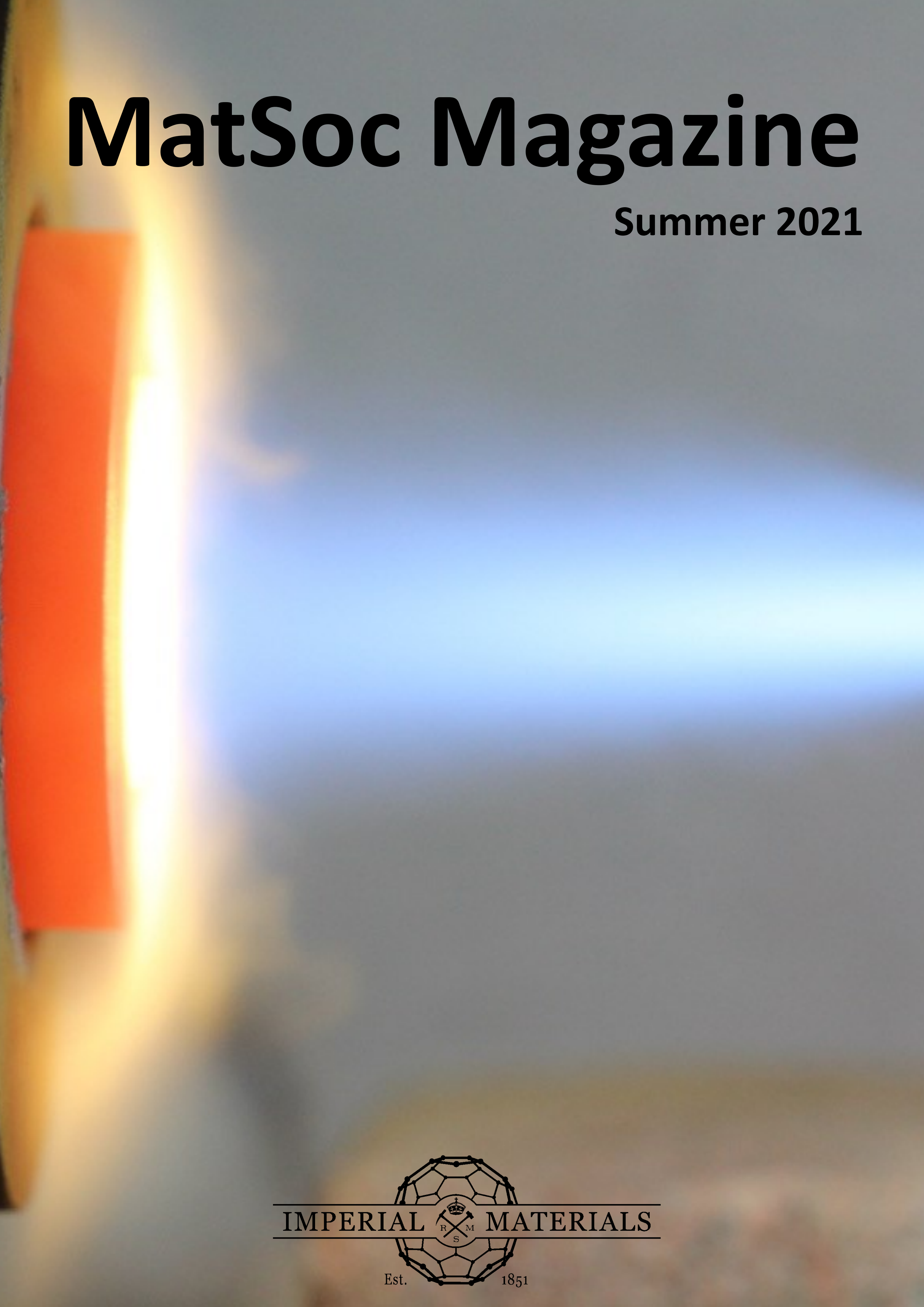
MatSoc Magazine

Summer 2021



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The Materials Society (MatSoc) is a student run organisation which aims to enhance the experience of students studying in this department at Imperial College London, and to promote Materials Science and Engineering both at university and in industry.

We achieve this goal through collaborative events, social functions, extra-curricular lecture series, and industry visits to engage with Materials Science beyond an academic environment.

Our society currently has 695 members, including undergraduate and postgraduate Materials Science students at Imperial, as well as other students studying other subjects who are interested in Materials Science and working in related areas upon graduation.

Bauerman Lecture 2019 (The Department has established a distinguished annual prize lecture - the "Bauerman Lecture" - named after Hilary Bauerman (one of the seven original students to enter the Government School of Mines in Jermyn Street in 1851).

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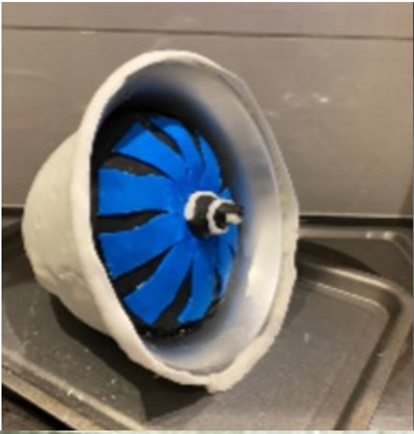

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Welcome to MatSoc Magazine

Editors Foreword

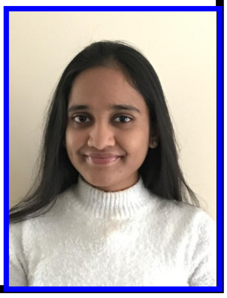
Welcome to the 2021 Summer edition of the MatSoc Magazine!

Producing the magazine in the Summer term, when exams are everyone's priority, was undoubtedly a challenge. However, despite my fears of struggling to fill the page quota (32 pages for a printed booklet), I am pleased to say that I have received an overwhelming response. This magazine includes a varied range of high quality articles about internal and external events and I am confident that this edition contains an article of interest to every individual.

To the freshers who will be reading this in October, welcome to Imperial, the Royal School of Mines and the Department of Materials. Articles of particular interest to you would be the ones on "Soft contact lenses" and "4D printing". These were written by Ben (1st year) and it is a great way to look at cutting edge science from someone who has been in your shoes. I would like to direct the older years to careers related ones like 'Careers in IP law' and 'Materials graduates in Shell'. I hope everyone would be able to find some time to read these articles in the holidays. I would also like to take this opportunity to introduce, **Adam Cliff**, as your next editor. I hope he finds this experience as enjoyable as I have.

Finally, I would like to thank everyone who contributed. As always, feel free to contact the writers or me for any comments about the articles!

Aishwarya Varanasi
MatSoc Magazine Officer 20-21



Welcome & 20-21 at a glance

President's address

Hey guys, Hope you are all doing well. A huge congratulations to all of you in making it through this year. With every up and down you must have faced, it is really inspiring that you were able to adapt to the new style of teaching with each new government guideline.

It was especially nice to see so many of you attending MatSoc events over the past term. The hard work George had put into organising the many 'Beyond University Lectures' over spring was received well, with a great turnout from the cohort. It was impressive to watch you guys really take up the information and knowledge our alumni and sponsors had to offer. Another thing that I took pride in was witnessing the talent all of you possess, whether it be comedic through the Jackbox party games; culinary, through the matsoc bake-off; or creatively, from our merch competitions or your talent show submissions.

