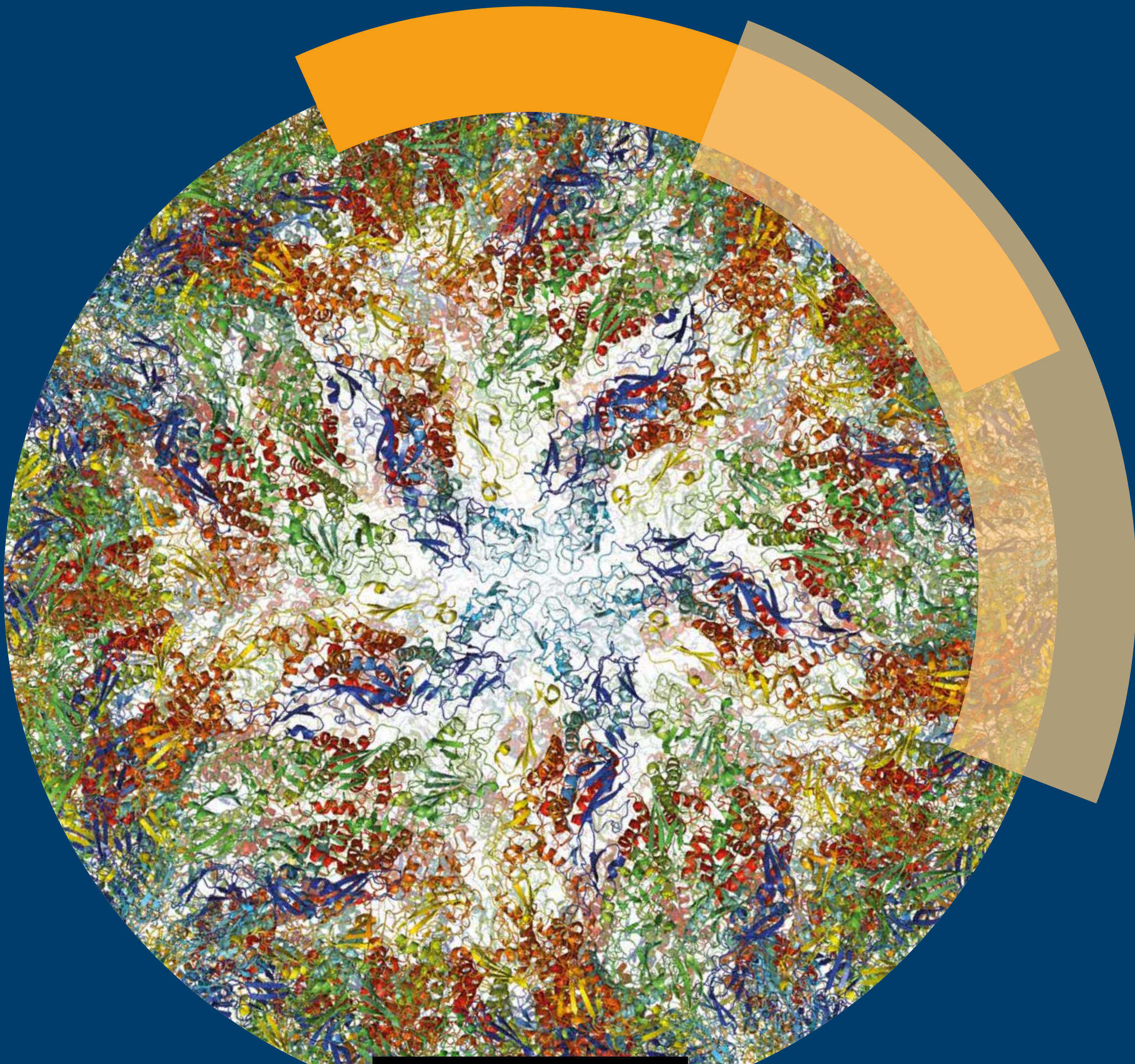


DISCOVERY

# Science Horizons: Research Frontiers

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

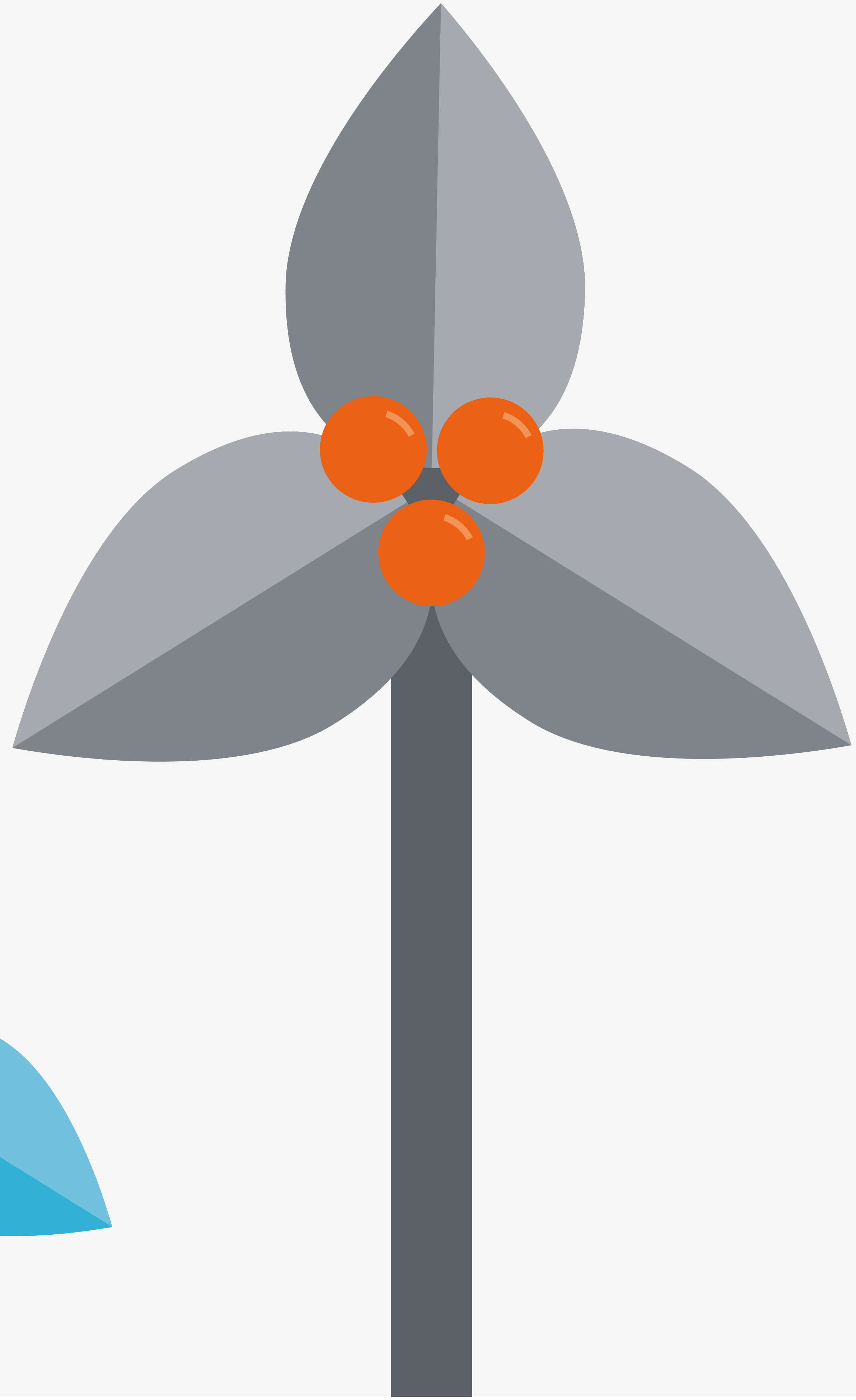
# Over the past decade, the global public research agenda focused on finding paths to sustainable prosperity.

