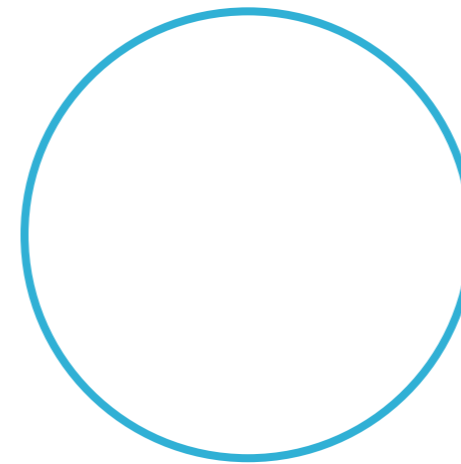


Sustainability

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.



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

## 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.

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



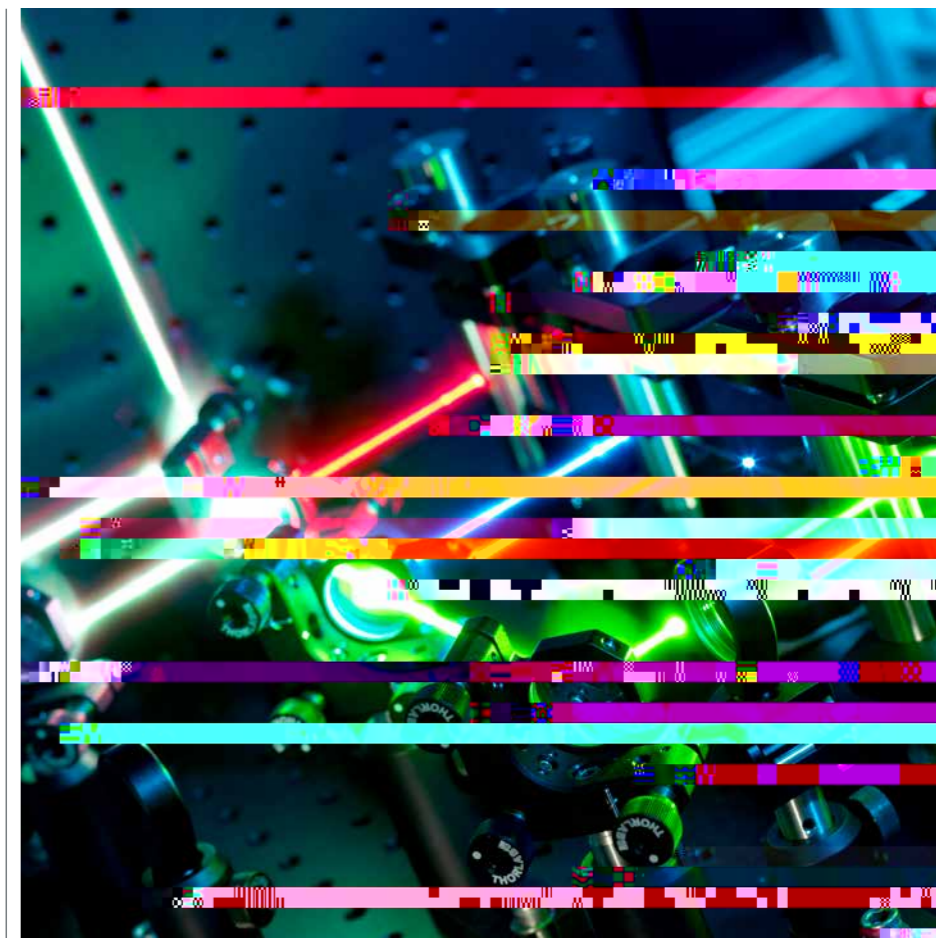
# Frontier techniques – smaller, faster, clearer, better

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

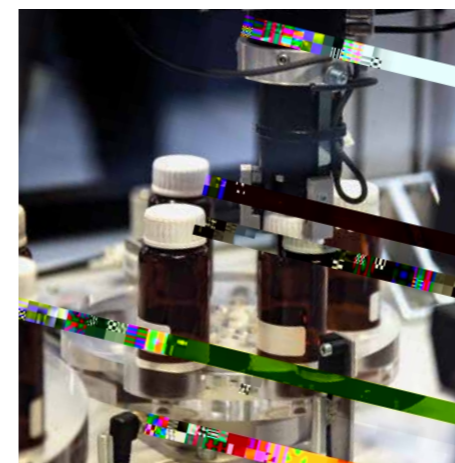
Chemical scientists have recently made enormous leaps in the science of measurement. These have already led to incredible discoveries and achievements based on that science, which allows us to see, create and manipulate at the atomic and molecular level with greater clarity and sophistication than ever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

