Hello and welcome to Resonance Issue 6! Whether you’re a seasoned reader, or you’re picking up a copy for the first time, I’d like to thank you all for your continued support as without you Resonance would not exist.

This is my first issue taking over from Zoe as the editor and I’d just like to commend her on the amazing job she did with the previous two editions. She made the job seem much easier than it is! I’m fortunate that I’ve had excellent support from Joe Clarke and would like to thank him for all his help in putting this issue together. With his wise input and the creativity of all of those who have contributed to this issue, I feel that we’ve made a sleek, informative newsletter that I hope you enjoy reading.

When the opportunity to take over as editor of Resonance was offered to me, I was pleased to accept the role as for me it holds some good memories. Back in 2012, I was a member of the first group of students, tutored by Prof. Simon Jones to produce a departmental newsletter as part of our “Skills for Success” project. One of my collaborators was Alex Stockham, who went on to set up Resonance, and another was Jenna Spencer-Briggs, who took over from Alex as the editor for issue three. I’m in awe at the initial hard work it must have taken to set up Resonance, and I’m proud to build upon the excellent foundations that they created.

This issue sees us celebrating one of our famous alumni, Prof. Fraser Stoddart, who was recently honoured with a Nobel Prize in Chemistry alongside Jean-Pierre Sauvage and Ben Feringa, for their work in the “design and synthesis of molecular machines”. We take a look at their work and also delve into the supramolecular chemistry currently taking place in our very own department. For those curious about our department’s history take a look at our feature on pages 13 and 14, and for those international readers over in Nanjing, we have a special article written by one of our colleagues about her experiences in Sheffield so far.

Happy reading.

Beth Crowston
The Nobel Prize in Chemistry 2016
The field of Supramolecular Chemistry has recently been awarded the highest accolade. We discuss the research behind the award and interview Prof. Mike Ward and Prof. Jim Thomas on their contributions to the field.

Departmental History
Zoe Smallwood discusses the changing face and facilities of the department in the first of a two-part feature.

From Mars to the Stars
The wide variety of chemical instrumentation on board NASAs Curiosity Rover is discussed as well as the potential of extraterrestrial life.
The summer of 2016 was drawn to a close with an event organised by a group of PhD students working at The University of Sheffield when they decided to host their own event to celebrate the work done by chemists that work across disciplines. The organisers felt that they were not given the opportunities to present their interdisciplinary work at other symposiums that focus on small, specialised areas of chemistry. Over 110 researchers from around the United Kingdom registered to hear how chemistry can be applied to physics, medicine, dentistry, and carbon capture, as well as viewing posters with a similarly diverse outlook. Talks from academics and shorter talks from early career researchers entertained the audience, with Seb Spain, Dan Jenkinson and Jamie Wright from Sheffield each giving a talk on the day. Other speakers included Natalia Sergeeva from Leeds, Carmen Galan from Bristol, and Duncan Graham from Strathclyde.

The event could not have gone ahead without the generous backing of the sponsors, which came from the Royal Society of Chemistry (both the Small Grants for Scientific Activities committee, and the Sheffield and District local committee), and industrial sponsors (StarLab, Fisher Scientific, Fluorochem, Asynt, TCI and Merck), representatives of which were present on the day. Prizes for the best poster and best early career researcher were kindly provided by The University of Sheffield Polymer Centre and went to Ben Allen and Vanessa Marcos respectively.

Overall, the event was a massive success and a group of PhD students from The University of Leeds expressed an interest in hosting the event next year, so keep an eye on your inbox for news of the next event!
Soft Matter Analytical Laboratory

The University of Sheffield’s brand new laboratory for categorising materials opened its doors in October 2016, Joseph Clarke brings you some of the details of this new laboratory.

Those students currently at the University might have noticed the redevelopment that has taken place around Mass Spectrometry on B-floor. Now it is home to the newest piece of analytical equipment and a new laboratory specifically built to image soft matter. Welcome to the Soft Matter Analytical Laboratory, also referred to as SMALL.

The new laboratory is the result of a £2 million investment, part funded by the Engineering and Physical Sciences Research Council (EPSRC). The project was completed in May 2016 and was officially opened at a dedicated symposium on the 7th of October 2016. The symposium featured guest lectures from leading researchers in the field and a speech from the Pro-Vice Chancellor.

At the heart of the new laboratory is the new Small Angle X-ray Scattering, SAXS, instrument. The machine is the first of its kind in the UK, equipped with a liquid gallium MetalJet X-ray source purposely built for the university by the French company Xenocs. In addition to SAXS, the laboratory is also equipped to perform rheology measurements, in which the flow of materials is studied.

The principal focus of the laboratory is the characterisation of materials. This includes polymers, colloids, films and proteins. From a chemical perspective one of the main uses will be in the study of polymers. The random order of polymeric chains leads to difficulties in characterisation. SAXS experiments can be performed on these disordered systems making it appropriate for structure investigation.

Furthermore, biological materials can be studied. Using SAXS and a combination of other crystallographic techniques, protein structure and, importantly, protein shape can be deduced. The advantage of using SAXS is that analysis is performed in situ, meaning proteins are analysed without having to move them into destructive media.

The experimental setup in SMALL is highly adaptable overcoming some of the challenges of studying thin films. The main challenge is the small surface available to image. Built-in to the apparatus is the ability to rotate any sample from a perpendicular path to a parallel pathway. This will skim the top of any surface resulting in a better scattering pattern.

Investment at this level is needed in this field. Measurements of this type were previously only possible at synchrotrons. This made it a lengthy and time-consuming process, since there are only a handful of these throughout Europe. Performing these measurements in-house will remove this barrier allowing characterisation in a fraction of the time.

The first results obtained from the laboratory have already been published. The paper appeared in September 2016 as a collaborative study between Dr Mykhaylyk and Prof. Armes.