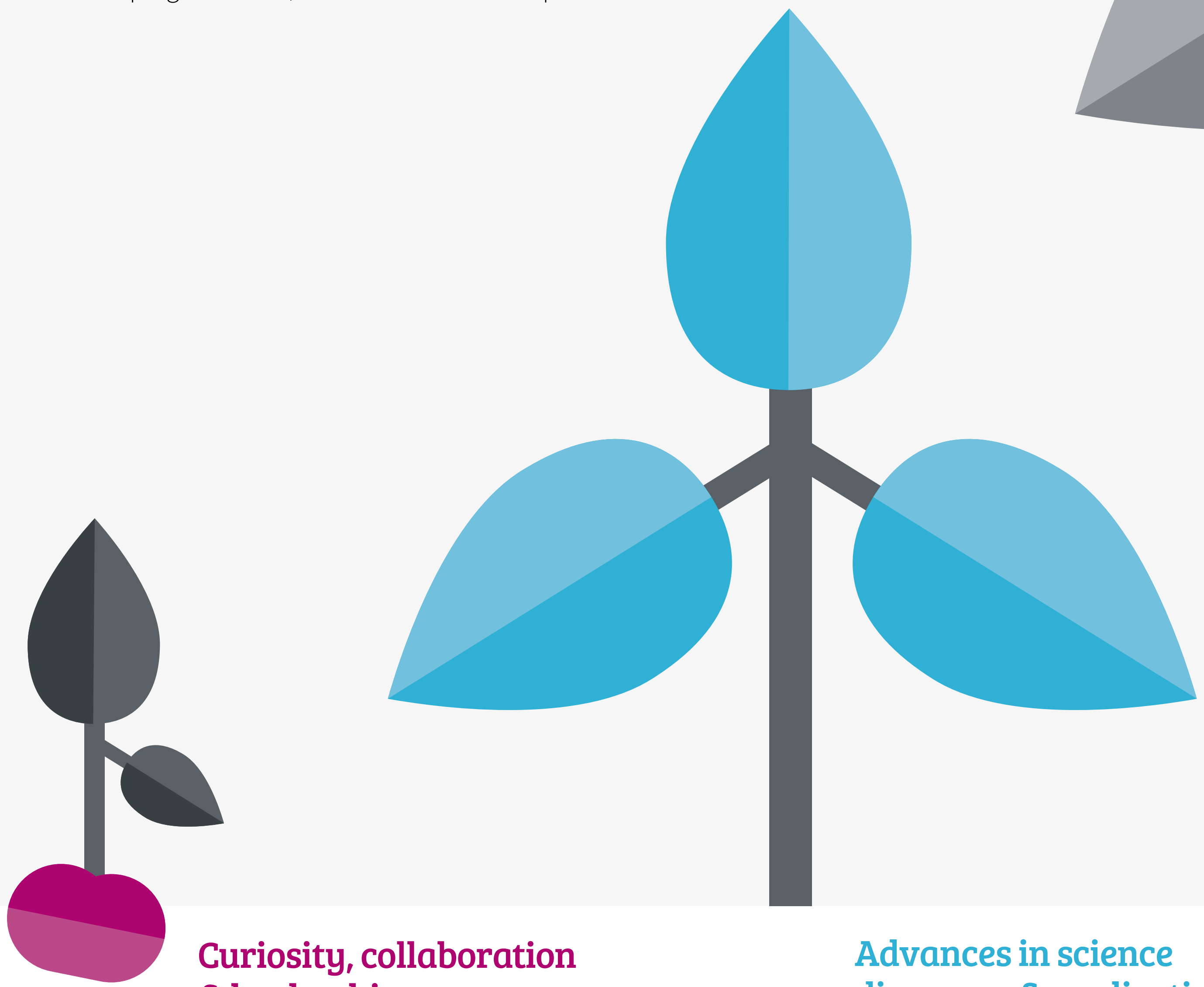
Driven by growing populations, escalating environmental concerns and the financial crisis of 2008, governments prioritised global challenges and industrial innovation when funding scientific research and development.

The chemical sciences will be central to advancing three dimensions of scientific research that will be essential to meeting this agenda:

- Solutions to global & industrial challenges
- Leading-edge questions
- Frontier techniques

These three are closely interdependent. The answers to leading-edge questions are necessary to advance frontier techniques – which in turn become the tools scientists use to discover the answers to questions across and beyond the chemical sciences. Both of these are critical to developing solutions, which leads to more questions.






**About Science Horizons**

Science Horizons is a Royal Society of Chemistry report into the direction, potential and needs of scientific research and development in the next 10-15 years, based on engagements with more than 750 leading scientists worldwide.

This first snapshot, Science Horizons: Research Frontiers, explores the amazing developments in science – particularly the chemical sciences – that will play a significant role in delivering sustainable prosperity for humanity.