I did feel that I missed out on meeting you guys in person in my last year here but am excited to see what the next year will bring for MatSoc. The committee have worked very hard to get sponsors this year and, although we were unable to spend it on our dinners and tours that we would have loved to hold, it means the following committee will have a hefty lump sum to hold (hopefully) a bumper year for those who have not been able to see what a fully functioning MatSoc is usually like. I will be leaving the society in the very capable hands of Jess and cannot wait to see what the new committee will achieve. For those who, like me, are saying goodbye to the department this year, I wish you all the very very best in your future endeavours and hope to see you all in the near future. I have thoroughly enjoyed the last four years in the department and you have all been a huge part of the great experiences I have had being a materials student here. I hope you all have an excellent summer and year to come.

Arinjay Jadeja

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21-22 MatSoc President's address

Hello everyone!

For those of you who don't know me, my name is Jess, and I am your MatSoc 21/22 President! Over the past three years MatSoc has truly become one of my favourite parts of being an Imperial student. From curries to bowling, lunch time lectures to tour, I have loved being a part of this community. Heading into my final year, I am excited to see how we will continue grow and develop as a society as I aim to uphold our current traditions as well as bring some new ideas into the community.

As we all know, this year has been a very strange one. Instead of our usual in-person events, online socials and lectures have become the new-normal. Although challenging, I hope we can all agree that AJ and the rest of the 20/21 committee have done an amazing job in keeping the MatSoc community alive!

I hope next year's events will be just as successful! Heading into next year one of my main aims is to reintegrate our year groups. Back in October, we were unable to hold our typical "Mums and Dads" event for the 1st years because of the restrictions. Having met a huge total of three freshers (all of whom are my children), I would really love to hold an event before term starts so that everyone can get together before the new cohort arrives. Another of my aims is to relight the spark that is the Geology/Materials rivalry! When I was in first year, Hill Cup (the Geology v Materials varsity) was one of the highlights of my year. We went Paintballing, Curling and had a very creative Bake-Off event. On a more academic/careers focused side, my main aim is the creation of the student-alumni mentor scheme. I hope you all have a lovely Summer, and I can't wait to see you all next term for another successful MatSoc year!

Jessica Dring-Morris
MatSoc President 21-22

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21-22 Committee introduction

Hi everyone, my name is Jess! My role involves ensuring everything runs smoothly within the committee while exploring new ways that MatSoc can help improve your university experience!! I am a current third-year student and your 21/22 MatSoc President. My favourite area of materials is biomaterials. I have a strong interest in the application of materials in medicine and heading into my 4th year I hope to specialise to explore this interest further. My favourite MatSoc memory has to be the Christmas Curry! This is always a great event and the perfect way to celebrate the end of first term.

Jessica Dring-Morris
MatSoc President 21-22

Hey everyone, I'm Yash and I am current second-year heading into my third year! Basically my role is maintain relationships with the department and our many connections to companies. I'll be working on the committee to make the careers fair the best representation of possible careers, many trips to industry as well as our "Beyond University" lectures. My favourite part of materials is metal alloys and their composites and the thing I'm looking forward to the most next year is the revival of in person events and lunchtime lectures. The Christmas Curry was my favourite MatSoc memory and I hope we can recreate it this year!

Yash Dwivedi
MatSoc Vice President 21-22

Nerojan Navaratnarajah
MatSoc Treasurer 21-22

Hi, I'm Nerojan. I'm a current second-year student heading into my third year. I am doing the nuclear materials course. My job is to ensure that a budget is set out for the year to effectively manage finances from the union and our sponsors, subsidise the great events that MatSoc organises and to make sure that there is still money left at the end! One of my main responsibilities is to keep a clear financial record and ensure that the rest of committee are regularly updated about it. My favourite MatSoc memory was the bowling event and I am looking forward to similar events next year with reduced COVID restrictions.

Hey, I'm Adam and I'm a current second-year heading into my third year! Most of what my role involves is behind the scenes, from organising and taking minutes at committee meetings to helping with any tasks that might be too much for just one person to take on. My favourite things about materials are semiconductor devices and wearing suits to the MatSoc formal dinners. I hope you all look forward to the coming year with our new merch that's going to be so good that you'll be proud to be a member of MatSoc.

Adam Wu
MatSoc Secretary 21-22

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21-22 Committee introduction

Hi everyone, my name is Abhi! I am a current second-year student heading into my third year. I intend to work closely with Nerojan and Adam to deliver an impressive line up of events, including, but not limited to bowling, the annual Christmas curry and an industry tour. My favourite area of materials is the theory and simulation of materials. My favourite MatSoc memory has to be the Christmas Curry! I am looking forward to watching everyone redevelop their social skills at all our socials next year.

Abhinav Rajendran
MatSoc Events Officer 21-22

Hi everyone, my name is Adam! I am a current third-year student heading into my fourth year. I am excited to be your MatSoc Publicity and MatSoc Magazine Officer for 21-22. Whether it be through posts on facebook or posters around the department, I'll make sure everyone knows about the event. I will also work towards greater engagement from everyone for the magazine. I love engineering alloys. My favourite MatSoc memory is the New Year's Dinner. I am looking forward to dressing up in suit for that next year.

Adam Cliff
MatSoc Publicity Officer 21-22
MatSoc Magazine Officer 21-22

Hi everyone, my name is Shreya. My role is to obtain funding for MatSoc's events from companies throughout the year, as well as to act as liaison between us and these sponsors. I have just finished my 1st year at Imperial and my main area of interest is renewable and green energy. My favourite MatSoc memory is completing in person and online scavenger hunts with my MatSoc family which got really intense at times. Next year, I am finally looking forward to some more in person events and meeting more people in the department.

Shreya Mistry
MatSoc Sponsorship Officer 21-22

Hey everyone, my name is Sohan. I will be the new website officer at MatSoc. My role is to keep the website updated with the latest editions of the MatSoc magazine, information on sponsors, up to date events calendar etc. I have just finished my 3rd year and will be heading into my 4th year in 21-22. I have a strong interest in biomaterials and will be pursuing that next year. My favourite MatSoc memory is the Christmas Curry. I am looking forward to our new website next year.

Sohan Ratajczak
MatSoc Website Officer 21-22

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Women at Imperial week

Women at Imperial is an annual event that takes place around International Women's Day (8 March). This year, over the course of a week, the college and the department celebrated women staff and students. This raised awareness of the support available across the College for women. This year the theme for International Women's Day was **#ChooseToChallenge**. This aimed to celebrate women's achievements, raise awareness against bias and take action for equality. In the Department of Materials, this week aimed to highlight the research and opinions of women in the department. There were interesting and insightful events lined up every single day.

One of my personal favourites was the one on **Wednesday** in that week — a "Women in Materials" talk and panel discussion. This was chaired by Dr. Eleonora D'Elia. This event focussed on the contributions female researchers (Dr. Leah C. Frenette and Sarah Fothergill specifically) had made during COVID-19. Both Leah and Sarah's talks were very inspiring. Leah is a research associate in the department of materials. She worked on advancing biosensing strategies at the point of care during COVID-19. Sarah is a PhD candidate in the Department of Materials who worked on Plasmonic biosensing in the time of COVID-19. Both Leah and Sarah spoke about their journeys in science to inspire more women to take up a career in science.