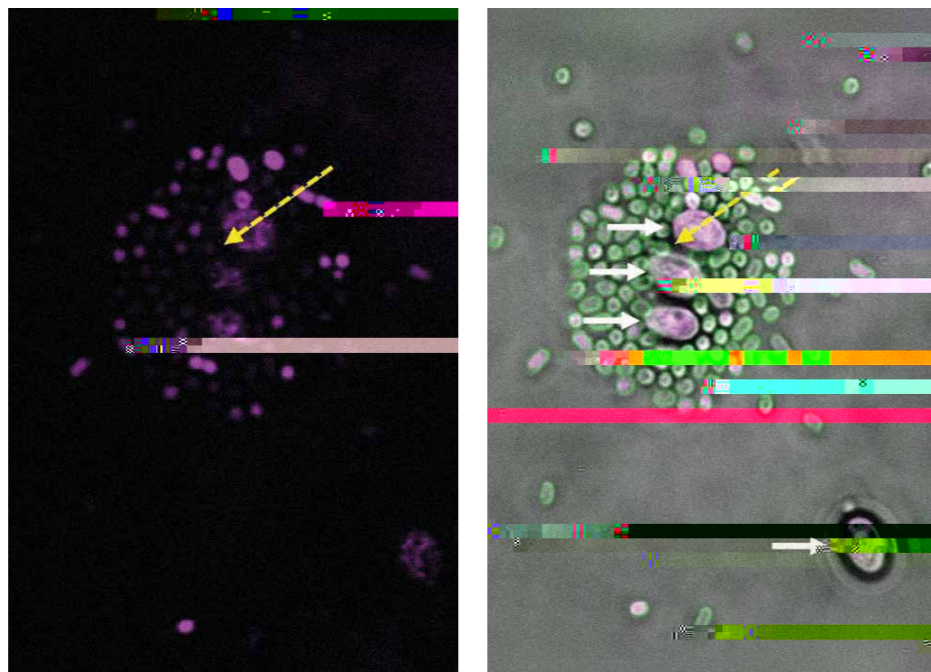


These incredible advances in our ability to explore the molecular world – and map it for everyone to see – help chemical scientists to answer the many unanswered fundamental questions of science, and to design the scientific solutions to global challenges.

