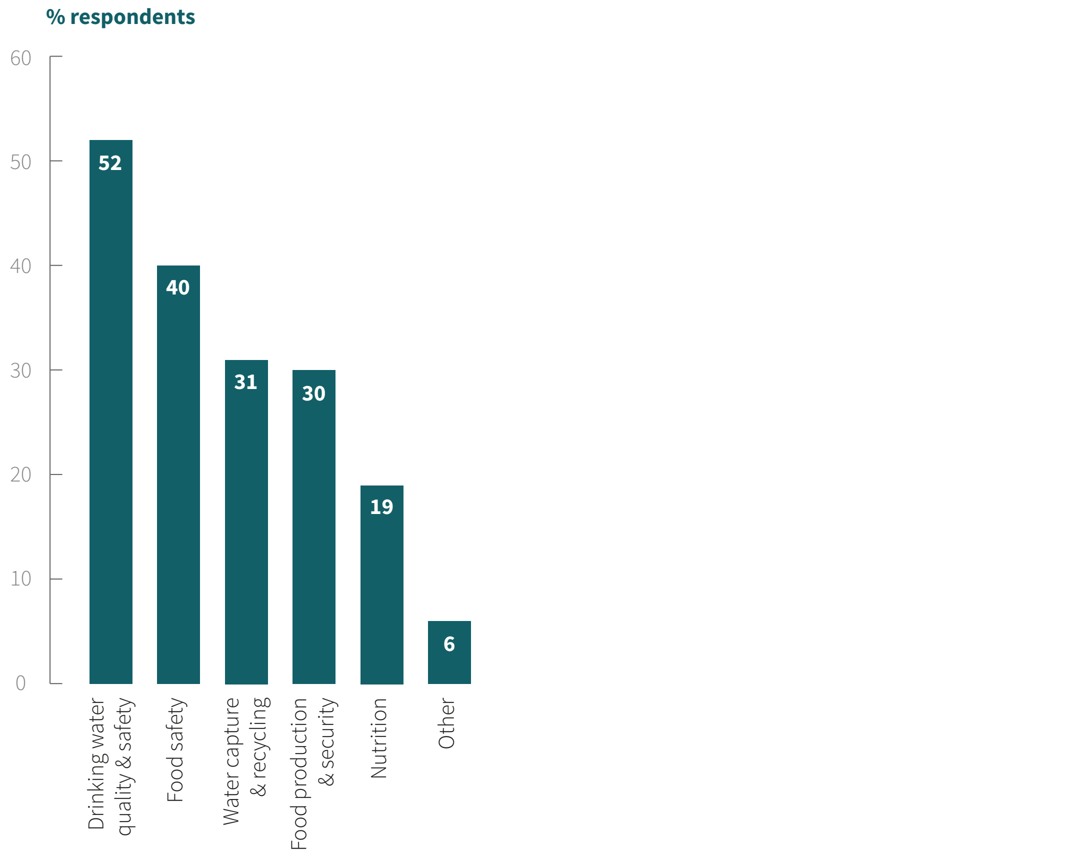
Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Does your research have potential application in any of these Environmental areas? Please tick all that apply. N=549