Dr. Leah C. Frenette

Sarah Fothergill

On **Thursday** the 11th, we had two events organised. The first one was all about building networks of early career materials women. This was a closed event for Materials Postdocs only. This event provided an opportunity to join the postdoc and fellow women for a casual coffee afternoon, with the opportunity to connect, swap expertise and share experiences of navigating as early career researchers.

The second event was on SPIE Women in Optics with Anita Mahadevan-Jansen, hosted by Dr. Jessica Wade and everyone was invited for this event. This is a monthly interview with women in the community to learn more about their research and hear their advice to other women in the field. This event was hosted by 2020 Diversity Outreach Award recipient, Jess Wade, this series is part of our efforts to encourage and inspire women to bring their ideas to light.

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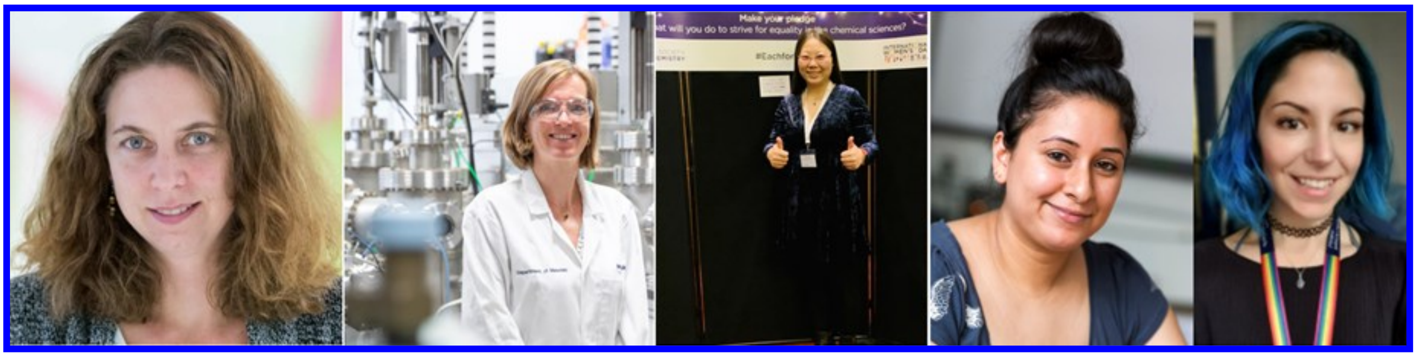
On **Friday** the 12th of March, there was a women's informal staff/ student coffee (closed event for Materials staff/ students only). This was a good opportunity to come to our unique 'virtual common room' experience to meet and chat with women from across the department. The aim of this event was to facilitate discussion amongst students and staff who might be able to offer advice or guidance or just chat in a fun environment. The event was hosted on the platform Gather. Town. This meant that people could walk around the common room, create small discussion pods or larger groups play a game together, check out the video on inspirational women or write on the shared whiteboard to give feedback or ideas for future events.



Pictures of some of the women's achievements the Department of Materials celebrated in 2021 March. From left to right: Professor Alexandra Porter, Professor Sandrine Heutz, Dr. Hui Yang, Raj Adcock, Dr. Eleonora D'Elia

After attending all of the events in the week I had realised that there were a lot of great women that work at Imperial College; right from my colleagues, teaching fellows and lecturers. All of their work and success inspires me.

I believe that it is very important to celebrate international women's day because women form a great proportion of Imperial College's multinational community. Every day, at Imperial I get a chance to work, exchange ideas, knowledge and culture with so many bright and successful women from all around the world. By celebrating this community and the great achievements of these women we can empower and inspire young women from all around the globe to get together and use the power of their voice to create a better and fairer world where everyone has equal rights and benefits no matter what gender, background or race they are coming from.

Careers in IP Law

In Spring term, we had a lunchtime lecture given by Isobel Stone (a Materials Science graduate from Cambridge) about pursuing a career in IP Law. The Q/A format summarises the key take-aways from the lecture.

IP law is relevant to all businesses, but can be core to the technology, engineering and pharmaceutical industries said Isobel Stone, an associate at Mewburn Ellis. Intellectual property (IP) is intangible property that is the output of human creativity and intellect [1]. IP law protects and regulates intellectual property through a system of IP rights. Core IP rights include patents, trade marks, copyright and design rights (the precise nature of the rights available varies by country). Roughly around half of the cases go to court: this will typically take place between 12 to 15 months after the start of the claim [2].

What does intellectual property law involve?

Intellectual property involves many different kinds of IP rights. When this is looked at very broadly as a typical transaction process, solicitors will generally negotiate over the licensing, assignment or generation of a right (for example, the allocation of potential rights arising from a joint venture). Patent attorneys on the other hand do the actual applying for and obtaining of registered rights. Though the lawyers may specialise in one or two particular types of IP rights in larger or more IP focussed firms, the work that they may do might be largely similar. Other kinds of lawyers exist, these layers litigate over IP rights. They argue whether they are infringed by another person or whether the right is valid.

Who are the clients in intellectual property law?

Where there are ideas there is IP. Clients could be individuals owning small businesses that make pop-up stages out of scaffolding, small and medium-sized enterprises (SMEs), and multinational technology companies. Some organisations might require IP only once in their lifetime and some organisations use IP right more regularly in their life cycle. Technology and pharmaceutical companies come across IP issues more regularly than other companies. In these industries, the value of the business is based on their IP rights. IP rights play a significant part in the development of new technologies, such as 5G or artificial intelligence, as well as pharmaceutical products, which can generate a degree of media interest.

What does a typical intellectual property law case look like?

An IP law case usually involves two companies – one company would sue another company for infringement of its intellectual property rights. Proceedings would be issued, and the opposing side would likely say they do not infringe the IP right and allege that the right was invalid in some way in their defence [2]. After the parties have set out their cases, there will be a case management conference to determine the appropriate directions to take the matter to trial (for example, what disclosure and evidence is required). Litigation concerning IP rights tends to be highly evidence based, though it varies as to whether the significant issues will turn on evidence of fact or expert evidence.

It can be harder to settle IP disputes than in other areas of commercial litigation, as often the stakes are quite high; parties usually face either being prevented from doing something or giving up (or limiting) the right to prevent others from doing something

The complexity, the value of the dispute and the right in question will determine the specific list in the Business & Property Courts (for example, the Intellectual Property Enterprise Court, the Patents Court or the genera Intellectual Property List).

What will a trainee lawyer in an intellectual property department do?

Trainees are likely to be involved in all aspects of case. They may be responsible for the administration of a matter, making sure everybody knows what they're doing and ensuring that key deadlines are kept, and they will attend meetings as part of the wider team. Trainees likely will also be involved in drafting, such as preparing (parts of) license agreements or court pleadings, and legal research.

What skills do intellectual property lawyers need?

IP lawyers need the following skills

- **analytical brain**
- a **willingness** to get to grips with things they don't understand
- **good team** playing skills (as intellectual property lawyers will often work on the IP aspects of other areas of law)
- **lateral thinking skills** (as IP disputes can be complex)

References

[1] "Understanding Industrial Property". World Intellectual Property Organization. Retrieved 2018-12-06.
[2] Intellectual property law: area of practice. [online] TARGETjobs. Available at: https://targetjobs.co.uk/career-sectors/law-solicitors/345798-intellectual-property-law-area-of-practice [Accessed 12 June 2021].