A Brief Introduction to SAXS.

The study of chemistry typically rests on the visualisation of matter which cannot be viewed by the naked eye. Instead we use techniques to provide information which can aid in the interpretation of what the structure is. For most undergraduates, this is limited to NMR, IR, and mass spectrometry from which characteristic peaks provide indirect evidence for a molecular structure. However in addition to these, one can use Small Angle X-ray Scattering to characterise materials in the range of nanometers ($10^{-9}$ m) to submicrons.

In SAXS, collimated X-rays are directed at a sample. The angle at which this X-ray beam is scattered is subsequently measured by a detector. This angle is often very small. Therefore, powerful machines are needed to detect the defracted pattern. The measurements generate a scattering curve, which is later interpreted to reveal information about the structure of the sample including its shape, its electron density and its internal morphology.
Interview

Resonance Welcomes the
Beth Crowston and Joseph Clarke both had the opportunity

Dr Ben Partridge

Dr Ben Partridge joined the chemistry department in June 2016, having taken up the position of Lecturer in Organic Chemistry. For Ben, the broad range of research conducted in the department made the decision to make the move to Sheffield easier, as he feels that his work on new catalytic methods for the synthesis of organic molecules will complement it well. Currently, organoboron chemistry and catalysis are two separate research areas in his group. However, Ben hopes to develop new, sustainable, catalytic methods by bringing them together with his work which takes advantage of frustrated Lewis pairs (FLPs). This approach has potential to make chemistry greener and more sustainable, as the FLP catalysts would be made from elements (e.g. boron, nitrogen, and carbon) which are more abundant, cheaper and more environmentally friendly than their transition metal counterparts.

Ben accredits his interest in chemistry to the fun experiments he carried out at home when he was younger, and to a particularly memorable teacher who demonstrated the technique of distillation to him when he was 11. He thought that it was “really cool” to see black goo be purified into clean, colourless fractions and wanted to learn more. After continuing to enjoy the subject at school, and then at degree level, his passion for chemistry motivated him to undertake a Ph.D. with Prof. Varinder Aggarwal FRS at the University of Bristol. After this, Ben was encouraged to take up a postdoctoral position with one of the world leaders in transition-metal catalysis, Prof. John Hartwig, at the University of California, Berkeley. Upon his return to the UK, Ben worked with Prof. Hon Wai Lam at both the University of Edinburgh and then at the University of Nottingham.

Outside of chemistry Ben is a keen cyclist. When he finally moves to Sheffield he wants to buy himself a new road bike to take advantage of the city’s close proximity to the Peak District. Currently, he still commutes to work from Nottingham and has only seen the sights between the train station and the department. However, he hopes that he will have plenty of years here in Sheffield to explore the city and the surrounding area. Ben also likes to cook for his friends and family but feels this doesn’t count as a hobby as it is “basically organic synthesis” just in the kitchen rather than the lab.

Dr Tim Craggs

Dr Tim Craggs has developed this technique to a particularly memorable teacher who demonstrated the technique of distillation to him when he was 11. He thought that it was “really cool” to see black goo be purified into clean, colourless fractions and wanted to learn more. After continuing to enjoy the subject at school, and then at degree level, his passion for chemistry motivated him to undertake a Ph.D. with Prof. Varinder Aggarwal FRS at the University of Bristol. After this, Ben was encouraged to take up a postdoctoral position with one of the world leaders in transition-metal catalysis, Prof. John Hartwig, at the University of California, Berkeley. Upon his return to the UK, Ben worked with Prof. Hon Wai Lam at both the University of Edinburgh and then at the University of Nottingham.

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Dr Craggs’ research focuses on single molecule FRET (Förster Resonance Energy Transfer) which is used as an experimental ruler in molecules, and is of particular use in the field of protein studies. Studying single molecules overcomes some of the averaging inherent to ensemble measurements (that typically involve many millions of molecules) and is performed by using minute concentrations. Measuring single molecules means different configurations can be identified. He is currently building his FRET machine, with the help of his level 4 masters students, with the hope of first measurements by Easter.

As well as an interest in biological chemistry, Tim is also a keen musician. In fact, he said that playing the violin in orchestras and string quartets helped to fund the final year of his Ph.D. studies. He also said he enjoyed singing and rowing during his time in Cambridge. Like a lot of academics Tim cycles to the University, with Sheffield’s hilly landscape presenting more of a challenge than Bristol.

Did you Know

FRET is a mechanism of measurement involving light-sensitive molecules called fluorophores. An excited donor fluorophore transfers energy in a radiationless process to an acceptor fluorophore. The efficiency of this transfer is dependent on the distance between the two fluorophores. Dr Craggs has developed this technique for protein structure measurements.

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Dr Tim Craggs

Drawn towards academic science from a young age by a strong scientific family background, Dr Tim Craggs has recently been appointed as Lecturer in Biological Chemistry at the University of Sheffield. After studying undergraduate Natural Sciences and a Ph.D. at Cambridge University, he had a series of domestic and international postdoctoral positions at Oxford, Yale and Bristol before moving to Sheffield.

Tim’s first contact with Sheffield came through a collaboration with Prof. Jane Grasby and through networking at conferences. His decision to move to Sheffield was influenced by its strong performance as well as collaborations with the physics department. A strong incentive was Imagine: Imaging Research,¹ a group of researchers who specialise in biological imaging, which fits well with Tim’s own research goals. This working environment as well as collaborations between departments, Tim tells us, is necessary for progression in his field.

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New Members of Staff
to discuss their interests in research and outside of chemistry.

**Dr Jonathan Foster**

He credits his secondary school teacher with sparking his initial interest in chemistry as he would impress the class with exciting demonstrations - “blown up watermelons, screaming jelly babies, and purple volcanoes all certainly got my attention.” However, it is the creative aspect of chemistry that keeps Jona fascinated as “it allows you to design new molecules and materials that have never existed before,” which in fact he now does on a daily basis as part of his research.