# Creating solutions – the chemistry of sustainable prosperity

Researchers expect that the solutions to major societal challenges – from environment and energy to human health and agriculture – will be underpinned by the chemical sciences. 99% of surveyed researchers stated that their work had potential application in at least one global challenge area.

Potential application of research to global challenge area (% respondents) and Top 4 application areas

**Environment** – 82%
- Substitution of toxic or hazardous materials
- Environmental monitoring and/or remediation
- Substitution of critical and scarce materials
- Waste recycling

**Human Health** – 74%
- 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

Tesla Model 3, fully electric road car

**82%**

OF RESEARCHERS AGREED IT IS THEIR "DUTY AS SCIENTISTS TO CONSIDER THE POTENTIAL APPLICATIONS OF OUR RESEARCH"

Not all research is designed with an end application in mind – some is curiosity-driven research that seeks to answer the fundamental questions about how our world works.

But more than four fifths of researchers we surveyed did agree that it is their duty to consider the potential applications.

For those who have designed their research to specifically solve challenges, many are focused on industrial challenges – whose solutions lead to, for example, advanced consumer products that are more durable, more recyclable, have higher-resolution screens or longer-lasting batteries.

# Leading-edge questions – understanding how our world works

Scientists' efforts to better understand the world around them has led to some of the most significant technological breakthroughs in history. Chemical sciences researchers are now looking for answers to an incredibly broad range of questions – from the inner workings of chemical elements to understanding the origins of life – to enhance our understanding of fundamental principles of science, without necessarily having any specific application in mind.

In Science Horizons we grouped the leading-edge questions that researchers are tackling 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.

*"Fundamental understanding at the molecular level and translation to function is where we have seen dramatic advances in the past decade which will only advance further over the next 5-10 years."*

**Professor Oren A. Scherman**
**University of Cambridge**

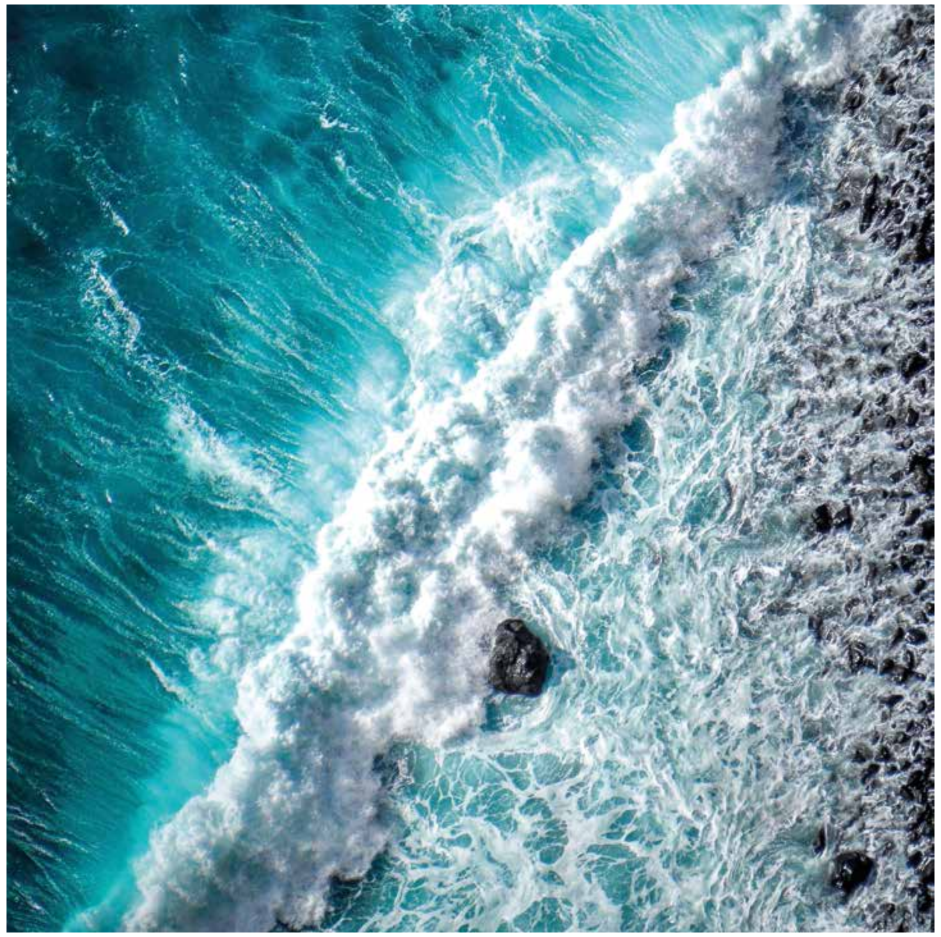
*"Chemistry underpins our iPhones, the paints on our walls and the medicines we take – chemistry is everywhere."*

**Professor Phil Baran**
**Scripps Research Institute**

Exploring new science in all of these areas adds to our understanding of the world – and also discovers entirely new properties, materials or reactions that lead to applications no-one could have guessed. Chemical scientists at the University of Hull created the first stable liquid crystals decades before they were used to create flat screen displays now found in every home and office.

Researchers are studying, creating and controlling matter across a huge range of scales: from individual hydrogen molecules to our entire atmosphere, and almost everything in between. They are increasingly using complex computer simulation to study and design new molecules and materials increasing their capacity and throughput.

In the interdisciplinary teams that study these questions, chemical scientists bring the atomic and molecular expertise for example, how certain types of chemical bonds affect living and non-living systems, or how to arrange atoms and molecules into structures that affect things like strength or electrical properties. They play a central role in understanding the workings of the molecular machinery of every unanswered question.



The chemical sciences are vital to understanding not only the very tiny, like the structure of viruses, but also the properties of enormous complex systems, like our oceans, atmosphere and even outer space.

