Issue 1 // Spring 2014
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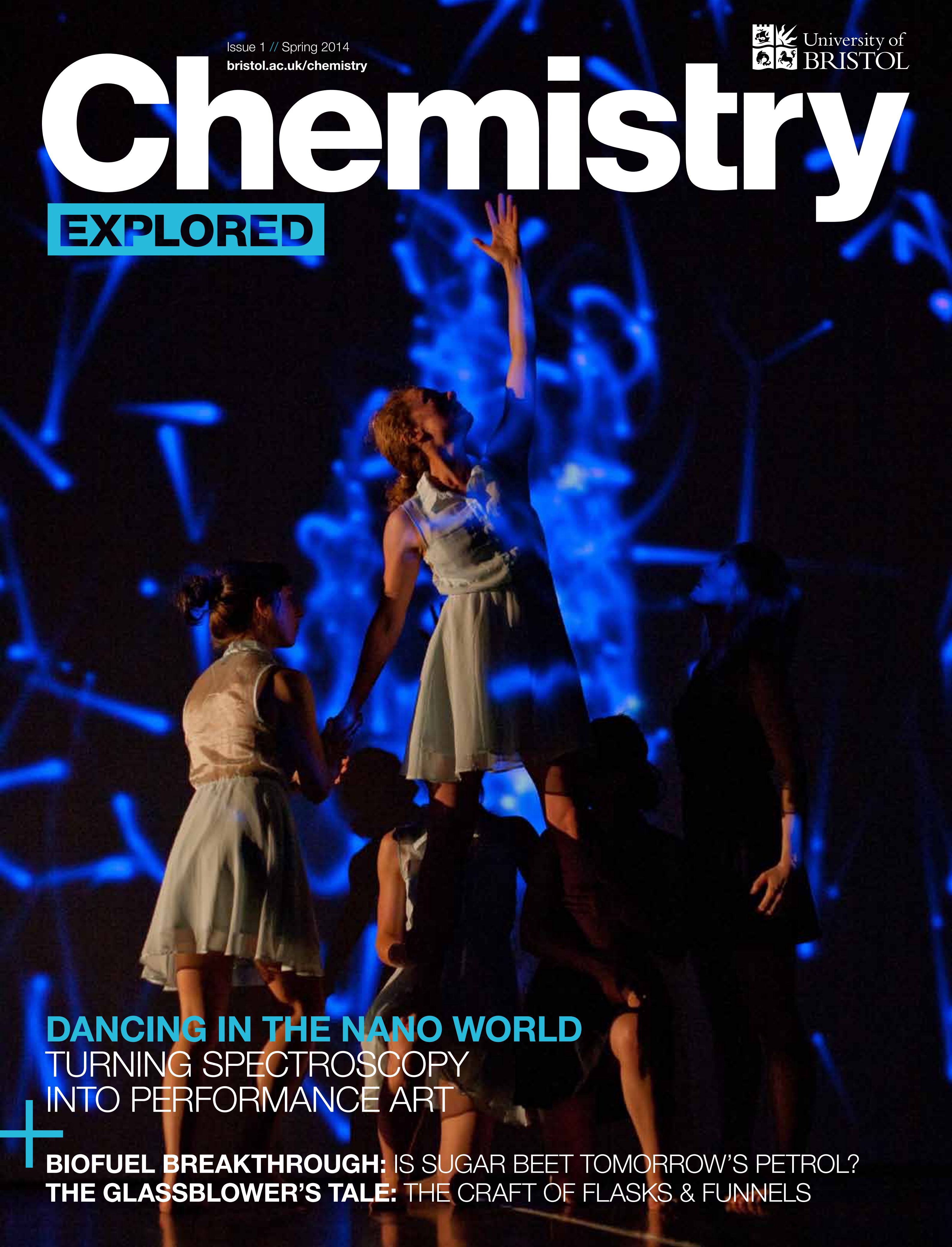
University of BRISTOL