His group are developing a new class of graphene-like two-dimensional nanomaterials called metal-organic nanosheets. Unlike graphene which is just made of carbon, these nanosheets can be assembled in a modular fashion using different combinations of organic ligands bolted together by metal-ions. The advantage of creating these two-dimensional sheets over the atto second timescale (10^-18 s) commonplace, where the process of electron transfer will be easily viewed. To research proteins effectively, spectroscopy at or beyond the pico (10^-12 s) timescale is needed. This requires very sensitive instrumentation which is currently not very common.

A major incentive for Adrien to move to Sheffield was the investment in the new laser facility, and the freedom to pursue his own interests. However, Adrien also praised the people of Sheffield, particularly their friendliness and openness in welcoming him to the city.

Outside of chemistry Dr Chauvet says nature is his hobby as well as his job, noting it was necessary when he worked in Switzerland to get out and about as much as possible. Naturally, he has been enjoying the Peak District where he cycles and walks, while also taking in the rich history. His office contains a plethora of plants and also a rather beautiful picture of the mountains of Switzerland.

Moving from laser physics to chemical spectroscopy, Dr Adrien Chauvet has recently been appointed as Lecturer in Physical Chemistry. Adrien studied Materials Science and then obtained a Ph.D. in biophysics, at Purdue University, USA, in 2012. He was then awarded a postdoctoral fellowship at the Polytechnical Federal School of Lausanne, in Switzerland followed by a senior postdoctoral position at the University of Geneva. It was from this position that he was hired to Sheffield.

**Dr Adrien Chauvet**

His main research interest lies in the area of biological chemistry, specifically, understanding the function and behaviour of proteins along the pathway of photosynthesis. Achieving a thorough understanding of the background of photosynthesis was a driving-force for the application of laser physics to the fields of biological chemistry, as Adrien says:

“Nature saw the perfection of one molecule to perform multiple processes. Learning from Nature can lead to advances in current technology.”

His current focus is on cytochromes, an electron transport protein. Cytochromes work within the cell membrane as both an electron and proton pump. This effectively turns the cell into a “chemical battery” with a positive and negative side. Even though, research in this field is still in its early days, advancing technology will soon make spectroscopy on three-dimensional discrete structures is that the sheets have a very large surface area consisting of a tuneable, periodic array of binding sites. This potentially allows you to do new things with these materials that you can’t do with discrete molecules. For example, the group are interested in developing them for a diverse range of applications such as creating new sensors to diagnose disease; more efficient catalysts for green synthesis; porous membranes for cleaning water and air, and new flexible solar panels.

Jona felt that joining the department here in Sheffield would benefit his research interests as it is very friendly and supportive, and is furnished with the equipment and expertise he needs. As a keen climber, he claims that the proximity of the Peak District didn’t influence his decision to come to Sheffield. However, as he and his wife recently had their first baby, his son has become a pretty all-consuming ‘hobby’ for the last 6 months instead.
The Nobel Prize in Chemistry 2016
Jean-Pierre Sauvage, Sir J. Fraser
“The design and synthesis of molecules that can move”

Sir Fraser Stoddart was awarded a third share of the Nobel Prize in Chemistry for his research in supramolecular chemistry. Sir Fraser has now become the fourth Nobel Prize Laureate associated with the department joining previous scientists Lord George Porter (1967); Prof. Sir Richard Roberts (1993) and Prof. Sir Harry Kroto (1996).

Sir Fraser joined the department as a research fellow in 1970 before becoming a Lecturer of Chemistry, and eventually being promoted to Reader in 1982. He finally left the University in 1990 to take up a position at the University of Birmingham before moving to the USA where he is currently Professor of Chemistry at Northwestern University in Evanston, Illinois. However, it was work that was performed in Sheffield that laid the foundations of research which would lead to his Nobel Prize award.

Research into Rotaxanes
Work conducted by Sir Fraser and the Sheffield research group in 1991 was cited and praised in the Nobel Prize announcement. This work was on the synthesis of molecules which would become known as rotaxanes. These are molecules where a molecular ring is closed around or threaded through a mechanical axle. The synthesis of rotaxanes often relies on intermolecular interactions, which drive the reaction, the most common of which is the stacking of aromatic rings.

The specific rotaxane that Sir Fraser synthesised relied on the stacking of aromatic rings along a linking chain. A ring closing reaction was performed which trapped the ring on the axle. Sterically bulky groups, in this case Si(CHMe2)3 ‘stoppers’ at the end of the chain prevented the newly formed ring from escaping. The exciting aspect of rotaxanes is the potential shuttling motion that can occur if there are multiple sites of interaction. This is an example of early work into the production of a molecular motor. Further research adapted this by changing the heteroatom to create systems where electrochemical oxidation or reduction, or even a pH-change, could lead to the ring ‘moving’ from one phenyl group to another.

Further research into rotaxanes led to several interesting features. These included the synthesis of a “molecular elevator” where the rise or fall of the rotaxane could be controlled; a molecular actuator which resembled muscle; and finally in 2007 of a rotaxane-based device with memory function. These devices used the fundamentals that were established in Sir Fraser’s 1991 paper. This single paper has led to the construction of tiny molecular based machines which have the potential to revolutionise technology in the future.


For more information visit the Nobel Prize
Jean-Pierre Sauvage’s contribution can be considered to be the lynchpin to the ‘design and synthesis of molecular machines’. Although rotaxanes and catenanes – two or more macrocycles interlocked – were already known structures, it wasn’t until Sauvage’s involvement in 1983 that they could be synthesised in any meaningful quantity. Whilst working on a complex consisting of two crescent-shaped ligands entwined around a central Cu(I) atom, Sauvage noticed the resemblance the structure had to a non-cyclised catenane. By connecting the open ends of the ligands and removing the metal ion, he successfully pioneered the templating approach to synthesising mechanically, interlocked machines. Many complex and intricate entities were to follow after this breakthrough, including trefoil knots and Solomon links.