Materials graduates in Shell

Shell (one of our sponsors) is an international energy company that aims to meet the world's growing need for more and cleaner energy solutions in ways that are economically, environmentally and socially responsible. Shell is one of the world's largest independent energy companies, operating in more than 70 countries and employing around 89,000 people. The challenge for the future is to continue to meet growing global demand for energy at the same time as reducing carbon emissions. Shell is an active participant in meeting this challenge. Through collective thinking, idea sharing and learning Shell believes that it can build the collaborations necessary to deliver the world with more, and cleaner energy.

In spring term, we had 3 materials graduates (Mabel Ntim, Joshua Jones and Sarah Hopkins) give a lunchtime lecture on how materials graduates could get a job in the energy industry. They not only spoke about the roles materials graduates undertake in Shell but also gave an insight into making successful applications to competitive graduate schemes like shell. The following pointers summarise some of the key takeaways for each stage of an application process for internships and graduate schemes.

Online application: a few questions and a CV upload

The Shell application form, like many other forms, consists largely of yes/no answers and options in dropdown menus, rather than opportunities to give detail about your skills and experience. For this reason, your CV must work extra hard to showcase your unique achievements. Shell like many other companies favours a traditional CV format with education and experience neatly listed in reverse chronological order.

CVs should be **clear and concise**. Pick out only a few key pieces of information rather than giving an in-depth account of each role.

For your education history, Shell suggests that you include information on any **relevant modules, projects, or dissertations**. This will help demonstrate your interest in and knowledge of your chosen scheme. Give an overview of what you did and what you learned. It is not necessary to list every module you studied at university. Instead, pick the modules you think are most relevant to Shell and the scheme you've applied for.

Shell highly recommends that you include your **achievements** and **outside interests** in your CV. This helps show you are well rounded and injects personality into your CV. Avoid generic interest such as listening to music or socialising with friends and definitely don't make things up. You need to be prepared to discuss your CV further in the interview.

Another idea would be that every company has got a set of **core values** it values. For example, they could have criteria like capacity, achievement and relationships. These qualities can be laid out in bulletin points within the sections of your CV; for example, as skills you've used in a particular job or hobby. Be specific and use quantitative details such as sales figures where possible to help illustrate examples. Reflecting the company's goals would be key to making applications shine.

Online assessments are timed cognitive tests and working style assessments. The following are tips for doing well on those:

Familiarisation is key

List out all the companies that you are applying to and google the online tests/ test providers. Familiarise yourself with their formats.

On demand video interviews are usually self-recorded video interviews to tell Shell (or other companies) about yourself. There are 3 broad types of interview questions asked:

- Motivational
- Competency
- Technical/ commercial awareness

Motivational questions are the far most common types of questions asked in interviews. The following questions are the most important.

- Tell me about yourself
- Why me
- Strengths/ weaknesses

Competency questions

Read up on **STAR** techniques.

Situation: Describe the situation and when it took place .

Task: Explain the task and what was the goal.

Action: Provide details about the action you took to attain this.

Result: Conclude with the result of your action.

Think about things like the competencies the program tests for. This informs what kinds of questions one can prepare for.

Interview/ Technical/ Commercial Awareness

Gauge the level of technical knowledge required from (job speculation, online)

Focus on the top-level fundamentals first before diving head first into the finer details

Stay on top of the news for a select number of issues

Final assessment centre consist of a virtual interview, a live session about a case study and an individual interview. It's important that you:

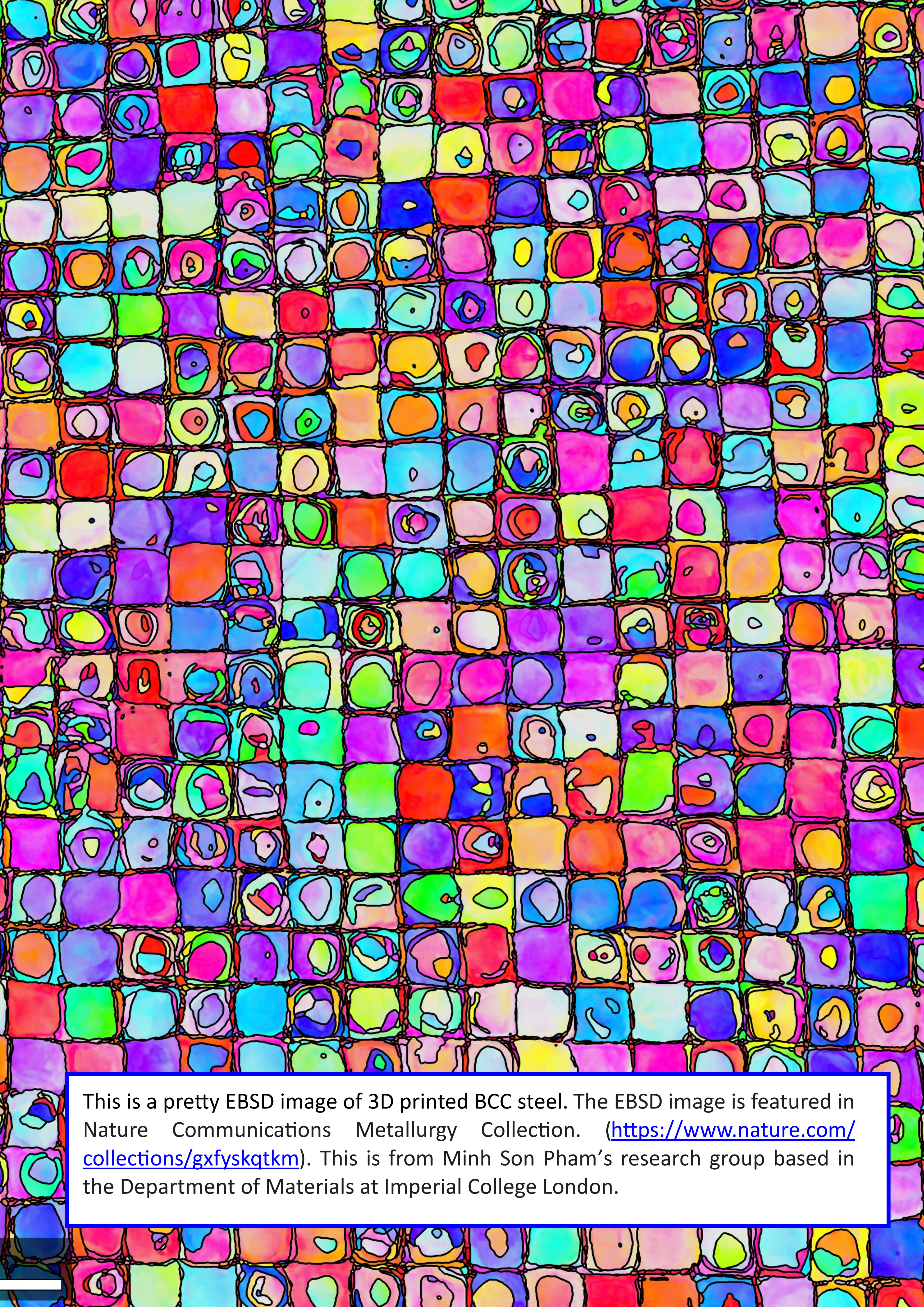
Are assertive during all exercises and don't dwell on any mistakes, instead concentrate on performing well in the next task.

Ensure that the assessors can see your working methodology.