Figure B3:
Areas of application for energy research



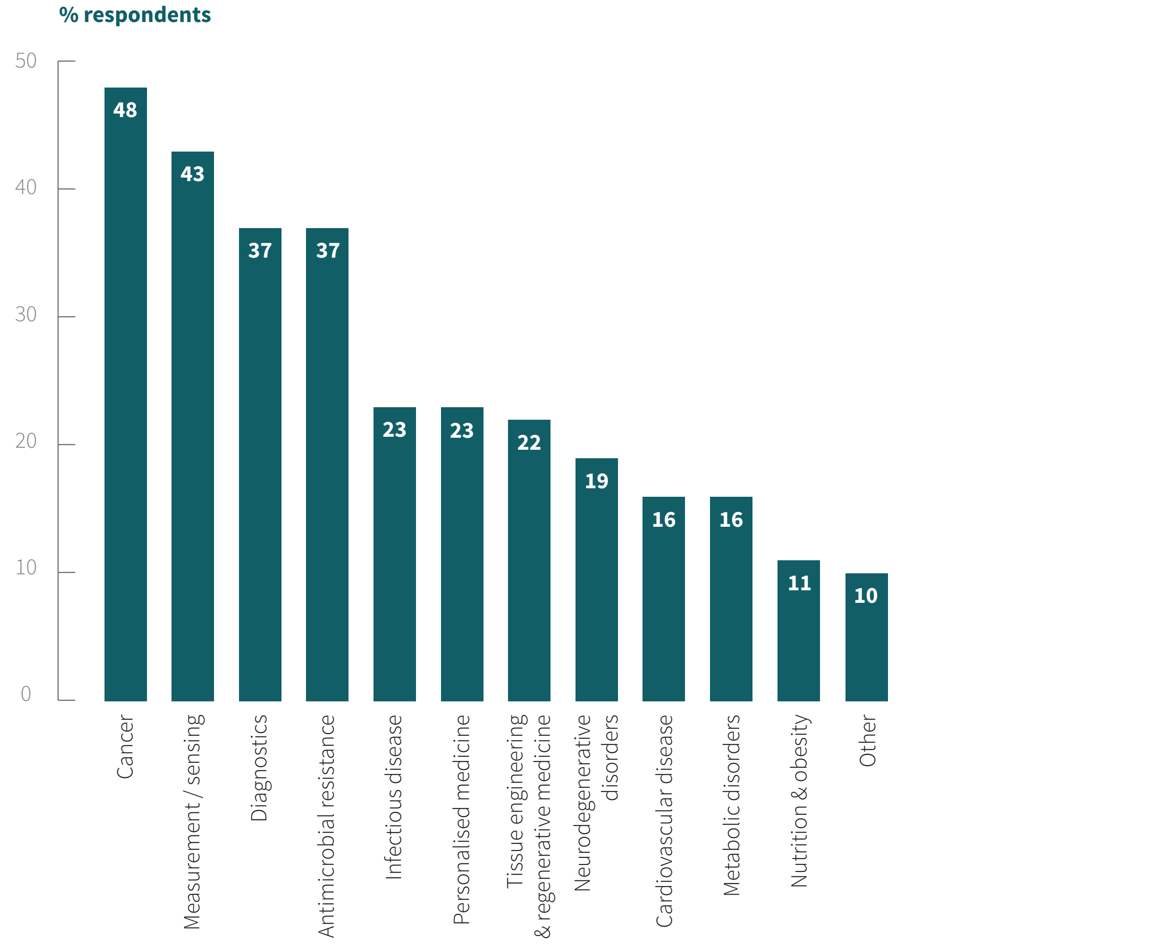
Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Does your research have potential application in any of these Energy areas? Please tick all that apply. N=553

Figure B4:
Areas of application for food & water research



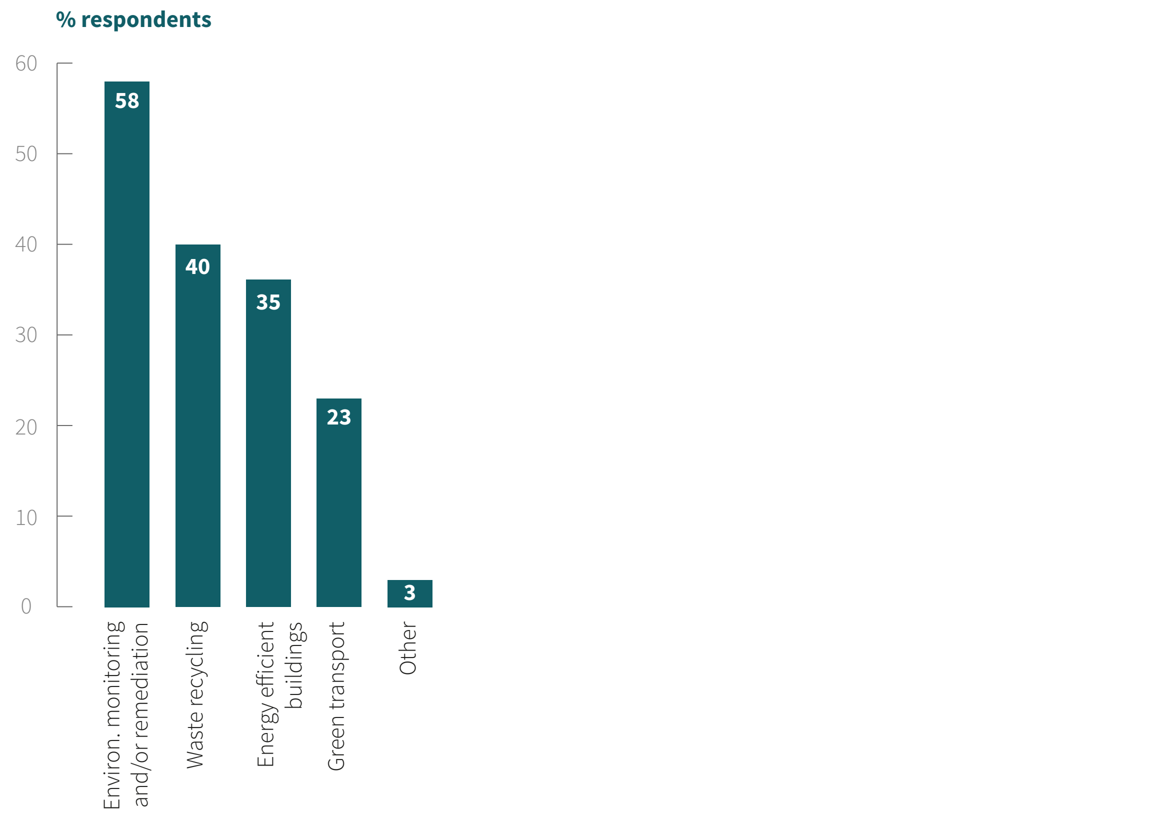
Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Does your research have potential application in any of these Food & water areas? Please tick all that apply. N=554