Ben Feringa built on Stoddart and Sauvage’s work by demonstrating the first example of controlled unidirectional motion similar to that seen in a rotary motor device.

The first device was based on a light-activated molecular switch, in which a molecule with isomerisable double bonds would alter its configuration when exposed to UV light, and then return to its original form upon thermal relaxation (as shown below). The compound can be thought of as consisting of two “blades”, and each irradiation-relaxation cycle would effectively rotate the “blades” by 180°. By preventing this rotation from reversing, the compound’s movements were essentially shown to mimic those of a propeller blade. Over the years astounding progress has been made by the Feringa group, with the fastest rotational frequency achieved so far being a staggering 12 million revolutions per second.

Taking their “molecular machines” even further into the realms of Nobel-prize-worthy work, the group have demonstrated that they can use their motors to move a microscopic object 10,000 times its size. Astoundingly, this movement can even be seen by the naked eye. The group has even designed and manufactured a “nanocar”; a structure comprised of four motor components that can be driven along a surface.

With the field of “molecular machines” flourishing, scientists now look to the future and speculate just how the ingenious field of molecular nanotechnology can be translated into real-world applications. With plenty of ambitious ideas currently being pursued, the one certain thing is that Stoddart, Sauvage and Feringa definitely deserve to share this prestigious accolade for the endless inspiration they have for tomorrow’s scientists.

Ben Feringa was awarded on the 5th of October to Stoddart and Bernard L. Feringa for their work on molecular machines.”
transcription factor proteins involved in recognising DNA. I thought, this is like genuinely synthetic biology, making something that’s completely abiotic but functions in a way natural systems do.

We started looking at DNA binding and found that this macrocyclic structure binds to DNA on the outside in precisely the same way a transcription factor called the TATA-box binding protein does. This protein is unique in that the whole thing binds on the outside of DNA. What piqued my interest was the fact that the emission properties of these macrocycles change when they bind to DNA, meaning you can probe DNA binding. What made it really interesting was the observation that these large molecules do go into cells. We found that when the compound went into cells, under the influence of light and oxygen, the cells died.

To cut a long story short, the compounds turned out to be sensitizers for photodynamic therapy. The building blocks that these compounds are made from are efficient at creating singlet oxygen on photoexcitation, but they don’t go into cells. The macrocycles we form from the building blocks do go into cells, functioning as a phototherapeutic. I was pleased to see that something that started off as a speculative thing has ended up having some possible future therapeutic leads.

I was doing a PhD at the University of Birmingham, when the head of department was Fraser Stoddart, who won the Nobel prize a few weeks ago. We used to get quite a lot of people coming to visit Fraser so we had a lot of seminars about supramolecular chemistry. My PhD was vaguely in the area and I just sort of thought I’d really like to pursue it. I applied for a position with people that were working in that area and I was lucky enough to get into a lab with Jean-Marie Lehn, who co-founded the area of supramolecular chemistry. One of the co-winners of the Nobel prize this year is an ex-PhD and post doc of Jean-Marie, Jean-Pierre Sauvage, who Prof Mike Ward worked for.

What drew you to the field of supramolecular chemistry?

I was doing a PhD at the University of Birmingham, when the head of department was Fraser Stoddart, who won the Nobel prize a few weeks ago. We used to get quite a lot of people coming to visit Fraser so we had a lot of seminars about supramolecular chemistry. My PhD was vaguely in the area and I just sort of thought I’d really like to pursue it. I applied for a position with people that were working in that area and I was lucky enough to get into a lab with Jean-Marie Lehn, who co-founded the area of supramolecular chemistry. One of the co-winners of the Nobel prize this year is an ex-PhD and post doc of Jean-Marie, Jean-Pierre Sauvage, who Prof Mike Ward worked for.

Could you tell me about your recent research or a recent publication?

I’ve got two interests really. One is to do with therapeutics, imaging and biological things. The other is trying to do self-assembly with building blocks which are in themselves interesting, either for photochemistry or electrochemistry. The last publication we had fused both. We made a variety of macrocyclic structures from building blocks; one in particular has a ruthenium centre. The final assembly has four metals in it, two of which are ruthenium, two of which are rhenium ion “connectors”. The interesting thing is they have a photo-excited state and so they’re luminescent. The thing that started me working on these systems was that they look like some transcription factor proteins involved in recognising DNA. I thought, this is like genuinely synthetic biology, making something that’s completely abiotic but functions in a way natural systems do.

We started looking at DNA binding and found that this macrocyclic structure binds to DNA on the outside in precisely the same way a transcription factor called the TATA-box binding protein does. This protein is unique in that the whole thing binds on the outside of DNA. What piqued my interest was the fact that the emission properties of these macrocycles change when they bind to DNA, meaning you can probe DNA binding. What made it really interesting was the observation that these large molecules do go into cells. We found that when the compound went into cells, under the influence of light and oxygen, the cells died.

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Could you tell us a bit about what your future research plans are?

An ex-PhD student of mine contacted me and asked if it was possible to collaborate and carry on looking at the compounds he developed during his PhD. This is quite unusual and obviously I was interested to work with an oncologist, who is his current boss in Oxford, and their studies have now got to the point where two of our therapeutic lead compounds are now being put into mice.

Within Sheffield, through collaborations with biomedical science and the medical school, we’ve got another set of systems which are getting to the point where they will be looked at as cancer therapeutics that will hopefully work by a different route to the traditional therapeutics. Theoretically they should work against cell lines that are resistant to normal therapeutics. There’s still a long way to go, but when I started this twelve years ago I never thought we’d get to this point.