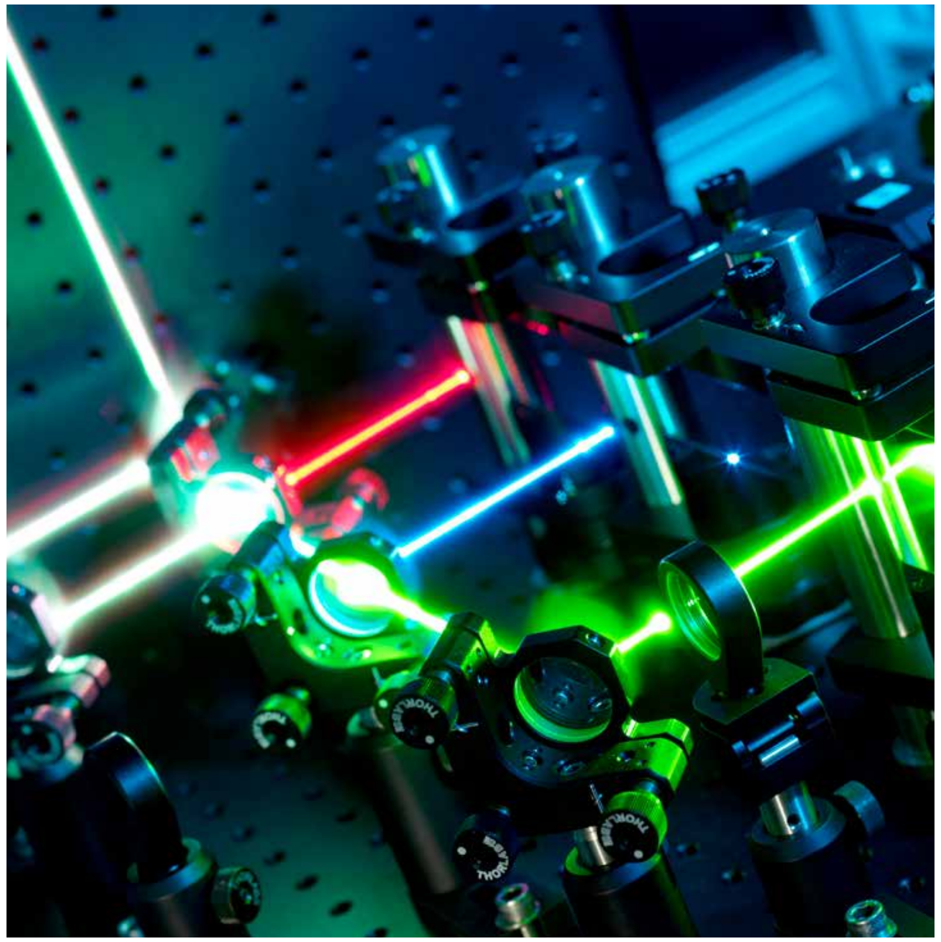
# Frontier techniques – smaller, faster, clearer, better

## Frontier chemical science techniques show us more detailed images of life and matter than ever before

Chemical scientists have recently made enormous leaps in the science of measurement. These have already led to incredible discoveries and achievements based on that science, which allows us to see, create and manipulate at the atomic and molecular level with greater clarity and sophistication than ever before.

- We can now see and measure events that happen not in the blink of an eye, but a billion billion times faster – like the vibration of a single atomic bond that signals the beginning of cancer-inducing DNA damage.
- We can use high resolution imaging techniques to gain crystal-clear pictures of not just the rough outline shape and size of a virus, but of the specific molecular structure that it uses to harm people.
- And we can combine these techniques and more to capture real-time visuals of chemical reactions happening in live cells and organisms – a huge step up from single, fuzzy images of dead bacterium samples.

**Advanced spectroscopic techniques and equipment allow scientists to explore the molecular world in greater detail than ever before**



**Advances in digital chemistry, including machine learning and automated laboratory equipment, will speed up the more routine and repetitive elements of chemical research**

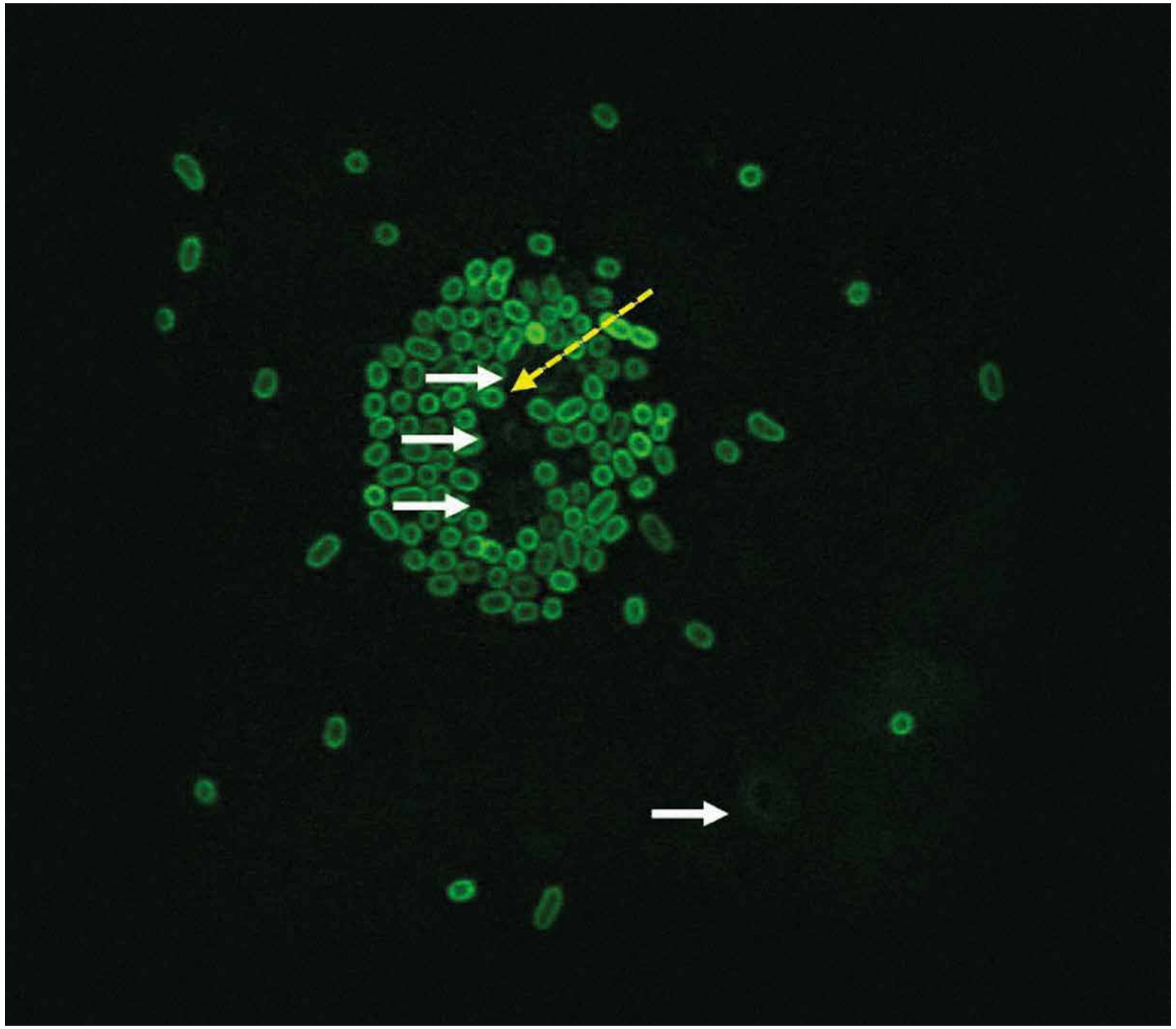
These incredible advances in our ability to explore the molecular world – and map it for everyone to see – help chemical scientists to answer the many unanswered fundamental questions of science, and to design the scientific solutions to global challenges.