Chemistry EXPLORED



DANCING IN THE NANO WORLD
TURNING SPECTROSCOPY INTO PERFORMANCE ART

+

BIOFUEL BREAKTHROUGH: IS SUGAR BEET TOMORROW'S PETROL?
THE GLASSBLOWER'S TALE: THE CRAFT OF FLASKS & FUNNELS

UPDATE

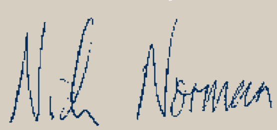
Welcome

As Head of School, it's a great honour to lead such a vibrant department that is home to so many fantastic colleagues and students. This issue gives you a taste of the innovative research and teaching that characterises chemistry at the University of Bristol.

From a research perspective, we feature a story about Protolife, an exciting new initiative which seeks to understand the molecular origins of the first cells. Elsewhere, Dr David Glowacki, one of our youngest members of staff, takes us on a tour of his acclaimed art-meets-science project, danceroom Spectroscopy. Continuing the creative streak, we feature an entry from the PictureIt… *Chemistry* blog, which uses imagery as the universal language of science.

You'll also read about what our undergraduate and postgraduate students get up to, and our award-winning outreach work, not to mention a profile of our extremely talented glassblower, Duncan Tarling.

I hope you enjoy reading this first issue of *Chemistry Explored*, and look forward to sharing more about life in Chemistry in future editions.



Professor Nick Norman
Head of the School of Chemistry

update

The latest news from the School of Chemistry

Tim Harrison shows school students the dramatic effects of liquid nitrogen on the local flora

Bringing chemistry to life in the classroom

BRISTOL ChemLabS Outreach has an international reputation for promoting chemistry to students of all ages and their teachers (*writes Tim Harrison*). Since the project's inception, we have worked directly with more than 300,000 students in 27 countries on five continents.

Much of the work in primary and secondary schools is carried out by trained students under my supervision. In recent years we've had the opportunity to help promote chemistry in Singapore, France, Malta, Jersey, Ireland, Namibia and South Africa. The quality of this work has been recognised with several national awards.

The engagement activities can be as varied as leading groups in hands-on practical work in primary schools, writing articles and giving talks and mini lectures to secondary school students.

More senior postgraduate and postdoctoral chemists, along with academic staff, are also engaged in aspects of up-skilling for practising teachers, in a variety of areas of contemporary chemistry.

On Wednesdays throughout the year, and most days in June and July, the undergraduate teaching labs are in use by school groups on day visits or residential stays. These are assisted in their practical work by yet more chemistry students.

Feedback is always useful. I gave two lecture demonstrations to 340 Year 10 and 11 students at Lliswerry High School, Newport, Gwent. Headteacher Alyson Mills commented: "Many thanks for bringing the 'wow' factor to my school today. The Key Stage 4 pupils have been talking about it all day and that is a fabulous testament to your delivery. The science was accessible and exciting and will be memorable."

Tim Harrison is Director of Outreach and Bristol ChemLabS School Teacher Fellow. www.chemlabs.bris.ac.uk

Selena on the roof of Africa, Tanzania, 2013

ON TOP OF THE WORLD

IN SEPTEMBER LAST YEAR, Undergraduate Student Administrator Selena Power decided to take on the challenge of Mount Kilimanjaro to raise money for the charity Hammer Out, which supports families and patients affected by brain tumours.

"It was a huge personal challenge that my sister and I undertook, to raise awareness about the fantastic work Hammer Out does supporting families like mine," says Selena. "I managed to hit my target of £4,000 – and climb 19,330ft – but decided to continue with the appeal and eventually raised £7,654."

So would she do it again? "I'd never attempt another mountain, but I have entered the Race for Life, the Pretty Muddy Run on Bristol Downs, and the Kamikaze Adventure Run."

Boom boom!