What would you say was the catalyst for the exponential growth in the field of supramolecular chemistry over the last 50 years?

I think the Nobel committee hit the nail on the head when they awarded this current Nobel prize for molecular machines. Within the media it’s been covered as nanotechnology, but really it’s a development of supramolecular chemistry. I think Jean-Marie had the kind of vision to advance the field and the three people that they have selected are the people that took that baton and moved it forward.

Jean-Marie is still publishing a lot of work in the area on devices, but certainly the three people the committee selected have started producing materials that could have real applications, in particular Fraser’s work in getting working memory devices on a molecular scale. I think the way forward now is to push that further. So for instance, I think over the next twenty years you might see molecular scale memory for computers.

1. Thomas et al., Chem Eur J, 2016, 17, 5996-6000.

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**Elemental Factfile: Iron**

*By Rachel Mowll*

Iron is the fourth most abundant element in the earth’s crust. It also makes up a large proportion of the earth’s core, although the exact composition of the core is unknown. In its elemental form iron is a grey metal, however it is most commonly found as the mineral haematite (Fe₂O₃). It has been used by humanity since prehistoric times. Iron played a large part in the industrial revolution with many innovations dating from this time such as the puddling and rolling techniques which allowed impurities to be removed and led to much larger scale production. The building of the railways in Britain in the early 19th century caused the demand for iron to skyrocket. The addition of carbon allowed steel to be created which is a hugely versatile material used in countless applications. There are many different types of steel depending on the application and these contain small amounts of other metals, for example chromium and nickel in stainless steel which of course was developed in Sheffield by Harry Brearley.

Iron is also used as a catalyst in some essential industrial processes. These include the Haber-Bosch process, forming ammonia from nitrogen and hydrogen, and the Fischer-Tropsch process which converts syngas (hydrogen and carbon monoxide) into hydrocarbon fuels. Different metals can be used as catalysts for the Fischer-Tropsch process but iron is relatively cheap so it is often used and is particularly effective for certain types of syngas which contain a higher proportion of carbon monoxide.

It is well known that iron plays an important role in biological systems and that it is important to get enough iron from dietary sources. This is because many proteins contain iron coordination sites. The most famous of these is haemoglobin. Haemoglobin is responsible for the essential process of transporting oxygen around the body in red blood cells. In mammals it is most commonly made up of four protein subunits, each of which contains one heme group, a porphyrin ring with an iron ion coordinated in the centre. The iron centre in each heme unit coordinates one oxygen molecule for transport around the body.

**Sheffield Steel:** [http://bit.ly/1I16YZn](http://bit.ly/1I16YZn)
**RSC factfile:** [http://rsc.li/1aJFfPg](http://rsc.li/1aJFfPg)
What drew you to the field of supramolecular chemistry?

I started during my PhD exploring the coordination chemistry of long polypyridines. We made some compounds and got some crystal structures, which turned out to be very exciting! These were some of the first examples of what we call double helicates. These structures have two metals in a central spine, and two ligand strands that coordinate around this spine and it looks like DNA and I thought, “well that’s cool”. This research generated some quite high impact papers because they were amongst the first examples of what we now call self-assembly: the ability of simple components, given the right conditions and geometric information, to come together into elaborate complexes under their own steam.

There are two approaches to synthesis, really. Conventional covalent bond synthesis is all about controlling covalent bonds. You can do a coupling here, an elimination there, an SN2 here, you can visualise a molecule and build it with complete certainty in lots of steps.

At the other end of the scale biology does interesting things with self-assembly. You can take very simple components, sit back and let them sort themselves out into remarkably elaborate structures. All of biology relies on self-assembly. It is a completely different approach to synthesis. So, it struck me as an interesting area and I’ve been playing with it ever since.

Could you give me a brief summary of your recent work?

There is a recent paper, that I’m sort of pleased with.1 We use the trick of self-assembly to make hollow capsules. Eight metal ions and twelve ligands spontaneously assemble to form a cube. You have a metal ion at every corner and a bridging ligand along every edge. It’s a nice example of self-assembly. Twenty components just zip themselves up to give a single structure because all the bits are complementary. It’s like putting a bunch of jigsaw pieces in a bag, giving them a shake, and finding the completed picture.

It turns out that these hollow cages bind molecules in the central cavity. This cage has a water soluble exterior, but the interior is hydrophobic. This means that, in water, anything that is hydrophobic will bind tightly in the cavity, size depending. For example, look at the crystal structure (see the structure on the left) of a cage/guest complex, with benzisoxazole sitting nicely in the cavity of the cage.

What we found in collaboration with Nick Williams, and this was really nice, is that the bound guest undergoes a reaction with base – the Kemp elimination. It’s not a particularly interesting reaction on its own, except that when performed in the cavity of the cage it’s accelerated by a factor of almost 1,000,000, which is a rate enhancement similar to what enzymes can do. It turns out this increased reactivity is related to the charge on the cage.

This cage has 8 Co (II) ions, so it has a charge of 16+. In solution under weakly basic conditions, it ion pairs very strongly, meaning the cage is completely surrounded by hydroxide ions. This means that from the point of view of the guest in the cavity the local pH is 14, even when a pH meter is telling you that the pH is 8. This strong ion pairing effect accelerates the reaction by providing a very high local concentration of anions. It is also potentially very general, because you can put a wide range of guests in the cavity of the cage and different ions around the surface of the cage. What we’re looking at is developing this as a general way to catalyse the reaction of any organic electrophile that binds in the cavity, with any anion you like! That’s a very exciting possibility.
What kind of applications does it have?

Potentially very general catalysis. The high positive charge will hoover up anions around the cage surface, so you can bring together any electrophile and any nucleophile in close proximity, and the reactions will work in water, which is environmentally friendly. If that works, it's very exciting, and Nick and I will be famous (hahaha). The field has changed a lot since Sir Fraser published his paper that led to him winning the Nobel prize.