Don't worry about the other candidates, and instead focus on putting your key skills forward.

Draw others into group discussions

Ensure that you understand the requirements of each task by quickly digesting the brief, and revisit this once you understand the overall challenge.



This is a pretty EBSD image of 3D printed BCC steel. The EBSD image is featured in Nature Communications Metallurgy Collection. (https://www.nature.com/collections/gxfyskqtkm). This is from Minh Son Pham's research group based in the Department of Materials at Imperial College London.

The Science Behind Soft Contact Lenses

Ben Schultes, a first year explores the idea of biocompatibility .

Millions of people depend on contact lenses to see every day. These lenses need to be carefully developed and manufactured so that they don't damage the eye and have the required optical properties. Because I've used contacts for the past 10 years, I decided to explore this topic in more detail and find out why some feel like shards of glass and others feel like nothing at all. The applications of specialized medical materials are vast, from permanent physical support to materials that stimulate regeneration and support the healing process. For obvious reasons, the most fundamental requirement of a new material designed for medical applications is biocompatibility. [1]

"But what is biocompatibility?"

A material is biocompatible when it has no unfavorable impact on the biological system in which it is placed. This means it either causes a favorable change, or has no impact on the system, and does not disturb it. In other words, it must be "free of toxic or injurious effects" and it must not "elicit an immune or other response in the recipient". [1]

Biocompatible materials can be developed through biomimicry, meaning that their composition or structure copies that of the biological system or environment where it is applied. These are referred to as biomimetic materials.

The first contact lenses were hard and made of glass. During the second world war, unfortunate plane crashes had fortunate consequences, as fragments of PMMA from the plexiglass windshield were implanted in the pilots eyes, and making the materials' biocompatibility apparent[2] (Although methyl methacrylate (MMA) is carcinogenic, its polymer PMMA is very unreactive and highly biocompatible [3]). Although these worked well and rigid gas-permeable (RGP) lenses are still used today, soft contact lenses are becoming increasingly popular because the material has similar properties to the ocular surface resulting in a much more comfortable fit.[4]

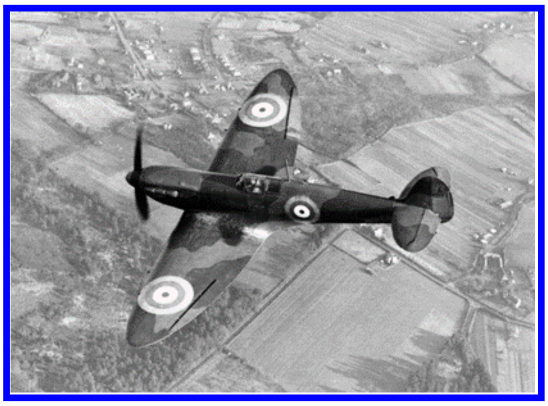


Figure 1 - British WWII Spitfire Plane [13]

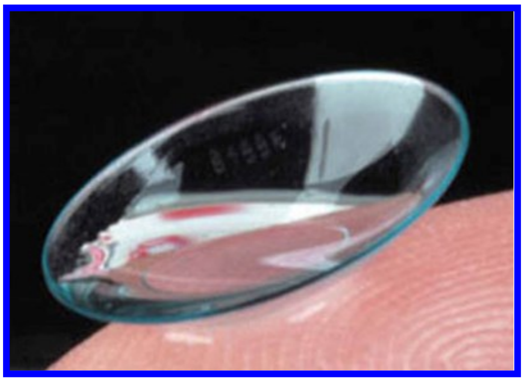


Figure 2 - A Hard Contact Lens [14]

Soft contact lenses are made of hydrogels which are saturated crosslinked polymer networks [5]. The higher the water content, the more comfortable the lens is to wear. A weakness of hydrogels are their limited gas-permeability. This has been improved by the development of silicone-hydrogels. Their higher oxygen permeability means that they can be worn safely for longer periods of time.

Common Polymers Used in Contact Lenses:

An example of commonly used polymer network in contact lenses is Omafilcon A, with 62wt.% H_2O. It is a hydrogel composed of 2-hydroxyethylmethacrylate (HEMA) and 2-methacryloyloxyethyl phosphorylcholine (MPC).

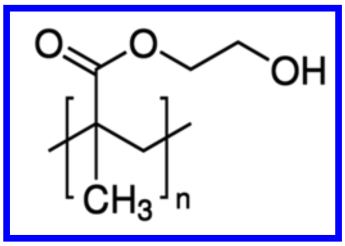


Figure 3 - poly(HEMA)[15]

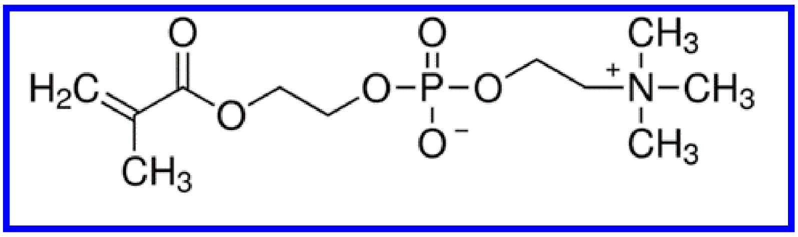


Figure 4 - MPC[16]

The $–PO_4–$ group in MPC is also found in molecules called phospholipids in human cell membranes. Additionally, the large and bulky side groups of the polymer increase the free volume in the hydrogel allowing it to absorb more water. Because of this, Omafilcon A mimics the composition and physical attributes ('squishiness') of the eye.

This hydrogel absorbs water in a very unique way. Poly(HEMA) is amphiphilic because its backbone and methyl group are hydrophobic but the hydroxyethyl group is hydrophilic. Poly(MPC) has even more hydrophobic groups, but it can still absorb water through a mechanism called 'hydrophobic hydration' because it is zwitterionic, meaning that it has positive and negative charges[6]. During this process, water molecules form a clathrate cage structure around the trimethylammonium group, $N^+(CH_3)_3$, where the water molecules are held in position by dipole-dipole attractions forming an almost crystalline structure that is often described as 'ice-like'[7]. This special hydration makes poly(MPC) very unreactive and biocompatible, since it doesn't disturb the biological system it is placed in.

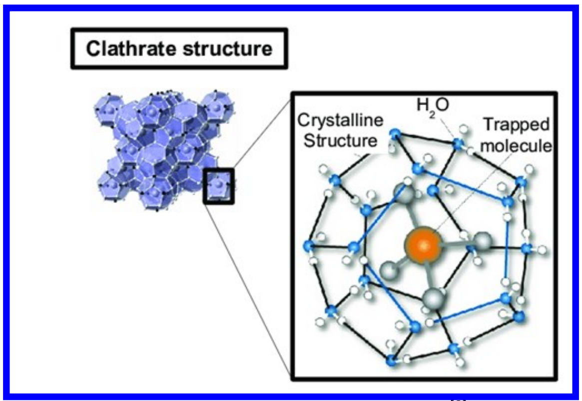


Figure 5 - Clathrate cage structure[8]