Professor Paul Wyatt, Director of Undergraduate Studies, took to the Bristol stage recently for a stand-up routine about the perils of the chemistry lab. Professor Wyatt joined the December lineup for Bright Club Bristol, which hosts gigs mixing academics with professional comics, and delivered an eight-minute set focusing on a surreal finger buffet held in the radioactive lab in his student days. "This is a room where you normally wear a space-suit to handle things, and yet everyone seemed happy to drink champagne and eat vol-au-vents there," he said. Buoyed by a positive reception, Professor Wyatt – who admits to doing a 'tiny bit of Footlights' as a Cambridge undergraduate – is already planning his next gig. **www.brightclubbristol.wordpress.com**

NEW ADVENTURES IN SYNTHETIC BIOLOGY

BUILDING CELLS from scratch and using bacteria to produce new vaccines – these are just some of the exciting ideas to be explored in a new research centre at the University of Bristol.

Funded by a £13.6 million grant from the Biotechnology and Biological Sciences Research Council (BBSRC) and the Engineering and Physical Sciences Research Council (EPSRC), BrisSynBio will bring together scientists from all fields, in order to develop new techniques and technologies in synthetic biology.

Centre Director Professor Dek Woolfson said: "We are over the moon. This is the culmination of hard work from a number of us over the past five years. It will allow us to begin some exciting multi-disciplinary research programmes."

Also in this issue...

News

Features

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With thanks to Dr Craig Butts, Ms Selena Power, Dr Jenny Slaughter, Dr David Glowacki, Mr Duncan Tarling, Mr Tim Harrison, Prof Steve Mann, Dr Mei Li.
Photography David Pratt

Students at work in the school's nuclear magnetic resonance labs

The beet generation

Prize-winning work on biofuels by young chemists means sugar beet is shaping up as a viable source of sustainable energy

WHEN ALEX SEARLE-BARNES and fellow student John Luckett made a novel discovery about the potential uses of an emerging biofuel, they turned to the University of Bristol to investigate further.

The collaboration between the Malmesbury School pupils and the School of Chemistry came about in 2010, when Alex and John had the idea to see how much ethanol they could extract from sugar beet. The University's researchers suggested they analyse their produce using the School of Chemistry's mass spectrometer and nuclear magnetic resonance spectrometer. This enabled them to prove the composition of their raw sugar beet fermentation extract by successfully distilling ethanol, while also identifying that the main fermentation by-product was butanoic acid.

The discovery went on to earn Alex and John a prestigious National Science and Engineering Competition (NSEC) prize, presented at the Big Bang Fair in 2011 by Professor Brian Cox.

The future looks sweet

In 2013, Alex made a further discovery – that butanoic acid derivatives, such as ethyl butyrate, were actually even more useful bio-fuels than ethanol. Working with Sofia Papadouli in the University of Bristol's Chemical Synthesis Centre for Doctoral Training, they successfully ran test reactions with hexanoic acid and ethanol.

But they found a sticking point in removing sufficient water from the fermentation broth to make the butanoic acid reaction efficient, posing new questions for Alex and the School of Chemistry and paving the way for further explorations.

"This is a perfect example of how students can apply science to real-world problems," says Craig Butts, Reader in Mechanistic and Structural Chemistry. "By coming to Bristol and using our labs and equipment, Alex and John were able to move a step closer to a really useful biofuel product.

"Will they be selling their ideas to Shell next year for millions? Probably not. But have they learnt a great deal to take into their scientific careers? Absolutely."

Energy from greens

Evidence for the potential of sugar beet as an alternative source of fuel has been increasing in the last decade. Its conversion to bioethanol and, more recently, biobutanol – a more energy-dense fuel – is already proving useful on large commercial scales. The British Sugar Biofuel Plant at Wissington in Norfolk is just one factory that makes use of the plentiful supply of sugar beet feedstock that is produced in the region. The use of ethyl butyrate is an even more recent development, as both an additive and a raw fuel, with companies modifying microorganism strains to increase fermentation.