What would you say has been the driving force behind the changes or the biggest change?

There are two things. One is the drive toward being able to mimic what biology does. Biology is just really clever chemistry. Cytochrome P450, for example can take a hydrocarbon and selectively oxidise it to an alcohol in aqueous conditions, at 1 atm pressure, at pH 7. About the only thing we can do with hexane is set it on fire! That controlled reactivity under mild conditions happens because enzymes are exquisitely selective and facilitate a particular reaction pathway. The fact that biology can do it means it is chemically possible. We've just got to catch up on 4 billion years of evolution!

We're just beginning to understand this complexity and we can make self-assembled systems that can start to mimic what biology does. In fact, a million-fold rate enhancement, isn't far off what enzymes can do.

The other impetus, and this is where the Nobel prize team came in, is towards completely artificial things. Never mind biology, we want to do things that don't exist in the real world. Feringa's clever chiral molecule undergoes a rotational conformation under the influence of light that allows it to actually walk across a surface. That's completely unnatural, but what fun! You can use the tricks of supramolecular chemistry to make molecules do functions that biology and nature have never dreamed of.

With the mimicking biology path, has a motive also been a push toward green chemistry?

When you start talking about the environment, it boils down to energy. Here's a statistic that might surprise you: enough sunlight hits the surface of the earth in 1 hour to provide mankind's energy needs for a year. Why are we short of energy?! What are we doing?! The answer is that we're not as clever as biology. We can't do photosynthesis in the way that biological systems do— it's hard! Reducing CO₂ back to some form in which you can burn it again, whether it's glucose if you're a plant or methanol if you're Julia Weinstein, is basically the way to reverse the destruction of the fossil fuel reserves. Biology does that using a very complicated supramolecular assembly – the photosynthetic assembly. There's a huge drive across chemistry and all the physical sciences to see if we can find ways to do the same thing. Harvest CO₂, shine light on it, reduce it to MeOH, you'd certainly get a Nobel prize for that. Then you've got a portable, carbon-neutral fuel based on harvesting the energy of the sun.

But a lot of the interest in supramolecular chemistry is curiosity driven, it's just fun! These are cute things, they're clever, so there's a lot of intellectual satisfaction in it. Being able to understand how molecules can manipulate themselves, and exploit the way in which they come together, is very satisfying.

Where do you see the field going in the next 25 years?

There are many people interested in these self-assembled cages and other groups have shown catalysis in the cavities. The direction it is moving in now is towards light harvesting. In my cage there are 12 naphthalene groups in the cage. If you put an electron deficient molecule next to normally fluorescent naphthalene it will transfer an electron to it, quenching the fluorescence. Suppose you put in the cage cavity an electron deficient molecule like CO₂. You've surrounded it with an array of 12 electron donors. Wouldn't it be nice if we could get multiple electron transfers to reduce CO₂. We've shown that if you put simple quinones in there you do get electron transfer. Next is to do it with two electrons simultaneously; reducing something by 2 electrons is much harder, because it must happen simultaneously. If you've got everything pre-organised so the electron donors are spatially close then you've got the possibility of multiple electron transfer to a guest handcuffed in the cavity. That's where we want to take it and some other people are doing similar things in the US and Japan as well.

The Beginnings of the Dainton Building

Before the chemistry department was even formed, the university had to be established! In the late 1800’s, there were several precursors to the university in the form of the Sheffield School of Medicine, Sheffield Technical School and Firth College, opened in 1828, 1884 and 1879, respectively. Firth College was founded and named after Mark Firth, the owner of a local steel business.

However, the situation at the School of Medicine was not good, and it faced closure. It was at this point that the city of Sheffield decided a university was needed, for the city to compete with others in the UK. The case was put forward to citizens in the form of a poster, asking people to contribute a penny towards the establishment of a new university for the city. The people of Sheffield responded, and £50,000 later (approximately £15 million in today’s money!) a campus was built on Western Bank for Arts, Science and Medicine. In 1905, the University of Sheffield was opened by King Edward VII and Queen Alexandra (see picture 1).

The Department of Chemistry was initially located a few hundred metres up the road, in the grounds of Firth Court (again named after Mark Firth, who founded Firth College). It was in no way the department we know today with chemicals being stored in air-raid shelters which had remained in the grounds following the World War II. It was later decided that a new venue was needed for the chemists, so what is now called the Dainton Building (the grey/white part that houses the foyer of the building we know today) was built. This was opened in the 1950s by the Duke of Scarborough, in a ceremony that took place in lecture theatre 1 and covered by the Sheffield Star newspaper (photo 2). The building was later named after Frederick Dainton, a chemist who was the Chancellor of the University between 1978-1997.

1. www.sheffield.ac.uk/about/history
the Department

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Dainton Building Renovations

The Dainton building has continued to evolve over the past seventy years. The Main Centre Block was quickly added to in subsequent years. First the East wing was built, in 1961, followed by the West wing, (also known as the Haworth wing) in 1964, which is the section of the department that backs onto the Arts Tower car park. The North Wing, also known as the Beaumont wing, quickly followed in the 1968. This block now contains the undergraduate teaching laboratories. As can be seen in photo 3, construction was not subject to the health and safety regulations we know of today.

The East Wing housed a library (where the entrance to the academic corridor is now), teaching labs and some research labs at the very end of the building, as well as some lecture theatres. The East Wing was host to a visit from the Duke of Edinburgh in 1971, whose visit resulted in crowds of people on the stairwell to try and get a glimpse of royalty. (as shown in picture 5).