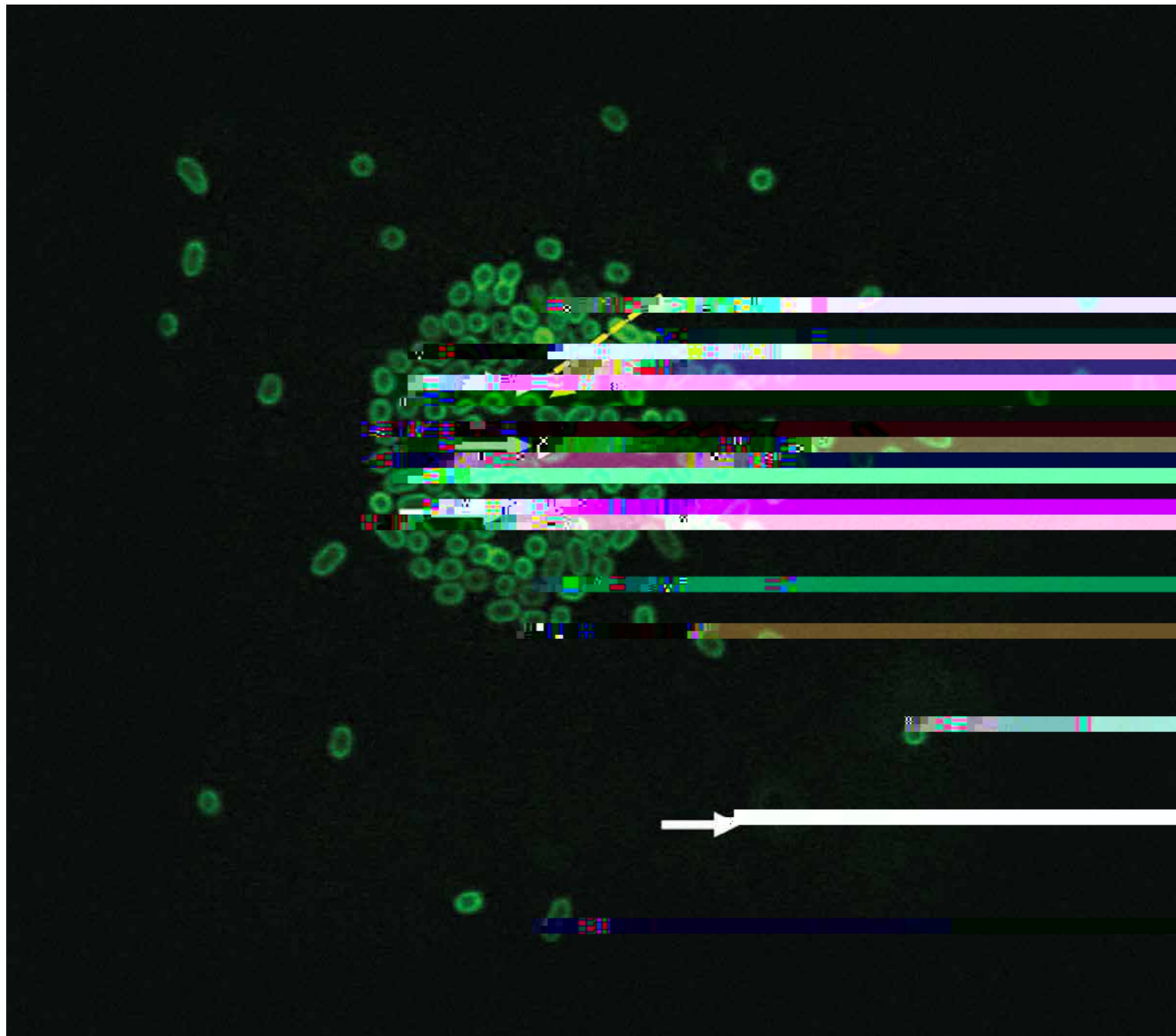
Chemical scientists draw on the skills and experience of the whole scientific community, bringing together the resources and expertise from different disciplines and countries. And they are taking advantage of powerful new digital and data techniques, like machine learning, computational modelling and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