Wissington factory produces up to 55,000 tonnes of bioethanol fuel

Source: www.britishsugar.co.uk

Duncan Tarling creates dozens of pieces of bespoke glassware every week

Mr Maker

Meet the craftsman who feeds the school's insatiable demand for laboratory glassware

OVER THE LAST 30 YEARS, Duncan Tarling has played a part in more experiments at the School of Chemistry than any other staff member – and yet he happily admits he's no chemist. Rather, he's the school's glassblower, responsible for creating hundreds of complex pieces of glassware every month – perhaps 100,000 pieces over the course of his career.

"I saw it advertised and thought it was something different," he recalls of his arrival at the University as an apprentice in the mid-1980s. Previously part of a three-man team, Duncan now operates solo from his back-room studio at the school's Cantock's Close site. Working to a verbal brief or a quick sketch, he can produce a simple piece of glassware in just a few minutes.

"Most things are made from hollow borosilicate glass tubes," he explains. "I buy them in widths from 4mm up to 100mm, plus separate joints and taps. The glass is melted with a torch or bench burner, and then formed into the shape you need. There's only about half a dozen processes in glassblowing really, you just join them all together."

More complex projects include glassware incorporating quartz – used for experiments involving ultraviolet light – which has a higher melting point than borosilicate and is therefore harder to work.

And while it might seem an anachronism to employ an in-house glassblower in a modern chemistry faculty, Duncan saves the school both money and time.

"A lot of the equipment they use in here, you simply can't buy off the shelf – you'd have to have it specifically made. I can make a quartz cell for £20 or so, whereas it might be £500 from a supplier. And you can have it in days rather than weeks."

Duncan's creative skills don't end in the lab either. In his spare time, he builds kit cars, and from time to time may be spotted driving his home-made Sylva Riot round the racetrack at Castle Combe in Gloucestershire.

2,000 yrs

Glassblowing dates back to the Middle Eastern cities of the 1st century BC Roman Empire. Similar techniques have been used continuously for 2,000 years.

2,282°F

Temperature at which borosilicate glass starts to melt (1250°C)

Dancing with molecules

What links Feynman-Hibbs molecular dynamics with the acclaimed violinist Nicola Benedetti? Dr David Glowacki – chemist, author and inventor of danceroom Spectroscopy – explains

Can you explain your danceroom Spectroscopy project?

I lead a project where we've made an interactive chemistry video game called danceroom Spectroscopy. Using a set of 3D sensor cameras connected to a computer with 5,000 processors, our video game lets you see your energy field and use it to control the motion of atoms and molecules.

In the autumn we hooked violinist Nicola Benedetti and her violin up to our system. She was able to control the graphics on a massive screen using both her motion and the notes she was playing on her violin. She'd never done anything like it before, and she loved it! We got massive applause at the end.

The following morning I participated in a panel discussion of the previous night's performance. There were musicians, music professors, experts in English literature and artistic producers. For a solid hour, they gave marks on the performance: what they liked, what they thought could be better, what they did and didn't understand.

You're a busy man. Can you describe a typical day?

About the only thing that I can guarantee in my job is that no two days are ever the same. Here's how my job works: I do pretty much whatever I like and I get a paycheck every month. In order to keep getting a paycheck, I try to make sure that, firstly, whatever I do increases the human knowledge that's already out there; secondly, I do a good job; and, thirdly, it gets other people excited.

It's pretty easy to satisfy these criteria, so long as I carry on with fun stuff, and so long as I find talented and energetic people to do it with. And whatever I do or whatever I find out, I never stop asking myself one question: 'Why?'

You frequently travel to discuss your research, what have you done recently?

In August I was in the USA for a meeting in Telluride, Colorado, which is so high up in the Rocky Mountains that the thin air can make people ill. The meeting was trying to figure out how enzymes work. Our bodies are human-sized chemical factories, and enzymes are little molecular machines that manufacture the chemicals we need to live. Without them, we're dead.

I wrote a paper last year outlining some new ideas for how they work, but lots of famous scientists disagreed with my ideas, and most of them were in Telluride. We basically had the equivalent of a playground fight, with some people on my side and some on the other side.