Figure B5:
Areas of application for human health research



Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Does your research have potential application in any of these Human Health areas? Please tick all that apply. N=554

Figure B6:
Areas of application for urban living research



Source: RSC Science Horizons Researcher Survey, 2018. Survey question: Does your research have potential application in any of these Urban living areas? Please tick all that apply. N=553

Interviews and workshops: examples of research advances in global challenge areas

The following are examples we heard from researchers in interviews and workshops when we asked about where they expect advances from chemical sciences research in the next 5-10 years. Examples vary in their level of specificity and some are relevant to more than one challenge area. As with the survey, some are also relevant to the sections on leading-edge questions and/or frontier techniques. By their nature they are illustrative and do not provide comprehensive coverage of all chemical sciences research.

Table B1: Energy

ENERGY	
Example topic	**Specific research examples**
Photovoltaics / solar energy	Developments in photovoltaics, eg building integrated photovoltaics and devices for indoor applications. One challenge is to develop light-weight, flexible materials with earth-abundant elements that can withstand real in-field conditions eg low temperatures for long periods. This requires fundamental research in areas like: exciton fission; development of new materials such as organics, perovskites, crystalline materials; system integration and methods to manufacture these devices.
Artificial photosynthesis	Developing artificial photosynthetic processes using catalysts to generate clean energy sources. This will involve fundamental advances in our understanding of catalysis and the materials that can support artificial photosynthetic reactions on a useable scale.
Chemical energy storage	Developing approaches to convert abundant electrical energy into chemical energy. Due to the revolution in natural gas extraction and also renewable energy, there is increased availability of 'cheap' electricity which can be harnessed to store energy in C-C, C-H, or C-N bonds and drive chemical reactions. A lot of work is done here but there is much more to do, to develop our understanding of how to produce energy carriers from low cost electricity sources.
Battery technologies	Developing improvements and alternatives to Li-based battery technology, eg lithium air batteries or alternatives such as sodium or magnesium are emerging technologies that need developments in electrochemistry, materials chemistry and other areas of research to reach the economies of scale for mass roll-out. Some of the key challenges are around improving energy storage density, speed of charging, cost and safety. A starting point is to use very advanced computer modelling techniques to understand structure/property relationships, eg how lithium ions move within these materials.
	Developing new methods for energy storage in wearable technologies. For example, fundamental advances in materials will contribute to the creation of more flexible, safer, smaller and environmentally friendly battery technologies.
	Advances in flow battery technologies for grid storage applications.
Metal-organic framework materials for energy	Translating porous materials such as metal-organic frameworks (MOFs) from lab-based applications to industrial-scale utilisation for energy capture, storage and conversion. Making the technology scalable and effective for commercial use is very challenging, for example creating pellets of materials for use in reactors).
Biomass fuels and feedstock	Development of biomass as a practical and scalable sustainable feedstock, eg developing selective and robust catalysts that can deal with inputs other than petrochemicals. This will involve advances in a number of areas such as enzyme chemistry and practical engineering to ensure scalability. The synthetic chemistry problem boils down to a few key chemical reactions that we still don't know how to do effectively – we need to work out how to carry out these reactions without using vast amounts of energy or solvent reagents some of which are toxic.