In 2005 the East Wing underwent an extensive refurbishment. During this time, the teaching labs were moved to their current position in the North Wing, and the Richard Roberts Auditorium replaced the smaller lecture theatres. In addition, the East Wing was renamed after Richard Roberts, a Nobel prize-winning chemist who studied for his degree and PhD in the department. (photo 8)

The next issue of Resonance will discuss some of the history of our department focusing on what happened to lecture theatres 2-5; the changing community in our department and finally the experiences of a past member of staff.

Zoe and Resonance wish to thank everyone who helped provide information, pictures, and memories of the department history, including: Elaine Frary, Richard Wilkinson, Prof. Mark Winter, Dr David Williams, Dr Sandra Van Meurs, Stephen Atkin, George Dodsworth, David Towers, Dr Catherine Smith and Dr Craig Roberts.
NASA has over 50 years of successful robotic missions to Mars and we are now perhaps as little as 15 years away from the first human mission. With increasing technological advances, we are able to send sophisticated spacecraft that can travel great distances, to learn and build on our knowledge of this distant red planet so that we can plan and pave our way to a new world.

One of the most famous robotic missions is the Mars Curiosity Rover. This travelling laboratory’s mission is to determine the planet’s habitability by analysing the Martian surface. One thing that NASA are hoping to detect are the building blocks of life.

Mars Curiosity Rover has a number of instruments on board to analyse samples on-the-go to achieve its goal. Of the spectrometers it carries, one of the most fundamental is ChemCam (Chemistry and Camera). To analyse the composition of the rocks on Mars, ChemCam fires a laser in a series of pulses that vaporises an area between 1 mm and 7 m away. Atoms and ions within the resulting gas are electronically excited, meaning that super-heated plasma will emit light as the atoms/molecules return to the ground state. ChemCam will detect these emissions and send the light through a fiberoptic link to the body of the unit and then to the spectrometer. The plasma light is then split into its constituent wavelengths. As each element has a “finger print” emission, the onboard spectrometer will determine the composition of the plasma and the abundance of elements within it. ChemCam can also recognise crystal structures such as ice and minerals, and assist in drilling of rock cores. This technique allows Curiosity to take as many as a dozen measurements from the rocks it encounters, per day, with no physical contact.

To determine whether Mars has the potential to sustain life, further study of the role water played in the formation of the minerals on Mars must be established. CheMin (Chemistry and Mineralogy), a mineralogy instrument on Curiosity, identifies the minerals and their abundance. Certain minerals are linked to different environmental conditions that existed when they were formed and with this, and by making comparison to our own planet, it can be determined if Mars bears any resemblance to our own planet at the early stages of its formation.

CheMin prepares samples by firstly drilling the rock it collects and then sieving powder into sample holders. X-rays are directed into the rock sample which will then interact, re-emit or fluoresce at energies that are characteristic of a particular element. X-rays are diffracted by minerals in a characteristic pattern, with this and the X-ray emissions, scientists can identify the composition of the crystalline structures of the samples that are collected on Mars’ surface.

One of the minerals studied is basalt. In particular there are two primary minerals within basalt that form when lava solidifies; olivine and pyroxene, both of which have been detected by CheMin. Jarosite mineral was also found within sedimentary rock by NASA’s Opportunity Rover, which indicates an oxidizing and acidic environment.

Human missions to Mars seem a distant dream, yet we are closer than ever to populating a new planet. Our scientific endeavours, to colonise new land or grow islands in oceans seems to be almost within touching distance. Human capabilities seem to have no boundaries given enough time and who knows we may end up on Mars someday.

Curiosity Facts
1. Launched 15.02 pm (GMT) on 26/11/2011.
2. Landed 5.32 am (GMT) on 6/08/2012.
3. Powered by the heat generated from the radioactive decay of plutonium-238.
4. Provides a mission lifespan of 687 Earth days. Although it is still functional today.
5. Aged exposed surface rock as 4.2 billion years old.

Curiosity factsheet: http://go.nasa.gov/2j1KN01
Mission Overview: http://go.nasa.gov/1cx7cGB
NASA image bank: http://go.nasa.gov/1KX0iyQ
NASA spectrometer: http://go.nasa.gov/1U22F7m
http://bit.ly/2j0fJ2

Images provided by NASA and NSSDCA
Have you ever looked up to the night sky and wondered, are we alone in the universe? As part of ChemSoc’s guest lecture series, Professor Brad Gibson from the University of Hull visited the department to give a lecture entitled Searching for Extra-terrestrials. Professor Gibson is the director of the E.A. Milne Centre for Astrophysics. This is a research institute that “pursues explanations for the wonders of the Universe” through academic research. It also offers extensive public engagement.

Professor Gibson spoke about the desire many of us share to find evidence for extra-terrestrial life. There are several examples from the past that people have taken as possible evidence, the most famous of which is the Wow! signal from 1977.1

Professor Gibson went on to discuss the well-known “Goldilocks Zone” for planets. This is the ideal distance from a star that a planet should be to have the potential to support life. He extended this idea to discuss the different zones of a galaxy that are most suitable for habitable planets. Too close to the centre of the galaxy and the planet would be bombarded with radiation too strong for life as we know it to exist. One must also account for the possibility of catastrophic events, such as supernovae.2

It seems for the time being, extra-terrestrial life is confined to the realms of science fiction.

There are other factors that must be considered for a planet to be a suitable environment for life to develop, aside from the obvious question: does it have water? For instance, consider the composition of the rocky crust of the planet. What effect will a different composition ratio of minerals common in our crust have on the potential for life? Fascinating questions and yet currently there are not many answers.

In addition, the Drake equation, which can be used to calculate the number of detectable alien civilisations in the galaxy, was discussed. This equation includes two types of unknowns: those that can be currently estimated or calculated effectively and those that are more philosophical.