5,000

the number of processors in the computer that runs the dS programme

21m

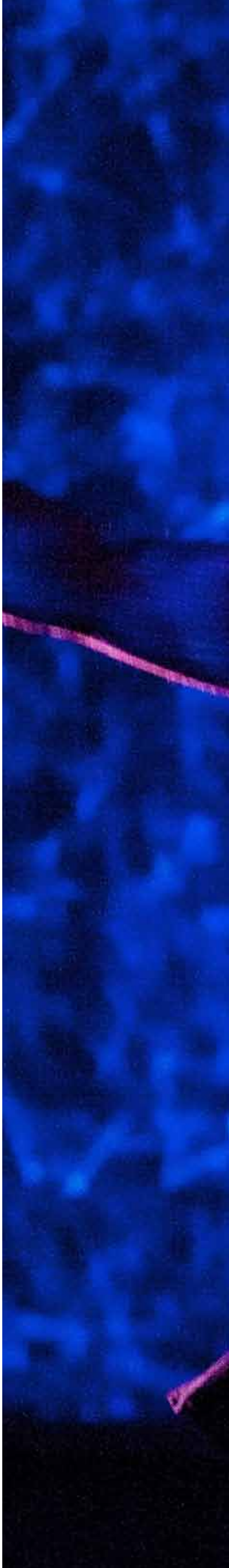
dS uses a 21-metre, 360 degree immersive projection dome

Also last summer, I attended a unique conference, held at the Kloster Seeon monastery in the foothills of the Bavarian Alps. The aim of the meeting was to bring together some exciting early-career chemists from the UK, USA and Germany in order to facilitate international networking across diverse chemistry disciplines. I presented in a session entitled 'Applied Theory', and had the opportunity to hear loads of amazingly talented scientists discuss their research across biochemistry, materials science, soft matter, theory and computation, organic chemistry, and so on.

And the future?

In 2013 I was awarded a Royal Society University Research Fellowship, hosted by the University of Bristol. My research fellowship is to carry out a programme entitled 'Beyond equilibrium: Ultrafast solution-phase dynamics and enzyme catalysis'. These fellowships are an amazing opportunity: they provide five to ten years of funding and a tremendous amount of intellectual freedom, so just my cup of tea!

For more details and video, visit danceroom-spec.com



danceroom Spectroscopy

How does it work?

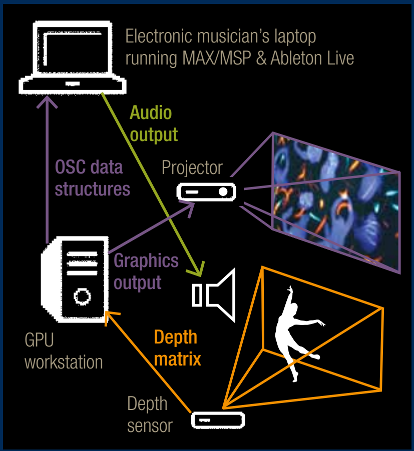
"This multi-award winning project is at the frontier of Sci-Art collaborations," says David. "It explores new languages and crossovers on the interface of physics research, interactive art, education, performance and technology. It interprets people as energy fields, allowing them to influence both graphics and sound, using their movement."

What's on the screen is a computer simulation of molecule movements, determined by Feynman-Hibbs molecular dynamics. Dancers are captured by 3D cameras and manipulated into energy fields during the performance.

Dr Glowacki told the Huffington Post: "On a fundamental level, the microscopic atomic and molecular interactions we have with our environment are energetic. Using physics-based molecular models, real-time supercomputing, and digital artistry, dS gives you a glimpse of your energy field, embedded in a sea of atoms and molecules.

"As you move, your energy field interacts with these atoms and molecules, affecting their vibrational dance, and generating sound and images. It's actually not so different from what's happening to you as you sit reading this article: trillions of invisible atmospheric molecules are microscopically battering you and momentarily interacting with your energy field at the point of impact."