Table B2: Environment, Food & water and Urban living

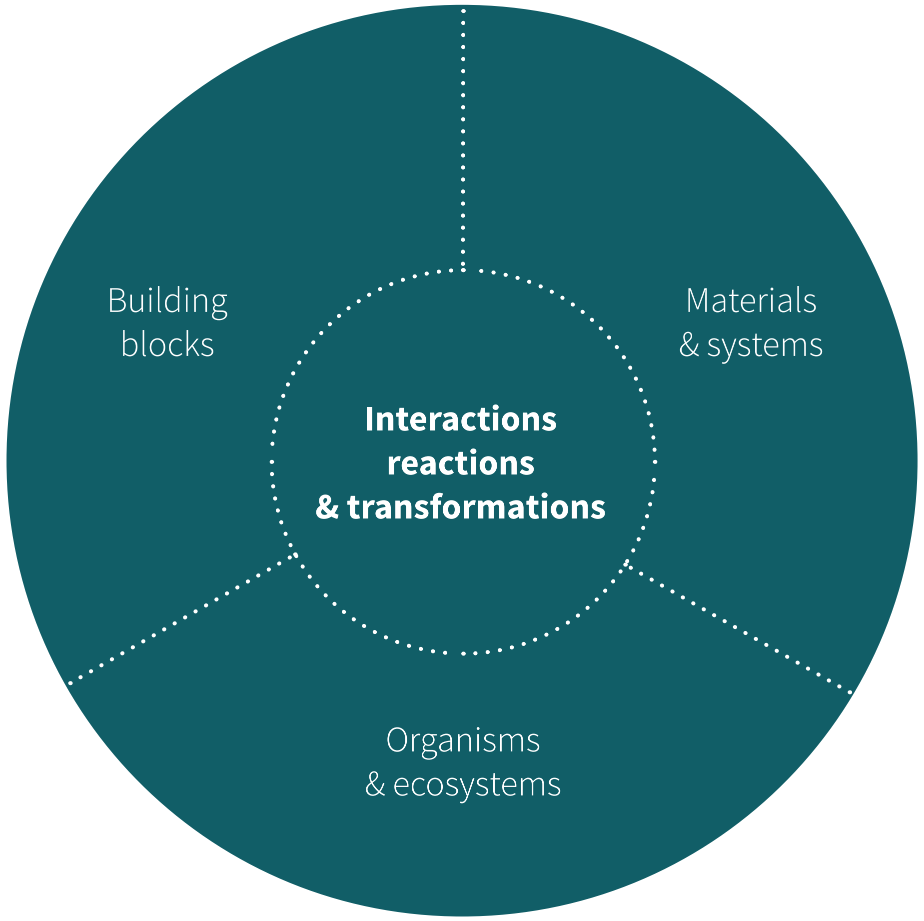
ENVIRONMENT, FOOD & WATER AND URBAN LIVING	
Example topic	**Specific research examples**
Circular economy	Developing new, low toxicity approaches to recycling commonly-used plastics that incentivise the economics of reclamation eg discovering enzymes that can carry out specific triggered degradations using metagenomic techniques.
	Advancing biological waste recovery – includes developments in areas such as catalysis and chemical applications of waste products or derivatives.
	Developing new polymer recycling processes as part of a 'circular economy' approach to manufacturing, eg a key goal would be the depolymerisation of polyethylene terephthalate (PET). Another area for development is catalysis – how can we transform plastics into products we want, for example to generate materials with higher value, longer lifetime, different uses?
CO_2 utilisation	Developing methods to capture and recycle CO_2 effectively into useful molecules and compounds. This will draw on developments in multiple areas to generate new catalysts and materials. The aim would be processes that are efficient at a modular or local level so devices can run at the site where CO_2 is being harvested, rather than at the scale of traditional chemical plants (requiring eg high temperature and pressure, multiple stages in production). Developments are needed in numerous areas, for example to produce porous materials for selective CO_2 absorption, sequestration and release eg MOFs, zeolites, oxides.
Nitrogen utilisation	Development of catalysts and systems for effective nitrogen fixation at room temperature and pressure from renewable sources, as alternatives to the Haber-Bosch process. This is important because nitrogen is an essential element in fertilisers.
Adaptive building materials	Development of new coating technologies that can change and augment as a function of the environment, eg materials that adjust the energy requirements of a building according to environmental cues.
Food production	Development of new natural preservatives and stabilisers.
Water purification	Advances at the interface of analytical chemistry and chemical engineering to develop new separation techniques with improved selectivity and affordability. This will have multiple applications from improving existing separations eg citric acid extraction, to advancing water purification eg separation of synthetic oestrogens, ephedrine, or pollutants.
	Development of technologies to enable the removal of perfluorinated chemicals from sources of water. One challenge is to find processes that break the very strong carbon-fluorine bond.
	Development of catalytic alternatives to chlorination for water purification.