# 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](http://www.combichem.co.uk)



# 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.

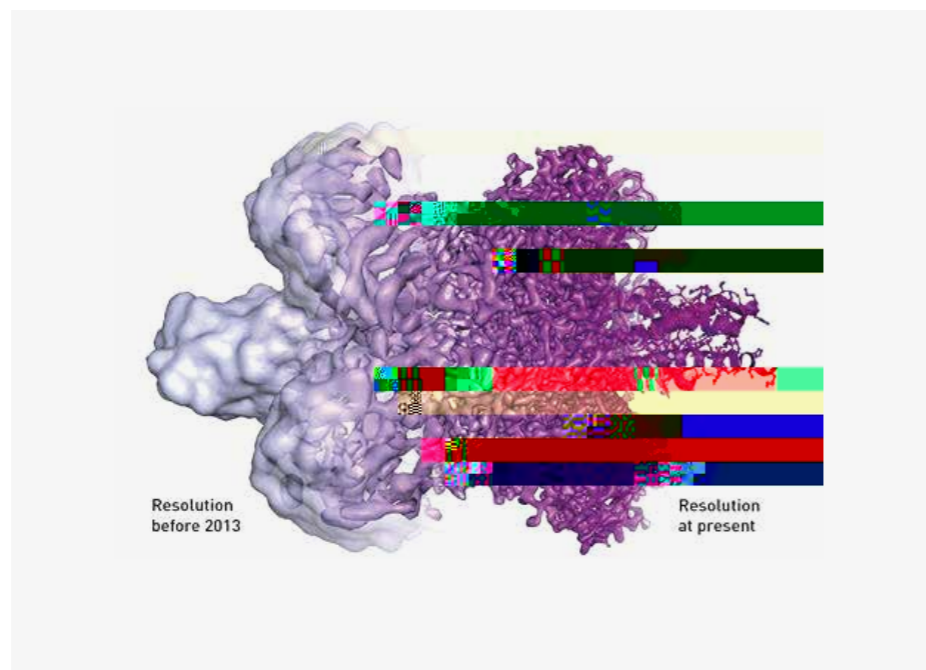
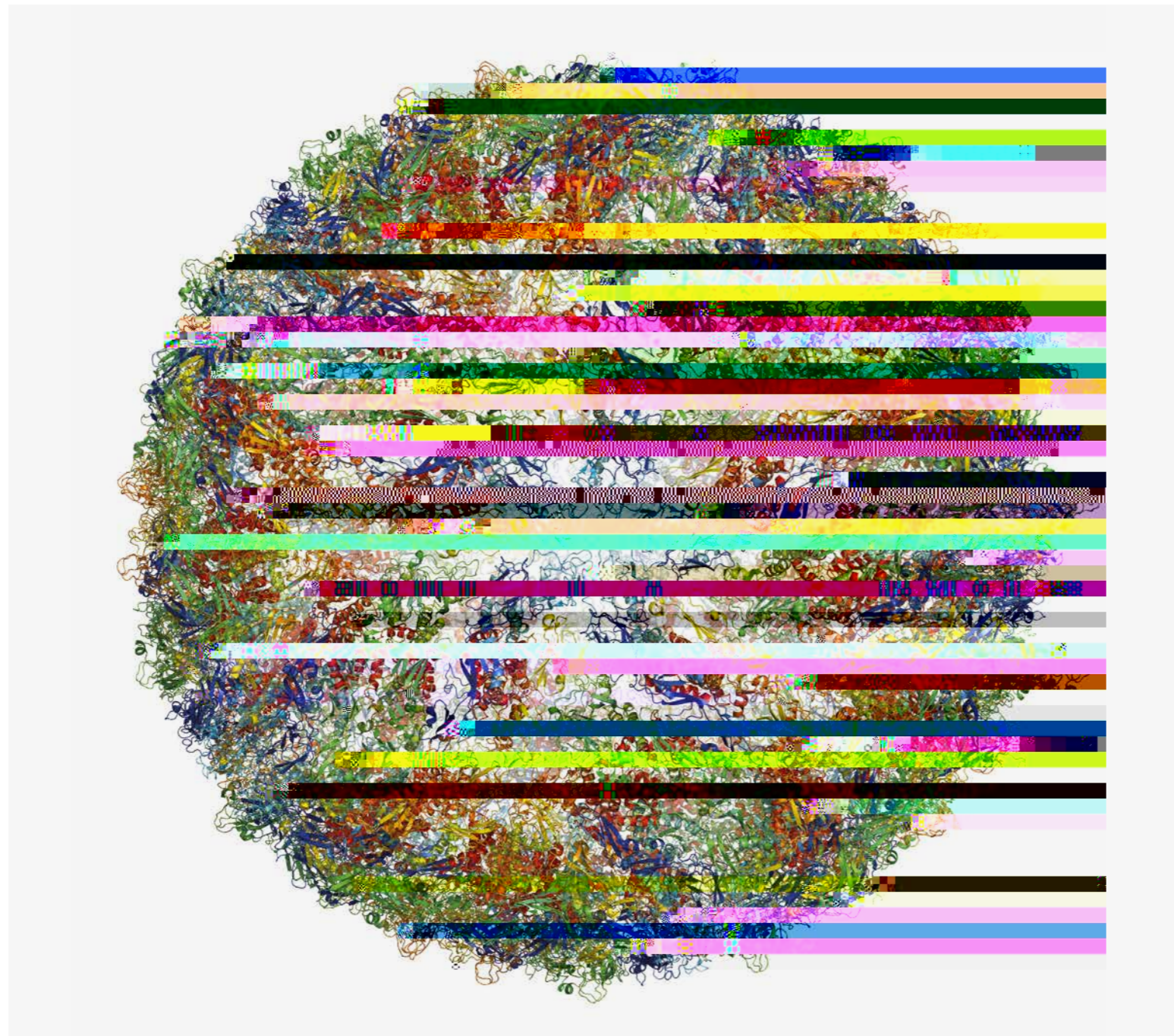
## Profile



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



# 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

*“As researchers we need to be open to new things, learning about different techniques and tools. We also need a*



# 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