Dr Glowacki discusses the dS project with dancers



Unravelling the origins of life

How did the first biological cells, the basic building blocks of life, form in a world devoid of biopolymers? That's the question that drives research in Professor Steve Mann's Protolife laboratory

As jobs go, searching for the origins of life takes some beating. But that is the goal of the school's Protolife laboratory and its leader, Professor Steve Mann. Conventional research in this area focuses on trying to produce ever simpler cells in which unnecessary functions are stripped away to leave minimal cells that could have formed with the smallest number of genes necessary for life.

Professor Mann, however, is taking a different approach. Could the first cells have formed through the spontaneous ordering of smaller molecules such as fatty acids or phospholipids into semi-permeable protocell structures? Could such self-assembly have resulted in the formation of structures capable of trapping the diverse range of reactive components necessary for primitive replication and metabolism?

Professor Mann's lab is designing experiments which demonstrate that simple protocells can form through self assembly, undergo self-reproduction to produce new protocells, and grow into larger structures as reactions proceed between the molecules trapped within the chemical micro-compartments.

"Five years ago my group was focused solely on nanomaterials chemistry; now, nearly everyone in the group wants to work on the chemistry of protocells because we are all incredibly excited to do new things, try out new ideas, and continue to push forward the frontiers between chemistry and other disciplines," says Professor Mann.

What is self-assembly?

Self-assembly occurs when molecules spontaneously aggregate together to form complicated ordered structures. The molecules are held together by relatively weak interactions such as hydrogen bonding or van der Waals forces. These interactions

Students at work in the Centre for Protolife Research, which is investigating the origins of cell formation

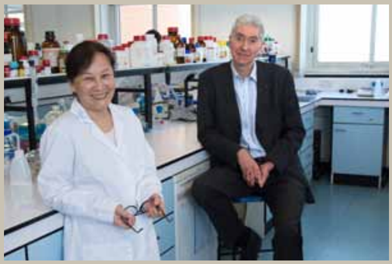
are often directional, so that the resulting structures take on characteristic shapes. Good examples of self-assembly include the formation of liquid crystals, in which large macromolecules align to form ordered phases with properties that are intermediate between those of a solid and a liquid, or the interaction of two polynucleotide chains in a double helix to form a strand of DNA.

The action of household detergents is also the result of self-assembly. Most aqueous detergents contain long-chain carboxylic acid molecules. At certain concentrations, these surfactant molecules aggregate together to form micelles.

The formation of a micelle maximises the exothermic interactions between the hydrophilic carboxylic acid head group and the surrounding aqueous solvent, protecting the hydrophobic hydrocarbon chains within. The resulting structure may trap otherwise insoluble hydrophobic molecules, such as fats or oils, allowing them to be transported, or in the case of detergents, washed away. At low concentrations, micelles are often spherical. However, at higher concentrations, surfactant molecules tend to form extended double layers of molecules in parallel sheets that resemble cell membranes.

Meet the chemists

Prof Steve Mann & Dr Mei Li



Professor Steve Mann is Director of the Centre for Organised Matter Chemistry, and Principal of the Bristol Centre for Functional Nanomaterials at the University of Bristol. His research is broadly focused on the chemical synthesis, characterisation and emergence of complex forms of organised matter, including models of protocell assembly. Professor Mann joined the University in 1998, following tenures at the universities of Oxford and Bath. He has published over 420 scientific papers, and was elected as a Fellow of the Royal Society in 2003. Outside academia, he enjoys running half marathons and playing the electric guitar.

Dr Mei Li recently took up the role of Laboratory Facilitator in the newly founded Centre for Protolife Research at Bristol, to manage the research centre and projects on protolife research. Her research activities involve a wide range of interdisciplinary fields across nanotechnology, materials chemistry, biology and physics. She has published nearly 80 well-cited research papers and review articles in major international journals. Her current research focuses on the design and construction of artificial chemical cells and protocell models based on spontaneous processes of inorganic self-organisation, construction of functional membrane of inorganic protocells and self-reproduction of inorganic protocells.