Table B3: Human health

HUMAN HEALTH	
Example topic	**Specific research examples**
Diagnostics	Advances in disease diagnosis, including identification of new biological markers and the application of technologies such as mass spectrometry and electrochemical analysis.
Drug design / discovery	Using new materials to deliver therapeutic molecules to different parts of the body.
	Development of new vaccines and related technologies eg encapsulated vaccines for improved stability and bio-availability, vaccines for malaria or new approaches to control vector borne diseases for example by sterilising mosquitos
	Applying our understanding of organic synthesis to improve design of molecules for medicine eg using digital technologies such as AI to predict metabolites and optimise drug metabolism and pharmacokinetics, developing new molecules that target difficult to reach areas of the body such as the brain, understanding disease mechanisms such as target versus off-target effects.
	Applications of MOFs in drug delivery, particularly cancer research. One research direction includes the use of molecular simulation and computational methods, eg using artificial intelligence / machine learning methods to find materials suitable for applications.
	Development of new antibiotics and advances in our understanding of drivers of resistance eg advances in bio-processing capabilities for large-scale natural product screening, advances in analytical chemistry for molecular-level analysis and characterisation.
	Continued advances in our ability to treat genetic disorders with targeted genetic interventions using our understanding of nucleic acid chemistry, eg targeted gene editing, nucleo-base modification and therapeutic oligonucleotides.
Advanced materials	Using materials like hydrogels as scaffolds for tissue regeneration to tackle conditions such as fistula.
	Development of bio-inspired materials for a broad range of medical applications, including effective drug delivery and wound healing.
Nutrition	Development of nutraceuticals (medicinally or nutritionally functional foods), which involves advancing our understanding of drug metabolism.
Personalised medicine	Personalised medicine/treatment requires the ability to measure the markers of disease at an individual level and develop therapies accordingly. This will involve developments in high precision and continuous measurement/monitoring, and chemists working with other disciplines is required to develop the sensors from research demonstration all the way through to cost-effective manufacture and deployment.
Synthetic biology	Development of smart molecules and systems that interface autonomously with living systems to drive positive health outcomes, eg reversible molecular switches that inform on the presence/absence of bacteria or toxic substances in living systems; artificial vision systems that can plug into the human brain or the introduction of new catalytic functions into human cells.

Appendix C

Leading-edge questions: specific research examples



The following are examples we heard from researchers in interviews and workshops when we asked about where they expect advances from chemical sciences research in the next 5-10 years. Examples vary in their level of specificity and some are also relevant to the sections on global & industry challenges and/or frontier techniques. They are by their nature illustrative and do not provide comprehensive coverage of all chemical sciences research.