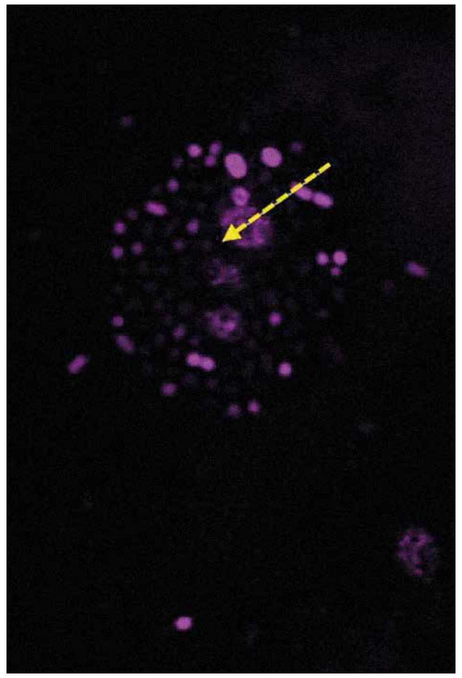
Chemical scientists draw on the skills and experience of the whole scientific community, bringing together the resources and expertise from different disciplines and countries. And they are taking advantage of powerful new digital and data techniques, like machine learning, computational modelling and robotics, to enhance and expand their scientific capabilities.

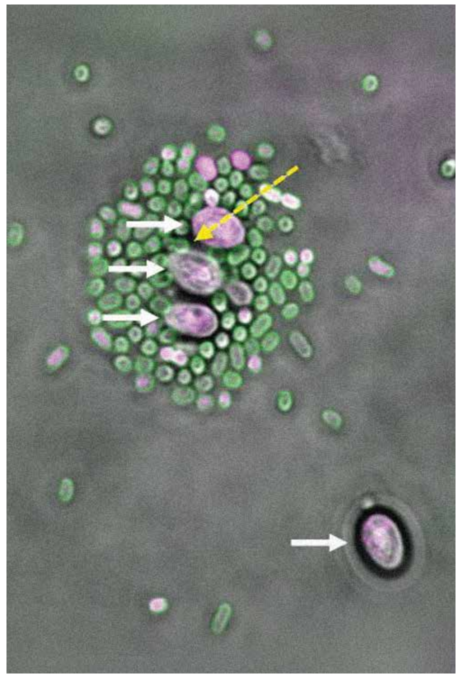
Today, chemical scientists are making amazing scientific breakthroughs and developing revolutionary technologies. With the right support and infrastructure, they can achieve even more for society and humanity over the next decade and beyond.

Case study 1

# Real-time lung infection diagnosis in ICU







In situ identification of Gram-negative bacteria in human lungs , allowing clinicians to diagnose and treat the infection immediately.

Patients on ventilators in critical care are prone to life-threatening bacterial lung infections. With limited bedside diagnostics available, often the only option is to move these critically ill patients to have an X-ray, which shows only shadows of a lung problem from which clinicians must infer a treatment plan.

Innovative chemistry and technology from the Bradley group and collaborators may change all that. They created a molecule that binds to specific bacteria and is detectable by a special fibre-optic camera inserted into a patient's lung. The resulting images clearly and immediately show the location and extent of the infection, allowing clinicians to diagnose and treat it there and then.