Picturing vanilla: a sponge cake, lab flasks and orchid flowers, relatives of the *vanilla planifolia* orchid

A flavour of science

The school's new PictureIt… *Chemistry* blog delves deep into the chemistry of everyday substances – including a certain flavouring for ice creams and cakes, derived from the vanilla pod. Here's an extract…

With *The Great British Bake Off* sparking people's interest in baking, the Victoria sponge is all the rage. But your bog-standard eggs, sugar, butter and flour would be nothing without the sweet, fruity fragrance of vanilla. This versatile, and notoriously expensive, flowering plant is used as flavouring in perfume and in aromatherapy, but is also useful for the chemist in the laboratory.

Origins

Vanilla was first cultivated by the Totonac people of eastern Mexico in the 15th century. In the early 16th century, the Spanish arrived in eastern Mexico, and it is from the Spanish 'vaina' that the word 'vanilla' originates, translating as 'little pod'.

Vanilla is obtained from a member of the Orchidaceae family plant, *Vanilla planifolia.* It is from the seed pods that the distinctive, identifiable flavour derives. The vanilla plant naturally grows only in tropical and subtropical regions and as such is the second most expensive spice that is commercially available, falling behind only saffron. This is because commercial cultivation of the plant is very labour intensive; for example, the flower needs to be hand-pollinated to mimic the natural pollination by hummingbirds and bees that are native to Mexico and Central America.

Interestingly, the distinctive smell of vanilla is not present in freshly-picked vanilla pods. This is because in the pods the vanillin is stored as β-*D*-glucoside and is not released until the pod is cured. During curing, some of the vanillin β-*D*-glucosidase is converted into vanillin, with the rest being converted, upon consumption, by enzymes in saliva.

Synthesis and uses

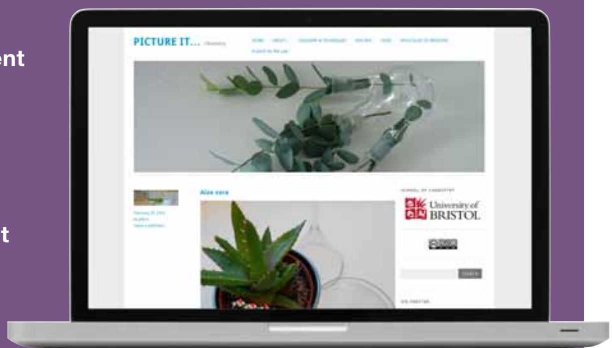
The smell of vanilla comes from over 200 odorant molecules, but the molecule that is the main contributor to the fragrance and flavour is vanillin. Because of the high cost of growing the plant, artificially synthesised vanillin now accounts for over 95% of all vanilla flavouring sold. The first industrial production of vanillin came from a synthesis starting from coniferin (found in the bark of pine trees) by two German chemists, Ferdinand Tiemann and Wilhelm Haarmann, in 1874.

The uses of vanillin are wide and varied. We are familiar with its prominence in baking and in chocolate manufacture, and even its involvement in the perfume industry, but a huge amount of the world's synthetic vanillin is used in the synthesis of other chemicals, such as pharmaceutical drugs. Not only this, but vanillin is used in food products, as an additive to mask

About the PictureIt... *Chemistry* blog

Dr Jenny Slaughter and Dr Natalie Fey started the PictureIt... *Chemistry* blog as a means of talking about science in a way that anyone can understand. Each post is written by a collaborative team, bringing together research and ideas from technicians, administrative staff, academics, undergraduates, postgraduates and school students. As well as vanilla, other recent postings comment on diverse topics including the properties of marmalade, spearmint, bananas and aloe vera.

You can read the blog in full at chempics.wordpress.com



VANILLA IS THE SECOND MOST EXPENSIVE SPICE THAT IS COMMERCIALLY AVAILABLE, BEHIND ONLY SAFFRON

unpleasant flavours that may arise from oxidative degradation of other chemicals in the food. Vanillin has been reported as having antioxidant properties in complex foodstuffs that contain polyunsaturated fatty acids.