Table C1: Building blocks

BUILDING BLOCKS	
Example topic	**Specific research examples**
Single molecule chemistry	Advances in analytical, computational and synthetic chemistry are coming together to enable us to have new levels of control of the study, manipulation and design at the individual atomic and single molecule level. Within analytical chemistry, advances in micro/nano-fluidic technologies and in spectrometry are very important for this field.
Main group chemistry	Systematic synthesis of compounds of main group elements to develop fundamental understanding of the properties of different elements and to develop compounds with novel applications, such as warm-white-light emitters driven by cheap, low-power continuous-wave infrared laser diodes; alternative metal compounds for use in batteries or development of new catalysts. This research also opens up unavailable bonding modes or unexpected structural features.
Carbohydrate chemistry	Employing organic synthesis alongside computational techniques to develop a fundamental understanding of synthetic carbohydrate formation asking questions such as how HCOH may be able to act as an initiator and chain carrier for sugar formation and how this occurs in environments such as space.
Quantum effects	Advancing our fundamental understanding of magnetic spin in materials and molecules, and how to control it. This will have important applications in electronics - from understanding and controlling spin at the level of single crystals to developing devices for energy generation or data storage.
Protein dynamics & structure	Advancing our understanding of the dynamics of protein structures using bioinformatics approaches to study the existing high resolution structural data and make predictions about new structures. This will allow us to further explore protein chemistry – not just thinking about relationships between structure and function but rather thinking of proteins as an ensemble of soft states, where different structural states facilitate different functions and roles in a protein. Using tools such as NMR can observe transient and excited states. This increased understanding has potential applications in fields such as medicinal chemistry, which relies on understanding of a protein in all of its receptive states to inform drug design. For example a third of all drugs today target G protein-coupled receptors (GPCRs) which have multiple states and structures. Using computational techniques it is possible to perform simple docking experiments of 10 million compounds over the course of a day to come up with new lead compounds.
	Protein cages are useful 'containers' for diverse cargo molecules such as proteins and metal nanoparticles and can serve as delivery vehicles, bio-imaging agents, reaction vessels and templates for controlled synthesis of novel materials. Strategies for designing and optimising these protein cages can draw on directed evolution techniques.
Ligand design	Many advances in organometallic and coordination chemistry depend on the design and synthesis of ligands to control molecular stability, structure or reactivity. Examples of the role of ligand design in advancing chemistry include the stabilisation of low-coordinate f-block elements as single molecule magnets, or the design of ligands which can accelerate C-H bond activation reactions.
Genomics & biological function	Using biophysical techniques to develop our understanding of the genetic alphabet with the goal of being able to build entirely synthetic systems to effect change in living organisms. For example using antibodies as a model system to understand the fundamentals of molecular recognition.
	Systematic structural and biochemical analyses of chromatin associated factors to reveal key features of selectivity and regulation among these factors. This will enable structure-based development of potent, selective, cell-active small molecule inhibitors of individual epigenetic regulatory proteins. The use of these chemical probes is highly complementary to genetic methods but more closely mimic strategies for therapeutic translation.
Lipid chemistry	Developing our fundamental understanding of lipid chemistry by using small tags and mass spectrometry to track their functions.

Table C2: Materials & systems

MATERIALS & SYSTEMS	
Example topic	**Specific research examples**
Intelligent polymer chemistry	Advancing our understanding of how mechanical and ionic forces trigger chemical reactions, in order to develop advanced 'autonomous' materials. With this knowledge, we could begin to design materials that respond to external stimuli to self-repair which could have applications to extend battery life or self-repairing coatings. For example, inspired by plant vascularisation developing materials with internal vascular systems to deliver catalysts intelligently to the area of need.
Bio-inspired materials	Understanding how nature facilitates CO_2 capture from first principles, for example within photosystem II during photosynthesis, to develop materials such as bio-inspired porous metal-organic frameworks with massive surface areas to harvest light energy.
	Development of new synthetic polymer biomaterials that mimic antifreeze proteins that are found in nature, which could be used to replace organic solvents like DMSO which has supercooling properties and applications in chemistry and biology research.
Molecular machines	Advances in development of molecular machines to allow mechanical coupling within dynamic polymer systems in order to amplify individual motions to achieve macroscopic functions in materials.
Advanced materials	Advancing our understanding of hexagonal boron nitride (h-BN), a layered material with a regular network of BN hexagons. This material has similar properties to graphite, but has been shown to be more thermally and chemically stable. Approaches for high yield synthesis of BN nanotubes and nanosheets are required to allow its development and potential application.
	Recent advances have used polymer matrices to make thermally conductive composites, increasing the original thermal conductivity by as much as 20 times. These polymers are useful for example to produce heat-release insulating packaging for use in cooling of electronic components. Applying these synthesis methods, eg chemical blowing, to produce new graphene materials, eg 3D strutted-graphene (SG).
Systems chemistry	Understanding the organisation and function of complex molecular networks in aqueous solution, including the impact of mechanical energy and the environment, with the goal of using directed evolution to synthesise life de-novo.
	Next generation systems chemistry – understanding more complex systems and reaction networks will require better models, measurement and data analysis. This can inform our fundamental understanding of living systems, eg cells. We have not yet developed the rules to construct such functional networks de novo, and one of the big challenges for chemists is the construction of functional far-from-equilibrium systems. Inspiration can be drawn by considering living cells as chemical reactors, and how these highly crowded reaction environments resist homogenization by limiting diffusion.
Chemistry of water	Advancing our fundamental understanding of the physical properties of water – structure, interfaces etc – and our ability to model water systems.
Molecular switches	Development of responsive materials / molecular switches whose behaviour is based on molecular structure or conformation, for example sensors and actuators that are activated by light.