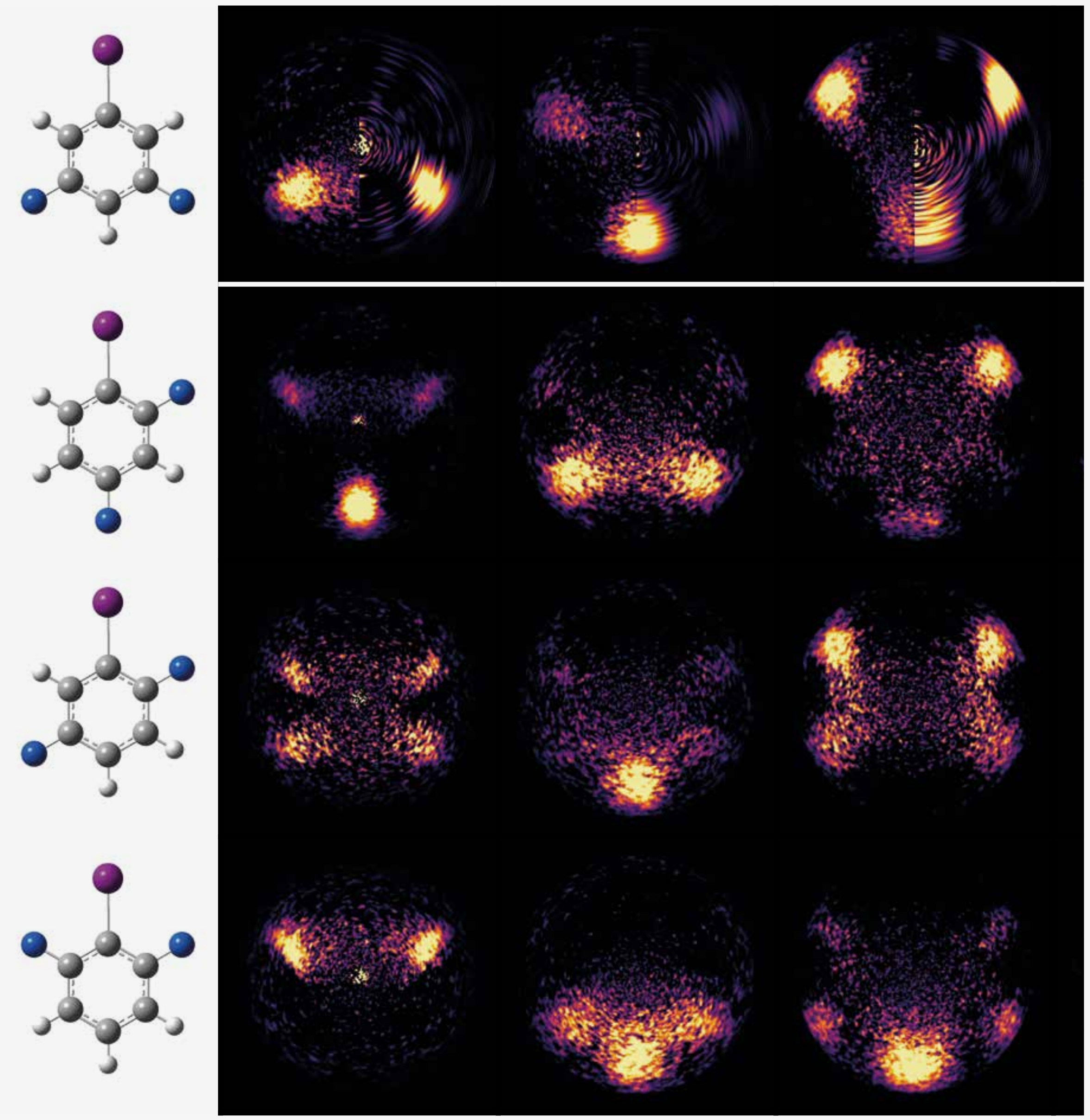
This will save lives. The Bradley group works closely with clinicians and medical professionals to ensure the technique is safe and practical. It will also help to mitigate some unnecessary use of antibiotics, at a time where antimicrobial resistance is a clear and present threat to humanity.

Profile

The Bradley group
Edinburgh
www.combichem.co.uk

Case study 2

# The fastest camera in the world




PImMS images recorded for (top to bottom) three different structural isomers of difluoroiodobenzene. From left to right, the columns show the relative velocity distributions measured for different pairs of atoms (iodine with hydrogen, fluorine with hydrogen, and fluorine with fluorine) when a laser is used to 'explode' the molecules. The images allow the three isomers to be clearly distinguished, and the structure of the original molecule to be determined.

Pixel Imaging Mass Spectrometry (PimMS) camera, creating 'molecular movies' by shooting at 80,000,000 frames per second.

In movies, frame rate makes a huge difference. The cinematic feel of 24 frames per second (fps) is a commonly-used classic; modern TV shows and sport benefit from a smoother 60 fps. To film a slow-motion video of, say, a water balloon popping, so that you can really see the detail, you need a camera that records several hundred or even thousands frames per second.

But what about watching molecules react? For that you need a camera built by scientists at the University of Oxford, which shoots at an equivalent of 80,000,000 fps. The team led by Claire Vallance and Mark Brouard combined new fast imaging sensors with mass spectrometry to create Pixel Imaging Mass Spectrometry (PimMS), a technique that gains information about molecules by breaking them apart, then measuring the size and speed of fragments.

With this new technique and equipment, the scientists can not only measure the mass and speed of the many thousands of fragments, but also their location and movement relative to each other – creating molecular movies showing an event that happens a million times in the blink of an eye. And, in contrast with the usual approach of sensing a single fragment at a time, PimMS can measure all the fragments in one go, reducing hours of work to a few minutes.

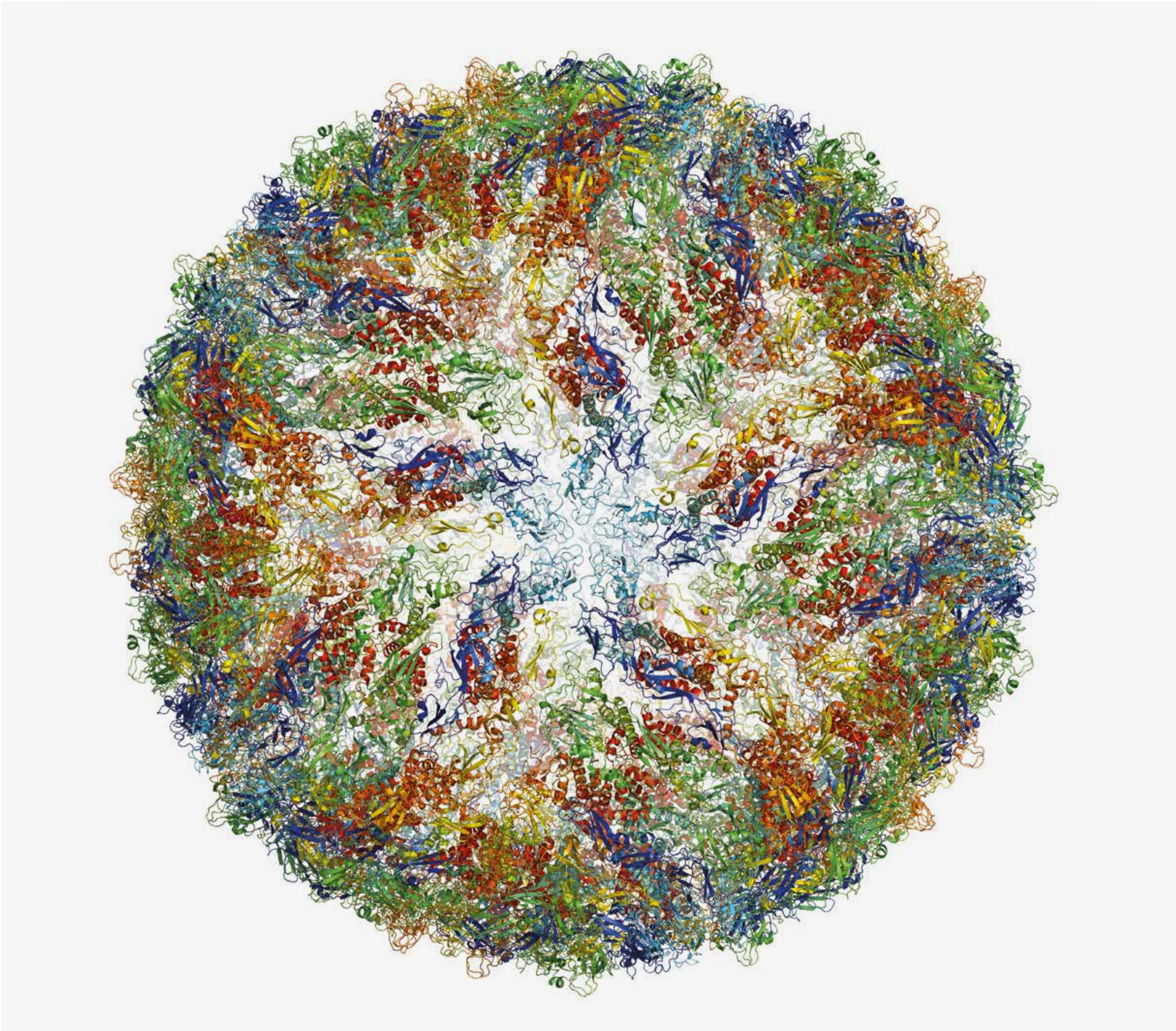
The scientists envision use cases ranging from measuring where in a tissue sample a drug has worked (eg chemotherapy) to measuring plant biology samples to improve crop yields.