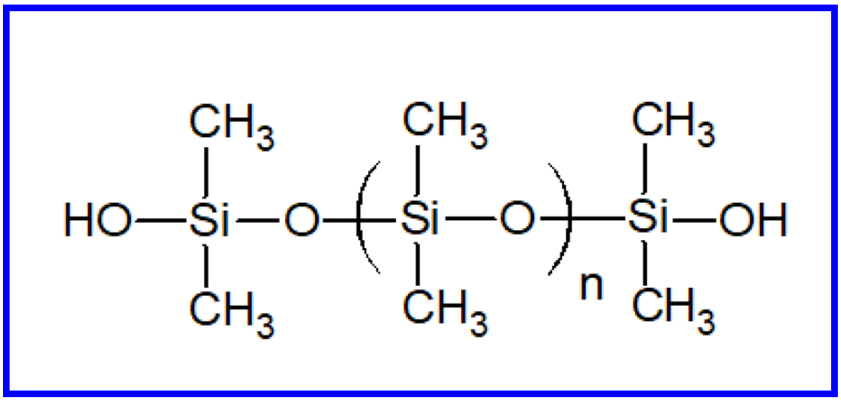


Figure 6 - Polydimethylsiloxane (Silicone)[10]

Silicone is highly gas permeable mainly due to its large free volume and backbone flexibility. Unlike conventional hydrogels where O_2 is transported by H_2O, in silicone-hydrogels oxygen diffuses through the free volume surrounding the polysiloxane chain, were the molecule is transferred between –SiO– groups and transported along the backbone.

Synthesizing a silicone-hydrogel was very challenging because of its hydrophobicity, which reduces fluid transmissibility. Scientists have been able to crosslink hydrophilic polymers with silicone and maintain sufficient water content[11]. Lenses were developed with water gradients ranging from 33wt% at the core to 80wt% at the surface. This mimics the water content of the cornea, improving the contact between the lens and the eye.

Figure 8 - Hydrogel Lens (Left) and Silicone-Hydrogel Lens (Right)[12]

Silicone technologies have taken decades to develop and are not yet very wide spread, but they are the future of contact lens materials due to their impressive biocompatibility resulting from their high oxygen permeability and water content.

What's next?

Biomimicry is vital in the development of contact lenses, as it is at a crossroads between optical and biological properties, and meeting all requirements can be challenging. Recent breakthroughs in materials science have allowed contact lenses to evolve from rigid and unnatural devices to soft contact lenses that work in synergy with the eye and have become practically unnoticeable to the patient. The risk of harmful side effects is being reduced, while comfort and optical quality are increased. We've overcome the initial hurdle of synthesizing silicone hydrogels, but it is still a very new technology. It is expected that silicone-technologies will only improve in coming years, so who knows what wearing contacts will be like in 10 years' time.

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Smart Materials and 4D Printing – When Materials Become Alive

Ben Schultes, a first year explores 4D printing.

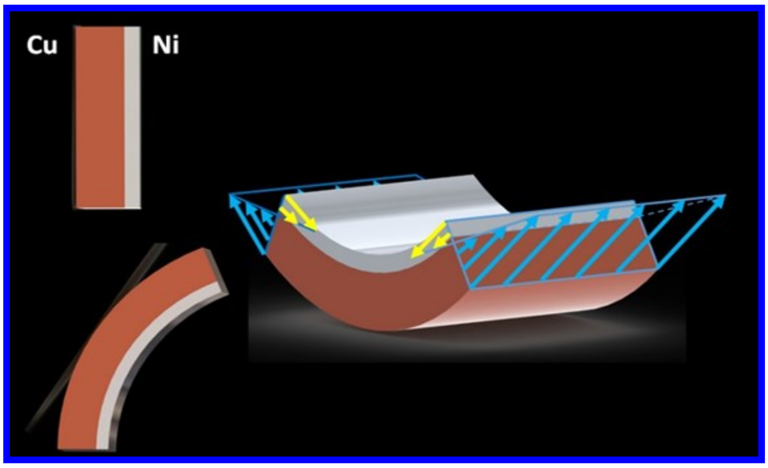
Many of the materials around us are static. Buildings are built to retain their shape and resist any forces that act on them. Most macroscale movement occurs by connecting static parts using joints, hinges, shafts, and so on. But if the materials we use become 'alive' and move themselves?

What are smart materials?

Smart (or programmable) materials are able to change their shape or properties when provided with an energy source. Their response is programmed into their micro and macrostructure and opens up a range of possibilities for intelligent, adaptive, or even self-assembling objects and systems. There are far too many smart materials to go into detail here, but they are all able to change their shape or properties due to an external stimulus. For example, moisture-responsive materials respond to water and humidity, such as hydrogels which can increase their size up to 200% by absorbing water. Photo-responsive materials react to radiation by breaking and forming bonds, or changing into a conformational isomer. Piezoelectrics are an example of electro-responsive materials, because they transform electrical energy into mechanical work or vice versa. For example, an electroactive polymer can change its shape and volume due to an electrical stimulus which can be used to make artificial muscles.[1] Thermo-responsive materials exhibit the shape memory effect, meaning that they can be deformed at low temperatures, but will change back to the original shape when heated. There are many types of materials that can do this, but the most common are shape memory alloys or polymers.[2]

What is 4D printing?

4D printing uses multi-material 3D printers and smart materials to produce pre-programmed intelligent objects that respond to an external stimulus in a predictable way, i.e. it adds the time dimension to the 3D object. By carefully choosing the smart materials (microstructure) and designing the macrostructure of the product, the transformation can essentially be programmed and embedded into the physical object. These objects then harness random energy from the surroundings and use it to make predictable changes. Smart polymers are particularly easy to use because they can be printed using conventional 3D printers, but using other methods such as electrochemical additive manufacturing, Imperial's Chen, X., Liu, X., Ouyang, M. *et al.* have experimented with multi-metal 4D printing.[3][4]



The figure on the left depicts an example of a way in which multi-metal structures can deform predictably.

How can we use smart materials to print shapeshifting 3D objects?

Smart materials tend to perform one function, so producing intelligent objects requires us to understand how and where to add smart materials into the structure. By controlling which parts of the object are passive (rigid and unresponsive) and which are active (smart and responsive), the sum of the small scale changes can produce a more impressive and complex macroscale change. As such, inherent programmability of an intelligent object lies in its geometry, because the geometry needs to channel the shape-changing response. The location, amount and shape of smart components in the structure must be optimized so that they work together. For example, if a shape memory polymer is used as a closing hinge, then its equilibrium position should be curved, so that when it is heated, the object folds. There should be no other hinge that impedes this movement.

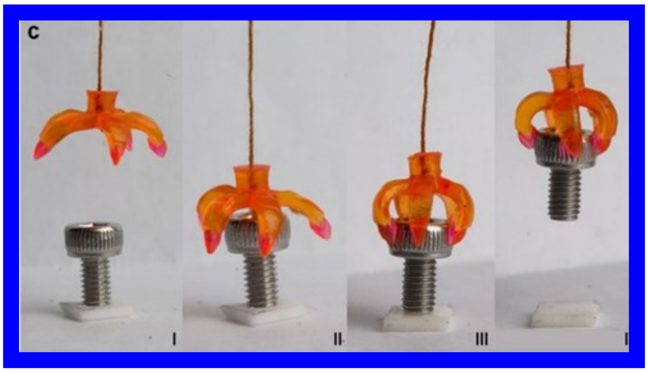
Because the geometry and structure can get very complex, software is used to simulate the movement of the object and calculate the printing pattern for the multi-material 3D printer. Computer simulation and mathematical modelling of the materials and the structure as a whole allows us to control the interactions of different parts, make forward and backward predictions of the object's movement and correct any errors in the geometry or choice of material.