Table C3: Organisms & ecosystems

ORGANISMS & ECOSYSTEMS	
Example topic	**Specific research examples**
Chemistry in the environment	Understanding the chemistry of the production of secondary aerosols in the air eg through oxidation of materials that are emitted, which can lead to the formation of very complex organic molecules. Understanding how these molecules form, and what they interact with is needed to inform methods to remove them from the atmosphere.
	Understanding the fundamental inorganic and organic chemistry that drives the behaviour and interactions of pollutants in soil and water, as well as their interaction with biological systems. Examples of contaminants include hormones, precious metals etc – in some cases, the intermediates formed by the breakdown of these pollutants are more toxic than the original forms. Understanding the chemistry will enable us to develop approaches for the specific removal or recovery of these pollutants from these environments, for example using photocatalytic methods and bacteria or enzyme engineering. Understanding their biological impact will require knowledge of toxicity, what comprises a safe level, the particular mix of chemicals present, and the uptake of these substances in living organisms.
Chemical ecology	Understanding the impact of micro plastics and nano-plastics on biological systems. We know they are accumulating in many animal species including birds, fish and humans, but have very little understanding of the implications of their presence.
	Understanding how birds navigate, for example how birds “detect” the Earth’s magnetic field and use this to navigate.
	Understanding the molecular basis of intercellular and interspecies communication, eg understanding quorum sensing.
	Advancing our understanding of the biochemical mechanisms that underpin the ability or inability of particular species to survive in specific environmental conditions, could provide insights to support the development of genetic interventions to increase survival rates of vital food sources in rapidly changing environmental conditions. This could help mitigate predicted environmental crises, for example, trout fish are expected to become extinct in a number of rivers in the near future.
Human physiology	Advancing our understanding of the human microbiome will help to inform such things as disease mechanism and drug interactions. This relies on developments in technologies such as new sensors that can be effective at point-of-use to accurately measure levels of specific microorganisms and molecular markers in the human microbiome. Measurement of the microbiome is a key step towards understanding its role in various health conditions involving the immune system but also its potential implications for autism and mental health.
	Advancing our understanding of the human brain and nervous system through neuromorphic computing – designing artificial neural systems based on the biological nervous system.
	Advancing our understanding of the molecular basis of mental health conditions.
	Advancing our understanding of the origins and mechanisms of human allergen responses, which will require advances in areas such as measurement within complex matrices.
	Interfacial chemistry to design drugs and treatments that have better molecular transport across membranes, in cells and to the brain. Examples include biologics, polymers and antibodies.
Chemistry of space	Understanding the molecules and chemistry of space using new instrumental techniques and light sources eg broadband microwave spectroscopy and terahertz radiation sources, combined with astronomical observations to advance our understanding of the development of life. New telescopes will allow us to probe in more detail than ever before which molecules are in space and why they are there. How are they made? Why are they in certain areas? Understanding the chemistry of how these molecules were made in an environment that was cold and where collisions occur every few days rather than collision rate of a typical chemistry experiment. These insights will help us understand why the universe is how it is, if there is life on other planets, eg evidence that there are amino acids or their precursors in space, and what materials and conditions were required for life to develop.