In the lab

Vanillin is also used by chemists in the laboratory; in thin layer chromatography and in the synthesis of other chemicals, such as the pharmaceutical drug *L*-dopa – used in the treatment of Parkinson's disease.

Vanillin is a white, crystalline solid, with a melting point of 81 °C. It is scientifically known as 4-hydroxy-3-methoxybenzaldehyde. The component functional groups present in the vanillin structure include an aldehyde, an alcohol, a methoxy group and the benzene ring. The presence of so many functional groups means that vanillin is a molecule that can undergo many different reactions.

There are at least ten ways to synthesise vanillin. The majority of modern-day syntheses are very similar to the original synthesis by Tiemann and Haarmann, but starts from guaiacol, which can also be obtained from the bark of pine trees. The most common method of industrial vanillin synthesis on a large scale is from the starting product eugenol, found in cloves, nutmeg and cinnamon.

More recently, lignin extracted from cow dung was utilised in the synthesis of vanillin. As well as the dramatically low production cost of synthesising vanillin this way (less than half the cost of synthesising vanillin from vanilla pods), this discovery benefits farmers too. Lignin does not readily decompose, and so the extraction of lignin from the excrement of grass-eating animals means the dung can then be re-used as fertiliser to improve soils. ■

Contributors: Hannah Haines-Horan, Nick Taylor, Natalie Fey and Jenny Slaughter

95%

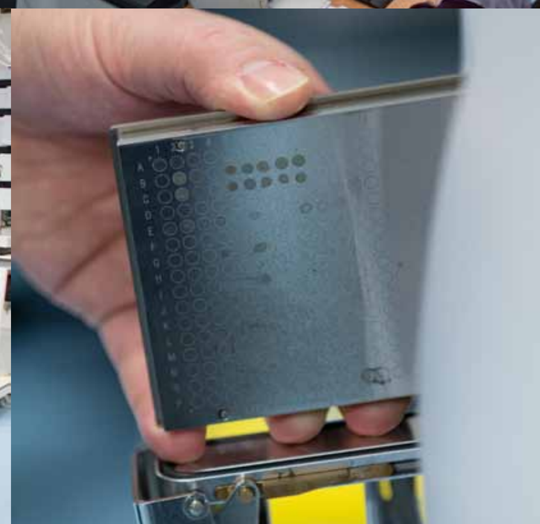
Artificially synthesised vanillin now contributes to over 95% of all vanilla flavouring sold

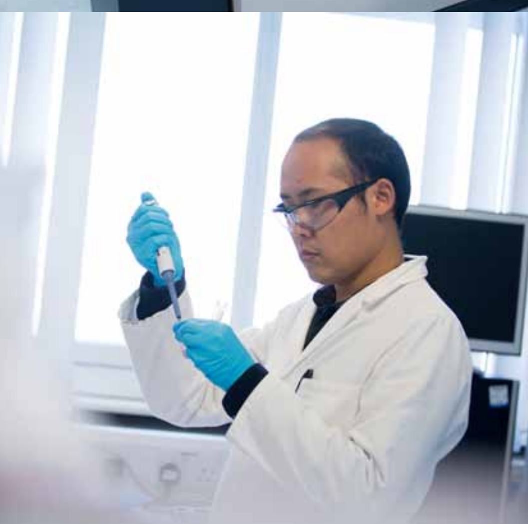
Meet the chemist

Dr Jenny Slaughter

Dr Jenny Slaughter is one of the two-woman team behind PictureIt... *Chemistry*. When not unravelling the interesting chemistry central to our everyday lives, she runs the advanced undergraduate practical laboratories.

As International Admissions Tutor, she recently visited Hong Kong, going to schools and colleges, meeting prospective students, staff and parents. When not at work, Jenny can be found 'hanging out' in one of Bristol's three climbing centres, or at one of the South West's numerous outdoor crags, escaping to the mountains in her camper van, or taking to the hills on her mountain bike. She's also a keen amateur baker and jam-maker, using the produce from her fruit and vegetable garden.





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