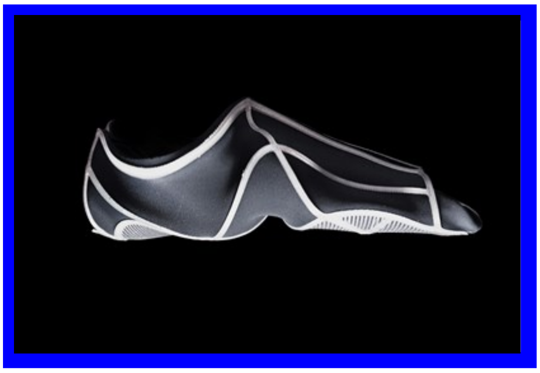
4D printed elephant origami structure. The 2D sheet folds into a 3D structure.

Origami is a great source of inspiration because it allows us to design complex 3D shapes from 2D sheet of material. Every origami structure has a unique crease pattern (i.e. the folds left in the paper when the structure is unfolded), so if smart material is deposited to recreate this pattern, it is possible to design a sheet of material that can self-assemble and fold into the 3D structure. 2D sheets are much easier to manufacture than 3D objects and the ability of the object to fold and unfold results in a vast range of applications. Origami-inspired geometries have been used in several space applications because of their ability to fold large solar arrays into small payloads, and more applications are being explored, such as shoes that fold around your foot.[5]

So, what can you do with 4D printing?

Designing objects that respond autonomously to external stimuli is so versatile because we do not need to control it with electronics; the material shape-shifts, so there are fewer parts which is more reliable over prolonged use. Further, because the structure is activated by the random energy of the surroundings we do not need to power it and it is more energy efficient. This allows us to have valves that open and close automatically due to changes in heat or flow-rate, foldable or self-assembling structures, and consumer products such as clothes that can measure bodily functions or adapt to body heat.[5] So far, mainly polymers have been used in 4D printing applications which can only operate in a limited temperature range. Now that Imperial researchers have demonstrated multi-metal 4D printing, much higher temperature applications are in sight.[4] The possibilities of 4D printing are endless, and it will be exciting to see how smart objects will impact our lives in the future.





Left: A 3D printed shape memory polymer gripper[6]. Right: A 3D printed shoe that wraps

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Materials Specialism focus: Modelling

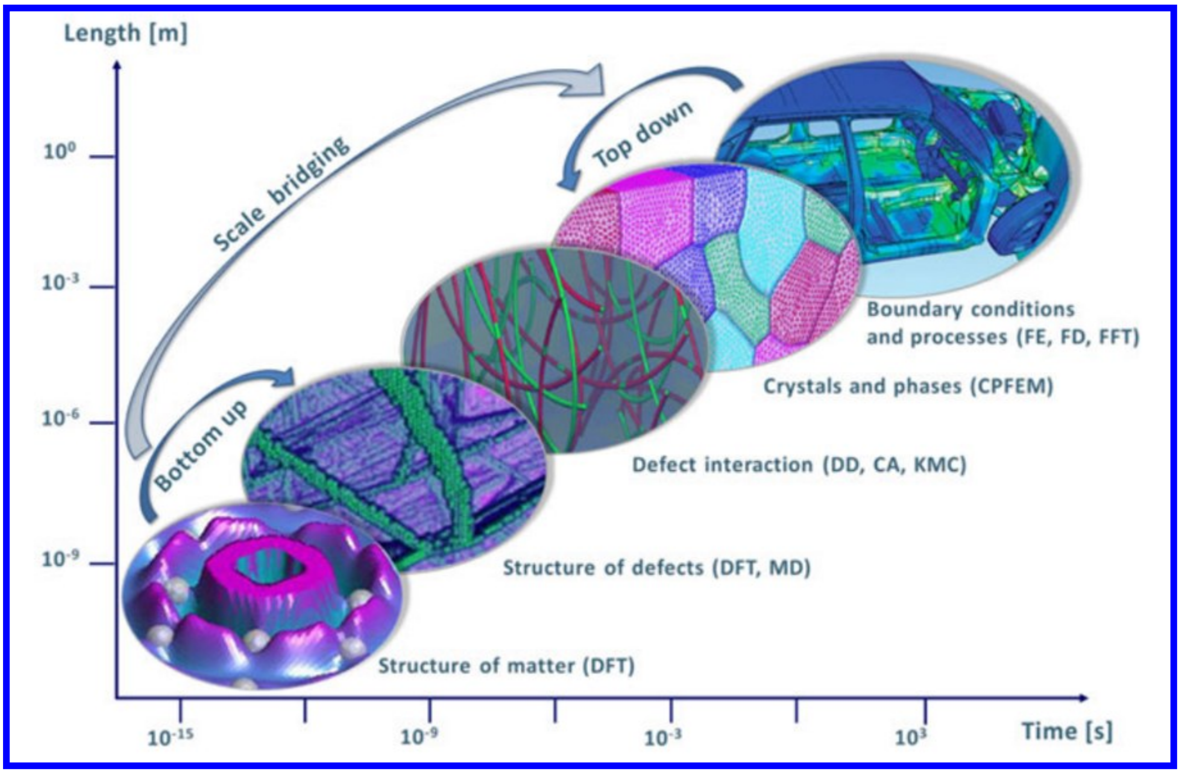
Aishwarya, a third year, looks the past and present of modelling materials.

In our daily lives, we are confronted by a multitude of materials-related phenomena whose essential role often extends over many scales in time and space. One example found at the very basis of life is protein folding. In this process, polypeptides fold into their characteristic 3D structure from an originally random coil.

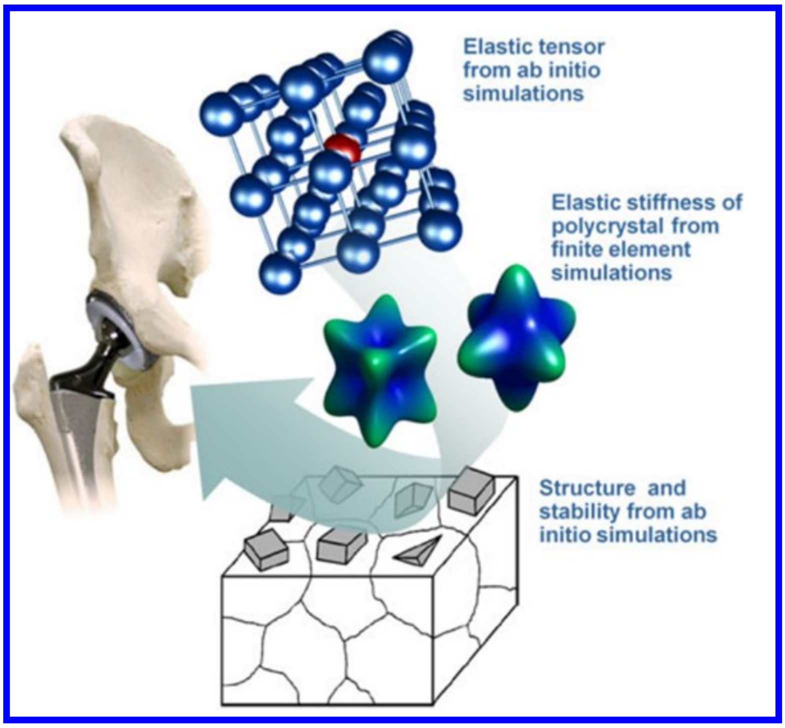
For most proteins, this structuring is essential to their function. While protein folding requires up to several minutes, the underlying chemical rearrangements take place within picoseconds through van der Waals and hydrogen bonds. In materials engineering, corrosion of metals is an essential process that destroys goods worth many billions of Euros every year. Beyond the purely monetary value, corrosion profoundly affects the safety of advanced products and processes, whose integrity and functionality society relies upon in fields such as energy, transportation, and information. While single electron transfer at a metallic surface occurs within femtoseconds and multiple oxide layers require minutes to form via diffusion and multiple reaction cascades, the macroscopic corrosion and decomposition of metallic structures proceeds over decades and even over hundreds of years.