Table C4: Reactions, interactions and transformations

REACTIONS, INTERACTIONS & TRANSFORMATIONS	
Example topic	**Specific research examples**
Light-matter interactions	Resolving the primary steps of light-matter interactions using ultra-fast microscopy, multi-dimensional spectroscopy and quantum computing to develop our understanding of biological processes triggered by light, eg DNA damage, photo protection in plants. For example the application of 2D electronic spectroscopy has led to new insights into the vibronic coherence in photosynthetic light harvesting complexes. Mastering the details of light-matter reactivity at the femtosecond level will also open up potential new applications for human health in areas such as cancer therapy or new methods to combat anti-microbial resistance.
	Advancing our understanding of photon conversion in order to enable harvesting of untapped parts of the solar spectrum into useful photons / charge carriers. Specifically, developing approaches for diffusion-free triplet-triplet annihilation up-conversion.
Protein interactions	Advancing our understanding of protein–protein interactions and how to intervene in or inhibit them; understanding how they fold, mis-fold and interact with other molecules in living organisms. Examples of where this is critical for advancements in human health include: peptide aggregation leading to amyloid formation implicated in Alzheimer's and Parkinson's disease; bi-molecular protein–protein interactions within intracellular signalling cascades; design of specific protein–protein interaction inhibitors.
Metallo-proteins	Advances in biological inorganic chemistry will deliver a step change in understanding metallo-protein function through molecular/atomic detail enabled by new measurement techniques. For example, we will be able to understand the conformational changes driven by chemical reactions which often happen at metal centres, or post-translational modifications such as phosphorylation that can drive/modulate protein–protein interactions. These advances will give us a much better understanding of how cells and their individual components work, and could lead to new antimicrobials; drugs for cancer and neurodegenerative diseases; an increased understanding of host-microbiome interactions; a better understanding of development; healthy ageing; new large scale production using cell factories; insights into light-energy capture; and CO_2 capture and recycling.
O_2 activation	Advancing our fundamental understanding of transition metal ions such as Mn^{-}, and Fe^{-} based catalysts in activating O_2. This will enable development of efficient and selective catalysts for O_2 activation with application in production of clean oxidants and use in fuel cells.
Complex organic synthesis	Advancing our understanding of C-H bond functionalisation – this has been a major fundamental synthesis challenge for chemists for many years, due to the highly inert nature of the bond. Most current systems rely on close proximity to a functional group to force reactivity – being able to selectively activate any type of C-H bond without any directing group, while allowing specificity, is the goal. Discovering new ways to activate C-H bonds will allow chemists to optimise a number of key industrial transformations for example in pharmaceutical research and also speciality chemical production.
	Discovering new routes for the synthesis of complex organic molecules. This will allow us to effectively synthesise complex molecules that could be screened for desirable properties such as pharmacological function.
	The Hexadehydro Diels-Alder reaction (HDDA) produces benzynes (aromatic systems containing, formally, a carbon–carbon triple bond), which are among the most versatile of all reactive intermediates in organic chemistry. The study of this reaction allows new modes of intrinsic reactivity to be revealed and exploited.

Table C4: Reactions, interactions and transformations (continued)

REACTIONS, INTERACTIONS & TRANSFORMATIONS	
Example topic	**Specific research examples**
Nanoparticles	Advancing our fundamental understanding of nanoparticle nucleation over multiple timescales using techniques such as microfluidic system transmission electron microscopy (TEM), allowing us to design robust and reproducible methods of production.
Next generation catalysts	Advancing our fundamental understanding of catalytic science by obtaining a detailed understanding of reactive mechanisms. Combining high throughput screening, advanced measurement and computational modelling techniques will allow us to discover new catalysts and combinations of catalysts that will improve the efficiency of reactions while also lowering the reliance on scarce and/or toxic elements. AI and machine learning are likely to become increasingly important in this field to inform design based on what we learn about structures and syntheses. These insights have application to a number of challenges, for example discovering high reactivity catalysts in CO_2 capture and developing improved solar energy storage materials.
	Using directed evolution techniques to create new protein catalysts as well as expanding the space of genetically encoded enzyme functions in order to catalyse synthetically important reactions not known in biology eg selective formation of C-Si and C-B bonds. These new capabilities increase the scope of molecules and materials we can build using synthetic biology and move us closer to a sustainable world where chemical synthesis can be fully programmed in DNA. Using directed evolution to optimise artificial reaction systems in living cells eg organometallic chemistry with artificial metallo-enzymes to enable Suzuki cross-coupling. Similar advances have been used to develop anti-malarial drugs such as artemisinin.

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