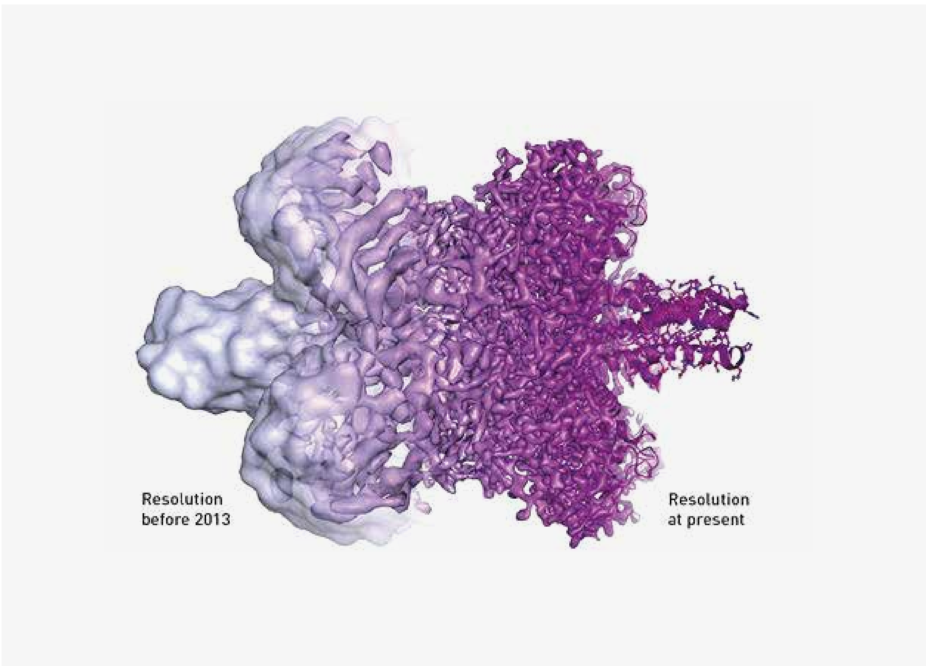
Profile

Claire Vallance and Mark Brouard
Oxford University
brouard.chem.ox.ac.uk

Case study 3

# Creating atom-level 3D images of viruses






▲ 3D image of the Zika virus at atomic resolution.

*Illustration, ©The Royal Swedish Academy of Sciences*

◄ The electron microscope's resolution has radically improved in the last few years, from mostly showing shapeless blobs to now being able to visualise proteins at atomic resolution.

*Image: © Martin Högbom/The Royal Swedish Academy of Sciences*

Traditional light-based microscopes can't see the detail of molecules – you just can't zoom in close enough. For that level of detail, scientists use electron microscopes that can resolve much more detailed images – but that power usually comes at a price, destroying biological molecules in the process.

Scientists recently fixed these problems and ushered in a new age of biomolecule imaging, with the invention and development of cryo-electron microscopy, for which they were awarded the Nobel prize in Chemistry 2017. By using weaker electron beams, improved image processing, and cooling water to act like a glass shield protecting the target, it's now possible to freeze live biomolecules in time and gain incredibly detailed, three-dimensional models of their molecular structure – down to individual atoms.

With a reliable technique to create these images, scientists have studied countless biomolecules in more detail than ever before – identifying the specific molecular machinery responsible for some antimicrobial resistances, and quickly creating a detailed model of the Zika virus following the 2017 outbreak in South America, enabling better detection and treatment of the virus.

Profile

Jacques Dubochet
University of Lausanne, Switzerland

Joachim Frank
Columbia University, New York, USA

Richard Henderson
MRC Laboratory of Molecular Biology, Cambridge, UK

Awarded the Nobel Prize in Chemistry 2017 "for developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution."

# Curiosity, collaboration and leadership

For science to fulfil its potential to answer fundamental questions, create solutions to global challenges, and contribute fully to sustainable prosperity, it needs to have the right environment.

Through Science Horizons we identified that curiosity, collaboration and leadership are essential enablers for science to best help society today and in the future.

## Curiosity

Research into the fundamental inner workings of life and matter – what we call discovery, or curiosity-driven research – has always been an essential element of science.

Much valuable research aims to solve a particular real-world challenge, or improve an existing process or product, and this has a hugely beneficial impact on society. But the value of understanding how and why atoms and molecules act in a certain way is not only adding to the body of scientific knowledge; it opens up new, unimagined frontiers of science and research.

94% of scientists we spoke to for Science Horizons said that curiosity-driven research is important for the advancement of the chemical sciences – and 70% agreed that funding agencies put too much emphasis on the potential applications of research.

Researchers from every country represented in the response base expressed concerns that the emphasis on societal challenges and economic growth has led to an imbalance in funding with insufficient investment in curiosity-driven research.