Computer modelling and simulation methods allow material scientists to study and predict material formation, structures, properties and performance from the nanoscale to the macro scale. These can be used in various areas of materials science like biomaterials science, nanomaterials, nuclear materials, advanced structural materials and functional materials.

For example, in biomaterials science modelling and simulation has been traditionally used to explore the interface between molecules and material systems. These biomaterial interfaces control many of the processes in living organisms like materials fouling and the spread of infection by germs. Typically, these simulations examine things like how nature produces shells, bones, and teeth, how cells and bacteria are able to bind to the surface and form biofilms.



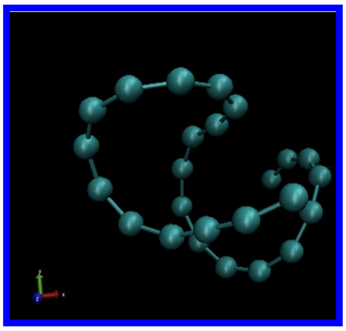
The figure above gives examples of different time and space scales encountered in the field of the mechanical properties of metals highlighting DFT (density functional theory), MD (molecular dynamics), DD (dislocation dynamics), CA (cellular automata), KMC (kinetic monte carlo), CPFE (crystal plasticity finite elements), FE (finite elements), FD (finite difference) and FFT (fast fourier transforms).

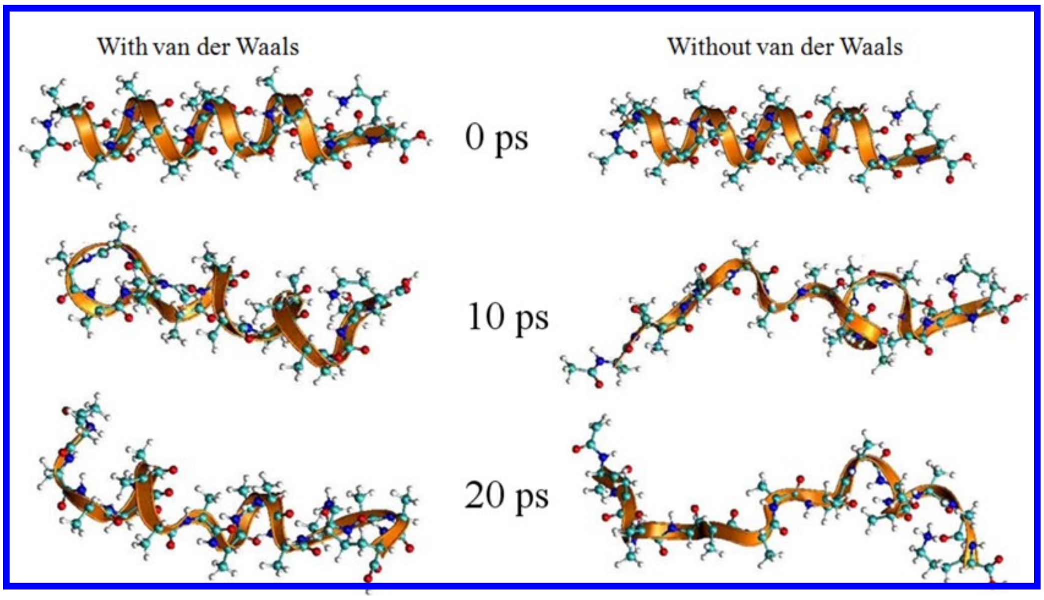


In the adjacent figure, the coarse graining procedure for the design of novel biomedical alloy grades using a multiscale model that starts with ab initio predictions and conducts the homogenization with a crystal-mechanical finite element method.

Current techniques being used

Predicting new compounds requires to explore the energy landscape of chemical systems, to determine the minima, the energetic and entropic barriers, and the locally ergodic regions of the landscape corresponding to stable and metastable compounds. These new modifications can serve as signposts for the exploring synthetic chemist, and provide information about the stability of e.g. solid solution phases at low temperatures thus complementing the efforts of the materials scientist. Such landscape explorations are performed on the atomic scale, using both empirical potentials depending on only the ionic degrees of freedom and high-level ab initio methods taking the electronic structure into account, in particular for the computation of the properties and the thermodynamic ranking of the modifications found. From the minima and the barriers separating them, one can determine the time scales on which the various phases are stable, and model and analyse the dynamics up to macroscopic time scales. Similarly, the modelling of syntheses requires the analysis of many processes occurring over a wide range of scales, such as chemical reactions between molecules, atoms and surfaces, diffusion in bulk and on surfaces, or the nucleation and growth of crystals. An example of this approach is a newly predicted phase of boron nitride in the β-BeO structure type.





The figure on the left is a Visual Molecular Dynamics (VMD) image of the polymer. Features like loops in the relaxed state are indicative of larger degeneracy. The figure on the right shows the evolution in time (snapshots after 0, 10, and 20 picoseconds) of a 15-alanine polypeptide at T = 1,000K. A high temperature is used in order to speed up the evolution. The interactions are treated using density functional theory together with the generalized gradient approximation (PBE). The left column shows the results employing a recently introduced PBE + vdW (van der Waals) approach.

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Future of this area:

The development of new materials, incorporation of new functionalities, and even the description of well-studied materials strongly depends on the capability of individuals to deduce complex structure-property relationships. A significant challenge in this field remains the “curse of dimensionality”. Even for the characterization of moderately complex materials, often a considerable number of parameters is required to characterize their composition and microstructure (or also processing conditions) uniquely. Modelling of materials is thus facing the challenge of high-dimensional parameter spaces, where numerous parameter combinations have to be sampled and studied thoroughly. Relying thereby on experiments is typically prohibitively expensive, given the often high-dimensional parameter space of interest. Thus, the combination of experimental and computational approaches is receiving increasing attention. The complex interdependencies in the resulting data sets can be studied using machine-learning approaches. Artificial neural networks and data-driven approaches can significantly help to identify, approximate, and visualize structure-property relationships of interest. This way, they can accelerate our understanding and effective utilization of complex hierarchical materials.

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Contact Information

Imperial College Materials Society (MatSoc)
Royal School of Mines, Imperial College London
South Kensington Campus, Kensington, London, SW71AZ
E-mail: materialssoc@imperial.ac.uk
Website: www.matsoc.co.uk

Editor:
Aishwarya Varanasi
MatSoc Magazine Officer
E-mail: av3418@ic.ac.uk

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Cover Background Image by Dr. Samuel Humphrey-Baker

White-hot sample, glowing red graphite holder, and blue flame from the high thermal flux testing of tungsten carbide cermets in an oxyacetylene flame.

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