The factors that can be calculated form part of the research that takes place at the E.A. Milne Centre and other similar institutions around the world. The more philosophical parameters, on the other hand, can easily be debated and are currently little more than guesses. As part of the lecture, Prof. Gibson entered reasonable estimates of the unknowns into the equation. The resulting number of civilisations in the Milky Way galaxy was just 2.3 Therefore, it seems for the time being, extra-terrestrial life is sadly confined to the realms of science fiction.

2. http://go.nasa.gov/2hsjkJD

The Drake Equation

\[ N = R \times f_p \times N_e \times f_i \times f_l \times L \]

N  “Lifetime” of communicating civilizations
R  Rate of formation of suitable stars in our galaxy
f_p  Percentage of those stars with planets
N_e  Number of planets per star that could sustain life like earth
f_i  Percentage of planets where life actually develops
f_l  Percentage of planets from f_i with intelligent life
f_c  Percentage of planets from f_l where technology develops
L  “Lifetime” of communicating civilizations

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Experiences of Life in Sheffield
Third Year undergraduate Jing Jing tells Resonance about her experiences adapting to British life in Sheffield as part of the 3+1 joint programme between the University of Sheffield and Nanjing Tech University.

The Christmas lights and markets are everywhere in this city. I am walking around in the city center with mixed feelings about the future.

I never regretted the decision to join the 3+1 joint program between the University of Sheffield and Nanjing Tech University upon graduating from high school. After finishing the three years of courses taught by the Chinese teachers and Sheffield professors, I finally came to Sheffield this August full of excitement and expectation.

Before going abroad, my classmates and I searched for some suitable accommodation. I thought it was more convenient and safe to live with people I was familiar with. In hindsight, it would have been beneficial to choose roommates from different countries to experience diverse cultures and to improve my command of the English language.

Undoubtedly, moving to the UK has been full of challenges. The first problem I needed to overcome was adapting to the British lifestyle and learn to live alone. This is the first time without my parents and deal with everything by myself. Luckily, my classmates and I are a collective community who can help each other.

I also encountered difficulties opening a bank account. It is clear that British banks are more careful checking the information more rigorously as I had to wait for them to post the cards and important information. I also struggled with cooking. But my roommates have helped me and I have learnt many new delicious recipes.

Like China, most courses in Sheffield are taught primarily through lectures. But, some projects require both individual and group contributions. For example, as part of the “Skills for Success” project in Level 3, I chose to be a part of the Chemistry Publicity Team. It was a challenging and wonderful experience for me where I grew up fast. It was in the first group meeting, I met the biggest difficulty - the language barrier. I was the only one from China in the group and, since it was my first year studying in the UK, it was a little hard for me to keep up with my peers when they spoke quickly. To overcome this, I participated in the interviews to enhance my listening and speaking abilities.

“The biggest advantage of studying overseas is to experience a different culture and country that will help you to build a brand new outlook of the world.”

Fortunately, my workmates were so kind and were able to help me. I was given the opportunity to demonstrate my individual strengths. I am skilled in graphic design and have some experience in publicity, so I put forward the idea of using posters as advertisement. I was mainly responsible for the photography of the advert and design of the final poster. My fellow students strengths played into my own weaknesses. They were able to perform the tasks that were communication heavy such as, collecting information on researchers, contacting interviewees, writing text and editing videos.

Studying at university are the most important years in my life, especially the year abroad. It is at university that I truly discovered what learning is about. I believe that the material taught isn’t as important as the ability to learn a new subject, and the experience analyzing and tackling new problems. It is also important to ask questions. The teachers were always telling us not to be shy and if we have any questions to ask.

Life in Sheffield is challenging and exciting. Fortunately, I have the help of many people, like my Chinese and Sheffield classmates, and my personal tutor and supervisor. There is no doubt that the biggest advantage of studying abroad is to experience a different culture and country that will help you to build a brand new outlook of the world. Studying abroad expands our horizons and enriches our life experiences, and also makes us more independent and enterprising. It is inevitable to encounter problems, but learning from the experience is something to treasure for the future.

Christmas is coming. I miss my family but I am looking forward to the new semester and the future.

10th biennial National Undergraduate Chemistry Laboratory Tournament

By Dr Julie Hyde

In July 2016, Dr Julie Hyde took a team of Level 2 students consisting of Amy Smith, Daniel Reader and Jack Watson to Nanjing University, China, to participate in the 10th National Undergraduate Chemistry Laboratory Tournament. This was a special honour and wonderful opportunity for them all, considering only two international universities were invited to take part.

The competition consisted of both a practical-related written exam and a mystery practical experiment, with all students receiving a medal and a certificate for taking part. The students commented that it was “a fantastic experience”, and allowed them all to appreciate education in chemistry in an international setting.
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Resonance Recommends

Our favourite sources of scientific communication.

Stuff to Blow Your Mind is a great podcast that discusses some fascinating topics relating to all disciplines of science and science fiction. It is produced by How Stuff Works who also have several other podcasts that discuss different things like how phenomenon work, such as radiation sickness and other interesting facts.

It's well researched and my personal favourites are those that discussed the moons of Jupiter and Saturn and also the Ig Nobel Prizes, prizes that celebrate the more unusual research. It is well worth downloading a podcast or two!

www.howstuffworks.com/
www.stufftoblowyourmind.com/

Events Listings

Charles Stirling Lecture Series
Every other Wednesday
starting February 15th

ChemSoc Lecture:
The Decontamination of Buildings after an Anthrax Attack
March 2nd

British Science Week
March 10th-19th

The Great ChemSoc Bake Off
March 24th

Chemistry Ball
April 29th

Various nights out, guest lectures and non-alcoholic socials to be confirmed.

More details can be found at: www.sheffield.ac.uk/chemistry/events
This Semester in Pictures

With contributions from: James Williams, Kittie Royle, Joshua Swift, Sharon Spey, Jo Buckley, Grant Hilb, Sara Bacon, Tim Manning and Joseph Clarke