**94%**

OF SCIENTISTS WE SPOKE TO SAID THAT CURIOSITY DRIVEN RESEARCH IS IMPORTANT FOR THE ADVANCEMENT OF CHEMICAL SCIENCES

**87%**

AGREE COLLABORATION WITH OTHER FIELDS OF SCIENCE IS CRITICAL

**81%**

AGREE INTERNATIONAL COLLABORATION IS ESSENTIAL

## Collaboration

Sharing knowledge, skills and resources is second nature to most scientists – from benefitting from another's expertise on a topic that affects your research, to access to international facilities.

Researchers highlighted collaboration as completely essential to advances in chemical sciences, with 87% agreeing that collaboration with other fields of science is critical, and 81% saying international collaboration is essential. More than 90% had collaborated with someone outside their field in the last five years.

Much leading chemistry research is highly interdisciplinary. When asked to classify their own research, more than three quarters of scientists chose two or more subfields, with an average of 2.7 fields for the whole group.

Researchers see the traditional reward and incentives culture in academia as holding people back from effective collaboration, especially earlier in a researchers' career when individual successes help to build their profile and reputation.

## Leadership

For science to make its best contribution, scientists have to lead those efforts effectively. Leaders in science need not just subject expertise, but the ability to imagine a research project, build and lead a cohesive team, and communicate its value well enough to get funding and visibility.

There is also a real 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, during a career stage when individual successes help to build their profile and reputation.

# Curiosity, collaboration and leadership

*"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**

*"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**

*"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."*

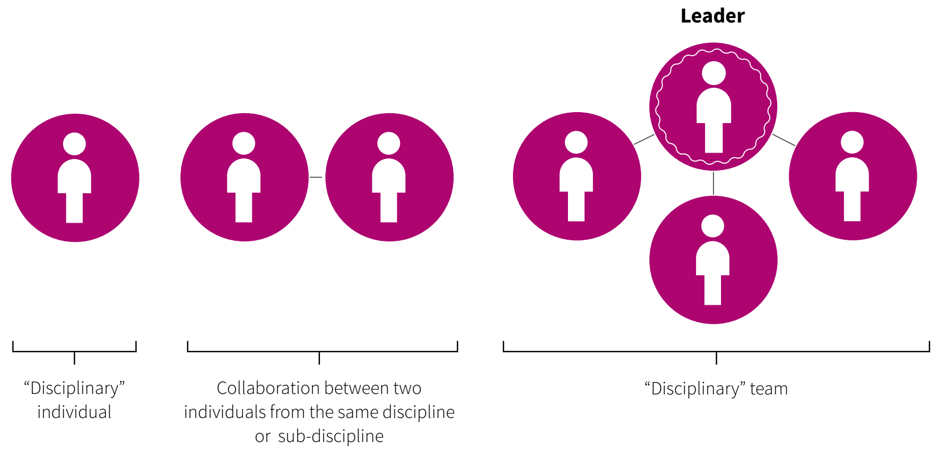
**Professor Helen Fielding**
**University College London**

*"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."*

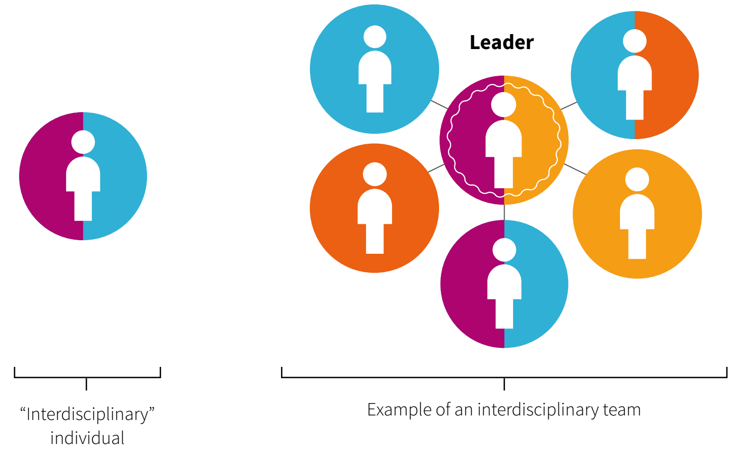
**Professor Bengt Norden**
**Chalmers University of Technology**

**Key**

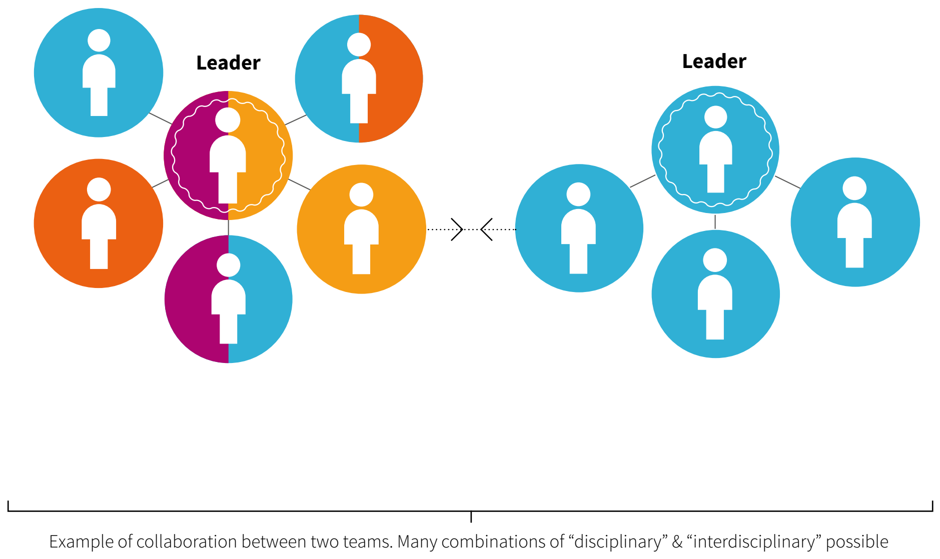

## Individuals and teams




## Interdisciplinarity




## Collaboration



# Taking advantage of a new golden age of discovery

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.

Chemical sciences researchers have a positive, confident vision for research today and in the future. There is a sense of agency and energy among researchers – they 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. 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.

To take full advantage of this, the researchers identified key themes that covered funding, collaboration mechanisms and research culture – alongside a call for scientists to be more proactive in shaping the research agenda, and for governments to recognise the importance of enabling the discovery research that will unearth incredible future scientific and technological advances.

*"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**

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